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QuantumSoft
Postfach 6613
8023 Zürich
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e-mail: profit@quansoft.com
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1 Introduction

proFit is an interactive tool for the investigation, analysis and representation of functions and data. It is designed for users in science, research, engineering and education. The key features of proFit 5.1 are:

- **Customized functions and algorithms**: Very powerful and simple Pascal-like syntax for defining mathematical functions, data transformation algorithms, drawings, and general macros.

- **Interactive parameter modeling and curve fitting**: Intuitive interface for modeling and fitting data. Various fitting algorithms. Optional restriction of parameter ranges. Support for y- as well as x-errors. Statistical error analysis for fitted parameters.

- **Professional plotting**: Accurate and flexible graphical representations of mathematical functions and numerical data. Multiple coordinate axes. Linear, logarithmic, 1/x, and normal probability scalings. Reverse scaling. Coloring of areas between curves and any axis. Editing of any part of a plot with standard drawing tools.

- **Drawing editor**: Support for standard drawing objects, Bézier curves, two different kinds of polygon smoothing, texts with sub- and superscripts, data point symbols, and any imported picture. Dash patterns are applicable to most drawing objects. Arrows are available for smoothed and un-smoothed polygons and simple lines. The drawing editor supports colors, views at different magnifications, and extended precision positioning of graphical objects. The floating point coordinates of drawing objects can be edited graphically and numerically.

- **Customizable graphical elements**: Dash-patterns, line thicknesses, arrows, error bars, and data point symbols can be customized. New arrows and data point symbols can be designed with a graphical editor and added to the standard drawing menus.

- **Extensive graphical output possibilities**: Support for PostScript™, PICT format, high resolution bitmaps, and QuickDraw GX™. Export of drawings with Copy&Paste, Drag&Drop, Publish&Subscribe, and EPS files.

- **Spreadsheet data management**: Spreadsheets for editing and transforming data. Predefined and user defined algorithms. Single precision as well as double precision data columns and text columns are supported.

- **Scriptability and Recordability**: Automatically record all your actions as a Pascal program or Apple Script for replaying them later.

- **Function and data preview**: Real-time automatic display of the current function and data. Interactive graphical editing tools for function parameters and data points..

- **Externally compiled code**: Import functions, algorithms, and other programs written in your favorite programming language or in Apple Script.

- **On-line evaluation of mathematical expressions**: Wherever proFit expects numerical input (such as in spreadsheets or dialog boxes) any mathematical expression can be entered.

- **Drawing from a program**: proFit programs can directly draw in proFit’s drawing windows to create drawings with high precision coordinates. These drawings are available for copying and pasting into other applications and for high resolution printing.
• *Macro programming*: Write complete macros to perform common tasks such as opening and closing document windows, fitting, importing and exporting files, etc.

• *Extensive on-line help*: Balloons and Apple Guide™ provide answers and explanations. A dedicated on-line help is available for function and program definition.

• *Powerful plug-ins*: Various external modules further increase pro Fit’s power, e.g. for contour plotting and 3D plotting of functions and data sets (3D plotting requires a Power Macintosh with QuickDraw 3D).

• *And much more...*: Such as Drag&Drop, Publish&Subscribe, Numerics algorithms, customizable data file import, etc.

What you need to run pro Fit:
pro Fit runs on Mac OS® with System version 7.5 or later. pro Fit requires at least 2 MByte (suggested 4 MByte) of free memory – if virtual memory is off, the Power Macintosh native version requires at least 3 MByte (suggested 5 MByte).
The QuickDraw GX features are available when running with the QuickDraw GX extension installed.
The QuickDraw 3D modules run only on a PowerPC machine with the QuickDraw 3D extension installed.

**How to read this manual**

This manual gives a full description of pro Fit 5.1. If you do not want to read it, you will still be able to find your way through pro Fit: pro Fit was designed to be used without a manual and most of its features are self explanatory. Extensive on-line help is provided. However, you will need to read the manual to efficiently work with some of pro Fit’s most advanced features.

Those of you who are already familiar with pro Fit 5.0 are referred to the last section of this chapter, "Changes between versions 5.0 and 5.1". Then you may go directly to the chapters giving in-depth information on the new features.

Those who prefer a beginner's introduction should continue with "Getting started", which gives an overview on the most common features of pro Fit.

A description of the basic concepts of pro Fit is given in the next section.
Basic concepts

proFit works with *data, drawings, functions* and *programs* (or, through *Apple Events*, with other applications or *AppleScripts*).

You can enter data into spreadsheet windows. Data can be transformed by built-in transformation algorithms, (e.g. sort, transpose, filter, Fourier transform, or mathematical operations) or by user-defined ones. Data can be text or numbers.

You can define your own data transforms by writing programs, which can access directly the data in the spreadsheet window. proFit translates these programs into computer code, which can be executed directly by the central processing unit of your computer. You can automate many operations using such programs or Apple Events and Apple Script.

**Functions** can be used for plotting, analysis and fitting. There are a number of built-in functions (such as log, cos, exp, etc.). You can define your own functions using the same simple, yet powerful definition language used to define other programs and macros.

Functions and programs can also be defined using an external compiler (external modules).

You can plot your functions and data sets in a drawing window. proFit offers most standard features of a drawing program, and the appearance of all graphical elements is customizable. proFit generates high resolution printer information for direct printing or for exporting data via the clipboard, Drag&Drop, or Publish&Subscribe.
Changes between versions 5.0 and 5.1

pro Fit 5.1 brings various new features. This is a list of the most important ones:

**Recording**
- pro Fit 5.1 is fully “scriptable” and “recordable”.
  pro Fit 5.1 can automatically “record” your actions into a program or an Apple Script. The program or script can then be run to repeat your actions. To record a program, use the commands “Start Recording” and “Stop Recording” from the Customize menu. To record an Apple Script, use a scripting application, such as Apple's Script Editor.

**Programming**
- The built-in programming syntax has undergone major improvements. Complex numbers are now fully supported in function and program definitions. Arrays and strings are also available. All predefined functions work with complex numbers. Parameters can passed as “var”. Many new commands have been added for fitting, plotting and other operations, making every single operation of pro Fit 5.1 accessible by a program. Most of the new commands use “named” parameters, i.e. a name precedes each parameter – this lets you omit parameters if you want to use their default values.

**Functions**
- Function parameter sets can be managed in a much more flexible way in pro Fit 5.1. Function parameters can now be stored with the function definition, with the function code, or with any other file, they will become available automatically when a function is added to the Func menu.

**Fit algorithms**
- New, special purpose fitting algorithms for linear regression and polynomial fit are available.

**Data Windows**
- Data windows can now have up to 16 million rows and columns as long as sufficient memory is available.

**Print Preview**
- A command “Print Preview” (in the File menu) lets you preview how your data-tables, functions, and drawings will look in print.

**Graphing**
- New features are provided for editing graphs: Axis labels can have a common prefix and postfix. Axes can be inverted (i.e. an axis can extend from 1 to –1).

**User Interface**
- The new user interface style and contextual menus introduced with MacOS 8 are supported.
- Some of the menus have been rearranged for better accessibility.
2 Installation

The installation procedure

Installation of pro Fit is very easy. Just double-click the self-unstuffing archive to copy all required files onto your hard disk.

Before installing pro Fit, read the “read me” file if any such file came with the package.

pro Fit versions

pro Fit 5.1 comes in three versions:

pro Fit 5.1 (ppc): A version of the application running native on PowerPC machines. This is by far the fastest version but it runs only on PowerPC machines.

pro Fit 5.1 (68k): A version of the application optimized for a Macintosh with a Motorola 680x0 (68k) CPU without floating point unit (FPU). This version runs on all Macintosh models but is not optimized for the Power Macintosh or for 68k models equipped with a floating point unit.

pro Fit 5.1 (fpu): A version of the application optimized for a Macintosh with 68k CPU and floating point unit (FPU). This version is faster than the non-FPU version but does not run on Macintosh models without a floating point unit. Neither will it run on Power Macintosh models.
3 Getting started

A first session

This chapter describes a typical proFit session. It shows how to enter new data, plot it, and how to fit a mathematical function to it.

Our data

The world’s human population is growing rapidly. Table 3.1 shows the number of inhabitants of this planet for the period after 1940

<table>
<thead>
<tr>
<th>year</th>
<th>population in millions</th>
</tr>
</thead>
<tbody>
<tr>
<td>1940</td>
<td>2200</td>
</tr>
<tr>
<td>1950</td>
<td>2500</td>
</tr>
<tr>
<td>1960</td>
<td>3000</td>
</tr>
<tr>
<td>1969</td>
<td>3600</td>
</tr>
<tr>
<td>1975</td>
<td>4000</td>
</tr>
<tr>
<td>1981</td>
<td>4400</td>
</tr>
<tr>
<td>1987</td>
<td>5000</td>
</tr>
<tr>
<td>1990</td>
<td>5300</td>
</tr>
</tbody>
</table>

Let us plot and analyze these figures.

Starting proFit

First install proFit on your computer, as described in the Chapter “Installation”. Then

- Double-click proFit.

proFit comes up with the following windows: The results window is used to output results of various calculations. The parameters window lists the parameters used by the current function and allows you to edit their values. The preview window shows a “real-time” preview of the current function and data set.

(Close these windows if you do not want them. When you need them again, choose their name from the Windows menu.)

Entering the data

First, you must enter the numbers given in Table 3.1 into a data window. To do this, you have to open a new data window.

1. Choose “New Data” from the File menu

An empty data window appears.
Data are arranged in horizontal rows and vertical columns. The topmost cell of each column shows the name of the column (by default ‘Column 1’, ‘Column 2’, etc.). The cells below contain the data of each column.

2. **Click into the first empty cell of column 1 and enter the first year, 1940.**

   We fill the first column with the years and the second column with the population. The first year is 1940.

3. **Click into the first cell of column 2 and enter the population in millions, 2200.**

4. **Repeat steps 2 and 3 to enter the other years and population figures in the following rows.**

   Enter the values given in Table 3.1. Note that you can use the arrow keys, the tab and the return or enter key to move from one cell to another.

5. **Enter the column titles, ‘year’ and ‘population in millions’.**

   Click into the titles ‘Column 1’ or ‘Column 2’ and enter the new names. Move the mouse to the vertical separation line to the right of the second column title, click, and drag the separation line a little bit to the right, so that you see the complete title. Your window should now look like this:
6. **Save the data by choosing “Save As...” from the File menu.**

You are prompted to enter a name for your file.

**Plotting the data**

Now that we have entered the data, we can display it graphically.

1. **Choose “Plot Data...” from the Draw menu**

A dialog box appears:

![Plot Data dialog box]

- **Plot into current graph**: unchecked
- **Open new window**: checked
- **X-axis**:
  - X1: lin
  - Auto range
- **Y-axis**:
  - Y1: lin
  - Auto range
- **Data window**: population.data
- **X column**: year
- **Y columns**:
  - Selected rows only
  - year
  - population in millions
- **Point**: unchecked
- **Connected**: unchecked
- **Line**: unchecked

Getting started 3-5
Here you can enter the ranges of the plot, the columns to be plotted, and more. In this introductory session we can use the settings as they are.

2. **Click OK.**

A drawing window appears, showing a graph of the data.

You can edit a drawing easily. For example, you can change most parts of the graph just by double-clicking.

3. **Double-click the vertical axis to change its range.**

(Double-click the vertical axis itself, not the numbers to the left of it!) A dialog box called “Graph Settings” appears, presenting the settings of the left y-axis:
You can change a variety of parameters here. Often you will use the edit fields First and Last to set the range of the axis. Another important field is the ‘Distance’ field that defines the distance between major tick marks.

4. Enter 0 for First and 6000 for Last, then click OK.

The vertical axis of the graph now starts at 0 and ends at 6000.

Double-click other parts of the graph or its legend to change other attributes. Try double-clicking the horizontal axis, the center of the plot, or the dot in the legend. You can also double-click any text in the drawing to change it. Or you can choose any of the drawing tools to add lines, polygons, text, etc.

A function to fit our data

The growth of a population can often be described by an exponential function of the type

\[ p(t) = p(x_0) \times \exp \left( \frac{t - x_0}{t_0} \right), \]  

(3.1)

where \( p(t) \) is the population at time \( t \), \( p(x_0) \) the population at an arbitrary start time \( x_0 \), and \( t_0 \) its growth constant.

Let us try to investigate the validity of this formula for the world’s population. We want to find the set of parameters for which equation (3.1) fits our data best.

1. Choose Exp from the Func menu
This brings the parameters window of the Exponential function to the front. It gives a description of
the built-in exponential function and its parameters:

The window is divided into three regions. The top region displays the function parameters, and lets you
edit their value. The bottom right region displays information on the selected parameter, the bottom left
region gives a short description of the function.

The function looks like this:

\[ y = A \times \exp \left( \frac{x - x_0}{t_0} \right) + \text{const}, \quad (3.2) \]

which is essentially identical to equation (3.1). The parameters window also displays the default values
for the parameters \(A, x_0, t_0\) and \(\text{const}\). Starting from these parameters, pro Fit can find a better set of
parameters for describing our data. But first you must define which parameters you want to fit, i.e.
which parameters you want to vary in order to approximate the data with the Exponential function.

As mentioned above, the starting time \(x_0\) is arbitrary. Let us set it to 1940.

2. **Click the number beside ‘x0’ in the parameters window and enter 1940.**
   This defines the parameter’s value.
   Since \(x_0\) is arbitrary, we do not want to fit it:

3. **Uncheck “Use for fitting”.**
   (The check box “Use for fitting” can be found in the lower right area of the window.)
   The parameter name changes from bold face to plain text. This indicates that this parameter is
   constant and will not be fitted.
   (Shortcut: You can also toggle the option “Use for fitting” by simply clicking on a parameter’s
   name.)

4. **Click the parameter name ‘const’**
   We don’t want to fit this parameter, either. The parameter name is not bold anymore and the option
   “Use for fitting” is unchecked now.

Before fitting, it is a good idea to assign starting values to the parameters that are going to be fitted, in
our case \(A\) and \(t_0\). This increases the speed of the fit and the probability of finding the best set of
parameters.
Reasonable starting values for our problem can be estimated easily:

\( A \) is the population in the year 1940, so we can set it to 2200 millions. \(-t_0\) (note the minus, it comes from the different definitions of Eqs. (3.1) and (3.2)) is the time within which the population increases by a factor \( e=2.71... \). Looking at the plot of the data in the drawing window, we can easily guess it to be between 50 and 200 years. Let us set \( t_0 \) to \(-100\):

5. Enter the starting values 2200 for \( A \) and \(-100\) for \( t_0 \)

Your parameter window should now look like the one below

Intermission: Previewing the data and the function

Above we have seen how to produce a graphical representation of the data in a drawing window and how to edit it. You can have a quick look at the graphical appearance of the data (without actively plotting it) by using the Preview window. This same window also shows you a graphical representation of the current function.

Select Preview from the Window menu. You should see the following window:

To the left of the window there are some controls that let you determine what the window must show, and if it must be a floating window or a normal window. To the right are some tools that can be used to edit and analyze the function and the data.

The window shows the current data set and the current function. If you change any function parameter the curve will change to reflect the new value (try it!). The window always shows a plot corresponding to the current set of function parameters and data points.

As you see, our first guess for the function parameters was not altogether bad, but the function doesn’t grow as fast as the actual data. The parameter set corresponding to the actual data set can be found by fitting.


Fitting

1. **Choose Fit... from the Calc menu**

   You can choose the data columns you want to fit:

   ![Fitting Setup](image)

   The data column settings are already ok. This box gives you also the possibility of specifying errors for the data points. For the moment, we don’t need to do this.

2. **Click OK to start fitting**

   Fitting is very fast. When it is completed, the fitted parameters are printed in the results window
The fit yields –54.8 years for $t_0$ and 2113 millions for $A$.

The Preview window automatically shows the function with the new, fitted parameters:

The function now approximates the data points quite well.

We can plot function (3.2) using the fitted parameters:

**3. Choose Plot Function... from the Draw menu**

A dialog box appears, displaying options for plotting the function:
We don’t need to change any of these options.

4. **Click OK to draw the curve**

   The curve is drawn in the graph. You can now rearrange the items in the drawing window to obtain a representation of data and theory like this one:

   ![Graph of world's population since 1940](image)

   **Defining your own functions**

   In the previous session you have fitted the built-in exponential function to your data. Fine. But what do you do if your model is described by some mathematical equation that does not appear among the built-in functions in the Func menu?

   Define your own function!

   proFit can work with virtually all functions you can think of. Let us look at an example:

   Imagine you want to analyze a function of the form
\[ y = a \sin(x) \times \ln(x) + b \]  \hspace{1cm} (3.3)

with the parameters \( a \) and \( b \). To define this function:

- **Choose New Function from the File menu.**
  
  This opens a new, empty function window.

- **Enter the definition of your function in the new window.**
  
  Just enter:
  
  \[
  a[1]\sin(x)\ln(x) + a[2]
  \]
  
  on the first line.

- **Click the "To Menu" button in the function window, or choose “Compile & Add To Menu” from the Customize menu.**
  
  This translates your function into computer code.

  pro Fit looks at what you wrote and sees that you used the variable \( x \) and the standard function parameters \( a[1], a[2] \). It therefore assumes that you want to define a new function and interprets your text accordingly.

  The new function is added to the Func menu, and the parameter window shows its default parameters.

  Your simple expression is replaced by a complete, syntactically correct function definition:

  ```
  function User_Function;
  begin
    y := a[1]\sin(x)\ln(x) + a[2];
  end;
  ```

  The first line defines the name of the function as it appears in the Func menu (User_Function is the default proposed by pro Fit. You can change it to something like LogSine). Then, enclosed between `begin` and `end`, there follows the definition of the function. In the third line the function is calculated (from the variable \( x \) and the parameters \( a[1] \) and \( a[2] \)), and it is assigned (" :=") to the variable \( y \).

  **Note:** An alternative way to define the same function is:
function logSine(ampl, offset:real);
begin
  y := ampl*sin(x)*ln(x) + offset;
end;

In this definition, the parameters of the function are defined in the function header. The names used in the header are then used in the function body. This is the syntax used for standard PASCAL functions. proFit uses the parameter names defined in the function header for displaying the parameters in the parameters window.

After adding the function to proFit, you can change its parameters in the parameters window. You can plot the function, use it for fitting, calculations, etc.

To plot it, you should first set its parameters to reasonable values, e.g. 1 and 0.5: Enter these values in the Parameter window and choose “Plot Function...” from the Draw menu. In the dialog box that comes up, select the plotting range (e.g. the x-axis from 0 to 5). If you already have an open drawing window, you should check the option “Open New Window”, otherwise your curve will be drawn into the existing graph.

Our sample function is not defined for $x \leq 0$. If you were to calculate it for a negative $x$-value, an error would occur. However, the function converges to $y = a[2]$ for $x = 0$. You may want to expand the definition range of the function by defining $y(x) = a[2]$ for all $x \leq 0$. This can be done easily with the following modification.

function logSine;
begin
  if x <= 0
    then y := a[2]
  else y := a[1]*sin(x)*ln(x) + a[2];
end;

(After having modified a definition in the function window, click the "To Menu" button or choose “Compile & Add to Menu” from the Customize menu to add it to proFit in its new form.)

Your function could even become much more complicated than this. You can define functions that contain more than one statement, as well as variables and procedures. You can use most elements of the PASCAL programming language for defining functions.

As we already noted above, it is also possible to implement the same function in such a way that it uses arbitrary names for the parameters instead of the predefined array element $a[1]$, $a[2]$:

function logSine(amplitude, offset: real);
begin
  if x <= 0
    then y := offset
  else y := amplitude*sin(x)*ln(x)+offset;
end;

The pro Fit package comes with more examples of function definitions. Look them up.
Writing programs

Besides defining functions for fitting and plotting, you can also define any data-generation and -transformation algorithms using the same syntax.

Let us have a quick look at a small program that fills the first column of a data window with the powers of two: 2, 4, 8, 16, etc. To define this program, again open a new function window (choose New Function from the File menu) and enter:

```plaintext
for i := 1 to nrRows do
data[i,1] := 2 ** i;
SetColumnName(1,'Powers');
```

Then click the To Menu button. This time pro Fit recognizes that you are defining a program, not a function. It adds the program to the Prog menu and replaces your text with the syntactically correct version:

```plaintext
program User_Program;
var i:integer;
begin
 for i := 1 to nrRows do
   data[i,1] := 2 ** i;
 SetColumnName(1,'Powers');
end;
```

Note that this program starts with the keyword program, and not function. The rest of it follows the same syntax as a function definition, with the exception that no “parameters” are used.

To run the program, open a new data window and choose “User_Program” from the Prog menu. The first column of the data window will be filled with the desired values.

In this chapter, you have seen some of the most important features of pro Fit. For in-depth information consult the following chapters of this manual.
4 Working with data

Data editing

The data window

The data window is organized in horizontal rows and vertical columns. It can hold up to 16 millions columns with up to 16 millions rows if enough memory is available.

To change the size of a data window (i.e. the number of rows and columns), click the resize field in the top left corner of the window.

To bring the first cell of the first column into view, click the home field (to the right of the resize field).

To insert or delete empty rows or columns, click one of the drag fields and drag the mouse.

To change the width of a column, click and drag the separation line between column titles.

Dragging down the info hook opens an empty area at the top of the data window. In this area you can enter general information or comments about your data:
When editing numbers in a data window, the arrow keys (↑ ↓ ← →) move the selection mark to neighboring data cells.

If you hold down the option key while pressing ← or →, the insertion mark moves horizontally within one cell.

The tab key moves the selection one column to the right. The carriage return or enter key moves the selection to the cell below.

**Selecting data**

You can select a **single cell** by clicking it.

- To select a **rectangular region** of data cells, drag the mouse from the top left to the bottom right cell, or click the top left cell and then click the bottom right cell while holding down the shift key.
- To select **all cells in a row/column**, click the row/column number field. To select several rows or columns, click and drag over the row or column numbers you wish to select.
- To select all cells in a column **starting from a certain row**, hold down the **option key** while clicking the topmost cell of the desired selection, or click the column number field and then drag the mouse down to the first row to be selected.
- To select all cells, choose **Select All** from the Edit menu.

You can create a **discontinuous selection**:  
- To extend or modify a current selection to a discontinuous selection of rows, click (and drag) into the rows to be selected or deselected while holding down the **command key**.
- Note that a discontinuous selection can also be created by selecting data in the **Preview window**. See also Chapter 6, “Preview Window”.

**Data types**

By default, each column of a data window contains numerical data, i.e. **real-valued numbers**. The precision and range of these numbers can be:
• $10^{-300}$ to $10^{300}$ with approximately 12 significant digits (double precision)
• $10^{-38}$ to $10^{38}$ with approximately 6 significant digits (single precision)

See Appendix B for details on numeric representations.

By default, a new data window opens with either single or double precision columns. The default type can be selected by choosing the command “Preferences” from the File menu. In the dialog box that comes up, click the “General” icon. See Chapter 13 for details.

A column can also contain text, up to 255 arbitrary characters in each cell. To switch between text and number formats, first select the column or columns you want to change and then choose Column Format from the Calc menu. Alternatively, you can also double-click the column number of a column you want to change.

After either of these actions, the Column format dialog box appears:

Check Text if you want the selected columns to contain text, check Numbers for numerical data. In the latter case you can specify their Range (single or double precision) and define the format for displaying numbers: select the number of digits to be displaced after the decimal point (decimals) from the Decimals pop-up menu. If you check the scientific option, all numbers will be shown in exponential representation (i.e. 1.34e+3 for 1340).

You can also enter the column width in pixels in the corresponding edit field. A second way for changing the width of a column is to click on the boundary line between column titles (the mouse cursor will change to $\leftrightarrow$ ) and drag it to the desired position.

### Entering data

You can type data in the data window, copy and paste it, or drag it and drop it everywhere you want.

Instead of entering a number directly, you can enter a mathematical expression, e.g. “exp(1)” or “6+sin(π/4)”, or any predefined function or variable. See Chapter 9, “Defining functions and programs” for more information about all the predefined keywords and functions you can use in mathematical expressions.
You can also import data from text files. See the Appendix C, “File Formats” for detailed information.

**Data transformation**

proFit offers various methods for transforming data: Numerical transformations, data reduction, sorting, transposing, and Fourier transforms. In addition, you can write programs that edit, manage, or create data in any conceivable way (for more information on writing such programs see Chapter 9, “Defining functions and programs”).

All the commands for transforming data are found in the Calc menu and they work on the data window which is in front of all other windows.

**Algebraic transformations**

To make simple numerical transformations on your data, choose **Data Transform** from the Calc menu.

The transformations you can carry out with this command are of the form \( y = \text{func}(x) \). You can define where the \( x \)-value comes from and where \( y \) has to be stored. You can also choose what function you want to use (note that some of these “functions” do not need an \( x \)-value).

The transformation is either by columns or on the current selection: Check **Selected Rows only** to only include selected rows in the calculation. Choose **Selected cells** to work on the current selection.
In calculations on the current selection, each cell \((x)\) in the selection is replaced by its transformed value \((y)\). In transformations by column, the cells of the \(x\)-column are transformed and stored in the cells of the \(y\)-column. You can select the \(x\)- and \(y\)-columns from the pop-up menus. (In these menus empty columns are marked with ‘\(\bullet\)’, columns already containing data with ‘\(\ast\)’, and text columns with ‘\(\dagger\)’).

Five different groups of transformations are available:

- **Simple arithmetics**: All these transformations are of the type \(y = x \text{ op } val\), where \(\text{op}\) is one of the operators \(+\), \(-\), \(^*\) (multiplication), \(/\) (division), \(^\wedge\) (power), \(\text{div}\) (integer division), \(\text{mod}\) (modulus).
- **Column arithmetics**: These transformations are of the type \(y = x \text{ op } \text{col}\). Again, \(\text{op}\) can be any of the operators mentioned above.
- **Differential / Integral**: These transformations return the discrete derivative or integral. The **derivative** is calculated as the discrete derivative of a column \(d\) that is selected from the menu to the right of the ‘\(\mathrm{d/}dx\)’ popup field, in respect to the \(x\)-column. The result is stored in the \(y\)-column according to the formula
  \[
y_i = \frac{d_{i+1} - d_i}{x_{i+1} - x_i}.
\]

The **integral** is calculated as the discrete integral of a column \(d\) over the \(x\)-column. \(d\) is again selected from the menu to the right of the ‘\(\int\) \(dx\)’ popup field. The result is stored in the \(y\)-column according to the formula
  \[
y_j = \frac{1}{2} \sum_{i=1}^{j-1} (d_{i+1} + d_i)(x_{i+1} - x_i).
\]

Sometimes you may want to integrate over a **single** column \(d\), or you may want to differentiate over a **single** column \(d\), according to one of the following equations:

\[
y_j = \sum_{i=1}^{j-1} d_i \quad \text{or} \quad y_i = d_{i+1} - d_i.
\]

You can do this by creating a column containing the numbers 1, 2, 3, ... (use the \(\text{fill(n)}\) command described under ‘Various functions’ below) and using this column as your \(x\)-column.

- **Various functions**: Here you can select various simple transformation functions, such as \(\sin(x)\), \(\exp(x)\), \(\ln(x)\), etc. Among them, you can also find the currently selected function of the Func menu, as well as the special functions \(\text{fill(0)}\), \(\text{fill(1)}\) and \(\text{fill(n)}\), which let you fill a column with the values 0 or 1 or with ascending values 1, 2, 3,... respectively.
- **Formula**: If you select this sort of transformation you are free to define any transformation statement you like. Columns are labeled by the character ‘\(c\)’ followed by their column number. You can use columns, constants, mathematical functions, or calls to user-defined functions in the Func menu. You can use the symbols \(i\) or \(n\) for the row number and (if you have chosen “Selection only”) \(j\) or \(m\) for the column number.

Examples:

\[
\text{x+sqrt(x)} \quad \text{an expression}
\]
\[
\tan(c10) \quad \text{tangent of values in column 10}
\]
\[
\text{CovarMatrix}(i,j) \quad \text{the covariance matrix of the last fit}
\]

The size of such a transformation statement is limited to 255 characters.

If the result of a calculation is not defined, either because a data field used for the calculation is empty or because there was an numerical error, the resulting data field is cleared.
**User programs**

proFit lets you define your own data transform programs or macros. These programs can perform data transformations in the data window, create a graph in the drawing window, etc. They are found at the end of the Misc menu.

Chapter 9, “Defining functions and programs” explains how to define such programs.

**Data reduction**

The command “Data Reduction” in the Calc menu offers several possibilities for data reduction, e.g. by averaging over several data points or by skipping part of the points.

To keep every n\textsuperscript{th} row and to remove all other rows, select **Keep every**.

To remove every n\textsuperscript{th} row and to keep all other rows, select **Forget every**.

To replace groups of n consecutive cells in a column by their average, select **Average over**. This option decreases the number of rows by a factor of n. (For example, if n=3, the values in the rows 1, 2, and 3 are averaged and the result is stored in row 1. The average of rows 4, 5, and 6 is then stored in row 2 etc.)

To replace every data value with the average of itself and its n-1 neighboring values in its column, select **Smooth over**. Again, the average of n values is calculated. In contrast to ‘Average over’, the number of rows is not reduced! (For example, if n=3, the value in row i is replaced by the average over the values in rows i–1, i, and i+1).

To transform only the selected cells, check **Selection only**. In this case only the currently selected cells (highlighted in the data window) are affected.

If the selection is discontinuous (whole rows only), the above algorithms are applied to each continuous block of the selection, one after the other. The various discontinuous blocks are treated separately and do not interact with each other.

To keep only the rows that are presently selected, check **Keep selected rows**. To remove all the presently selected rows, check **Remove selected rows**.

**Sorting data**

To sort data, choose **Sort...** from the Calc menu:
Use the pop-up menu to select the column to be used as a reference for sorting. You can sort by ascending or by descending values.

All the rows in the data window will be rearranged according to the new order in the sort column. To order only the selected part of the data window, check Selection only.

Note that you can only sort by columns that contain numerical data. You cannot sort by columns that contain text.

Transposing data

The command Transpose in the Calc menu exchanges the rows and columns in the active window. It automatically resizes the data window to make sure that all the data fits into it.

Statistical analysis of a data set

The command Statistics... in the Calc menu lets you calculate statistical data of a one-dimensional data set.
The data set that will be analyzed by the statistical algorithms can either be a **Single column** (use the popup menu to define it), **All columns**, or only the **Selected Cells**. If you specify a single column or all columns, you can check **Selected rows only** to only use the data in the selected rows.

The following statistical values are calculated from a set of data \(x_1 .. x_N\) and are printed to the results window:

- The number of valid values \(N\) in the data set.
- The median of the sorted data set (central value for odd \(N\) or average of the two central values for even \(N\))
- The minimum (smallest value) and the maximum (largest value)
- The sum of all valid values \(S = \sum_{i=1}^{N} x_i\)
- The mean \(\bar{x} = \frac{S}{N} = \frac{1}{N} \sum_{i=1}^{N} x_i\)
- The variance \(Var = \frac{1}{N-1} \sum_{i=1}^{N} (x_i - \bar{x})^2\)
- The standard deviation \(\sigma = \sqrt{Var}\)
- The mean absolute deviation \(ADev = \frac{1}{N} \sum_{i=1}^{N} |x_i - \bar{x}|\)
- The skewness \(Skew = \frac{1}{N} \sum_{i=1}^{N} \left[ \frac{x_i - \bar{x}}{\sigma} \right]^3\)
- The kurtosis \(Kurt = \left\{ \frac{1}{N} \sum_{i=1}^{N} \left[ \frac{x_i - \bar{x}}{\sigma} \right]^4 \right\} - 3\)

The **Skewness** characterizes the degree of asymmetry of a distribution around its mean. The **kurtosis** measures the relative “peakyness” or flatness of a distribution.

**Fourier transforms**

proFit can calculate Fourier transforms of numerical data. A Fourier transform is a transformation of numerical data from the “time domain” into the “frequency domain”, or vice versa.

If you have a one-dimensional set of real valued data points, \(h_k (k = 0 .. N-1)\), the **discrete Fourier transform** \(H_n\) of these points is given by

\[
H_n = \sum_{k=0}^{N-1} h_k e^{2\pi i kn/N}, \quad (1)
\]

where \(n\) goes from \(-N/2\) to \(N/2\) (\(N\) is assumed to be even). The inverse Fourier transform is the inverse operation: It allows the calculation of data \(h_k\) in the time domain from data \(H_k\) in the frequency domain by

\[
h_k = \frac{1}{N} \sum_{n=0}^{N-1} H_n e^{-2\pi i kn/N}. \quad (2)
\]
Note that $h_k$ as well as $H_k$ can be complex values.

A classical interpretation of the Fourier transformation is the following:

A signal $h(t)$ is sampled at a regular time interval $\Delta t$, resulting in a set of data points $h_k = h(\Delta t k)$. The Fourier transform of this set of data corresponds to the frequency spectrum of the signal. $H_n$ corresponds to the amplitude of the signal at frequency $n/(N \Delta t)$.

Note that the maximum frequency of the frequency domain is $f_c = 1/(2\Delta t)$, the Nyquist critical frequency.

The Fourier transform and its inverse can be calculated with two commands in the submenu Fourier Transform of the Calc menu: FFT and Inverse FFT. (“FFT” stands for “Fast Fourier Transform”, an efficient algorithm for the calculation of the Fourier transform.)

These built-in algorithms assume that the data set $h_k$ of the time domain is real-valued and not complex. In this case the frequency domain data set $H_n$ is complex but we have $H_n = H_{-n}^*$ i.e. the values at positive frequency are the complex conjugate values at negative frequency. It is therefore sufficient to calculate only the positive frequency spectrum of the Fourier transform.

Note: The built in Fourier transform works on real valued data in the time domain. To work in complex data, use the external module “FFT” that comes with pro Fit.

To carry out a Fourier transformation, bring the data window with your data in the time domain to the front and choose FFT from the Fourier Transform submenu:

Select the column that contains your time domain data and the columns for the real and imaginary parts of your frequency domain data. If you check the box Calculate frequency, you must enter the time interval between two points of the time domain (Data interval) and a column (Frequency) for the frequency values of the frequency domain data.
Instead of calculating the real and imaginary parts in the frequency domain, you can also calculate their absolute value and complex argument (check **Amplitude and phase**, instead of **Real and imaginary parts**).

To calculate the inverse Fourier transform, select **Inverse FFT** from the Fourier transform submenu. The dialog box that appears for this command is very similar to the dialog box we have just seen:

Your input data are the complex values in the frequency domain. You select the columns for the real and the imaginary parts, or, alternatively (when you select **Amplitude and phase** instead of **Real and imaginary parts**), you select the columns for the absolute value and the complex argument of your data.

The output column contains the real valued data points of the time domain.

If you want to calculate the time range (in seconds) for your output data, check **Calculate time**, enter the frequency interval between consecutive data points of the frequency domain, and select a column for the time values.

Note that if you have $N$ points in the time domain, you obtain $N/2+1$ (complex) points in the frequency domain and vice versa.

The FFT algorithm works only for $N = 2^m$ (where $m$ is a positive integer), i.e. for $N = 2, 4, 8, 16, ...$ If the number of input data points is not a power of two, then the missing values to the next power of two are assumed to be 0.

For further information on the subject of discrete Fourier transformations see e.g. W.H Press et al., *Numerical Recipes*, Cambridge University Press (Cambridge, 1989).
Defining a data set to work on

Some of proFit’s commands access data in the data windows. If you have several data windows open at the same time, proFit uses some rules for selecting the data window it works on:

- The transformation commands in the Calc menu work on the active data window (the window in front of all other windows). If the active window is not a data window, these commands cannot be used. (Example: the Data Transformation... command is only enabled when the front most window is a data window.)
- Some other commands use the front most of all data windows. It does not matter if windows of other kinds are in front. If the active window is not a data window, these commands look at all the windows behind the active window and work on the first data window they find. This will be the data window that is closest to the front. (Example: the Spline function uses the data window that is closest to the front.)
- The commands for curve fitting and for plotting data display dialog boxes where you can choose the data window from a pop-up menu. (Examples: Plot Data... and Nonlinear Fit...)

The data window containing the data used in a particular operation is called the current data window in this manual. The current data window is either the foremost data window or the window you have selected yourself.

When a data window is used as the current data window by a function or by some commands, four of its columns can have a special meaning. They are the default \(x\)-, \(y\)-, \(\Delta x\)-, and \(\Delta y\)-columns. You can define these columns using the pop-up menu that appears when you click the column number of a data window while holding down the command key:

For example, the ‘Spline’ function uses the data in the \(x\)- and \(y\)-columns of the foremost of all the data windows (other windows of a different kind, e.g. a drawing window, can be active).

A small ‘\(x\)’, ‘\(y\)’, ‘\(\Delta x\)’ or ‘\(\Delta y\)’ in the head of a column marks the default columns.
5 Working with functions

Functions supported by proFit are of the form \( y = f(x) \) and can have one or more parameters. You can use these functions for fitting, plotting and analysis. This chapter gives an overview of what you can do with functions.

proFit has a set of built-in functions, that you can use “as-is”, and gives you the possibility of defining your own functions. To do this, you can use the built in programming language (see Chapter 9, “Defining functions and programs”), or you can write your functions in your own compiler and import them as modules (see Chapter 10, “Working with external modules”).

A list of the currently available functions can be found in the “Func” menu.

Introduction

A function in pro Fit has the form

\[
y = f(x, a_1, a_2, \ldots a_n)
\]

where \( x \) is its argument and \( y \) its value. \( a_1, a_2, \ldots a_n \) are the parameters of the function. An example is the polynomial function, one of pro Fit’s built-in functions:

\[
y = a_0 + a_1 x + a_2 x^2 + \ldots
\]

You can select the function you want to work with from the list in the Func menu. When you do this, a short description of the function and its parameters appears in the Parameters Window. As an example, the polynomial function has the following parameters window:

![Polynom Parameters Window]

Parameters

In the Parameters window you can view and set the parameters of the function.

The upper part of the window lists all the parameters of the function. It also contains a popup menu where you can save parameter sets for later use (see below). The lower left part of the window gives a short description of the function, the lower right part lists some properties of the currently selected parameter. What you can do here:
editing To change a parameter, click its value field and enter the desired value. Hit the tab key or the enter key to move to the next parameter.

copy, paste You can copy and paste parameter values between the parameters window and data or text windows using the Copy, Cut, and Paste commands from the Edit menu. If you choose Copy with no parameter value selected, all parameters are copied to the clipboard, separated by tabulators. If you choose Paste with no parameter value selected, the text on the clipboard is assumed to contain several values separated by spaces, tabs or carriage returns, which are then used to change all parameter values.

limits A parameter can have upper and lower limits, which are displayed in the lower right part of the Parameters window. These limits are used to constrain the parameter during fitting and function optimization. To change a limit of a parameter, select the parameter and enter the limit in the corresponding field. To remove a limit, select the parameter and clear its limit.

fitting mode To change the fitting mode of a parameter, check or uncheck the option “Use for fitting” in the lower right part of the window. If you check this option, the parameter will be varied during fitting and optimization, otherwise it will be kept fixed. The fitting mode of a parameter determines the style of its name in the Parameter window. Parameters with names displayed in bold face will be varied during a fit. Parameters displayed in normal type face are kept fixed during a fit. As an alternative to using the “Use for fitting” checkbox, simply click the name of the parameter to toggle its fitting mode.

Setting one of the parameters of a function to be equal to the value of x

You can enter the expression '=x' when changing the value of a parameter in the parameters window:

The selected parameter is forced to be equal to the current x-value of the function.

If you want to study the dependence of a function upon various parameters, you can define your function as a function of parameters only, without explicitly using the variable 'x'. You then designate the parameter treated as the x-value by entering '=x' for its value in the parameters window.

If you explicitly use the variable 'x' inside a function and also define a parameter to be equal to x, both will have the value of x: A function like y:=a[1]*sin(x) becomes the function y:=x*sin(x) if a[1] is set to be equal to x in the parameters window.

If you define your own function, you cannot use this feature for parameters that you use in the procedure first because x is not defined in the procedure first. If you set a parameter to be equal to x, its value will be undefined in first. (See Chapter 9, “Defining functions and programs”, for more details.) If you plan to set a parameter equal to x, never use it in the function first.
Using functions

The following explains what you can do with functions. It does, however, not describe how to plot or fit functions – these topics are covered in Chapter 8, “Fitting” and Chapter 7, “Drawing”.

Calculating function values

You can calculate the $y$-value of the currently selected function for a given $x$-value by choosing Calculate Function($x$) from the Calc menu (the name of this command changes – it always uses the name of the currently selected function):

You can calculate the $y$-value of the currently selected function for a given $x$-value by choosing Calculate Function($x$) from the Calc menu (the name of this command changes – it always uses the name of the currently selected function).

If you click OK, the function is calculated for the given $x$-value, its $y$-value is printed in the results window, and the dialog box disappears.

If you click Do It, the function’s value is displayed in the dialog box and written to the results window. The box does not go away and you can calculate other values of the function immediately.

If Use fitted params is checked, the resulting parameters of the last data fit are used for calculating, otherwise the parameters displayed in the parameters window are used.

Choosing Tabulate Function($x$)... allows you to create a table of the function’s values in a data window. You are prompted for the first and last value of the table and its step width:

If you enter a numerical value for Step, the function is calculated at equidistant $x$-values. If you enter ‘auto’ in the field ‘Step’, proFit chooses the $x$-values at which the function is calculated by using a special algorithm that decreases the distance between calculated points wherever the function is strongly
bent.
To tabulate the function at the values of the $x$–column of the current data window, enter ‘points’ in the field ‘Step’.
Instead of ‘auto’ or ‘points’ you can enter a single ‘a’ or ‘p’.

**Optimization of functions**
The command **Optimize** from the Calc menu lets you find the maximum or minimum of a function by varying the function parameters and/or its $x$-value.

If you check **the active parameters**, the algorithm will vary all parameters that are presently marked as active (i.e. which in the parameters window have a bold face name and “use for fitting” checked). The parameters are only varied within their limits, if such limits are specified.

If you check **$X$**, the algorithm will vary the function’s $x$ value. Otherwise the $x$-value is kept fixed at the given value.

The settings under **precision** affect the accuracy and speed of the calculation. If your function is slow, you should first choose a low precision and, once you are satisfied with the results, choose a higher precision.

**Print full description** controls the amount of information to appear in the results window.

Note that the command “Optimize” is designed for multi-dimensional optimization. If you only want to vary the function’s $x$-value but not its parameters, you should use the faster command “Extrema” described below.

**Finding roots**
The **Analyze** submenu in the Calc menu allows you to calculate the roots, the extrema and the integral of a function:
Roots

The roots of a function \( f(x) \) are those values of \( x \) for which \( f(x) \) takes a given value, such as 0. To calculate the roots of a function, choose **Roots** from the Analyze submenu (menu Calc).

![Roots of Polynom(x)](image)

Here, you can select the range within which to look for roots. This range is divided into a given number of sub-intervals.

Example: If you look for the roots \( f(x) = 0 \) of a function between \( x = 0 \) and \( x = 1 \) and specify ten sub-intervals, proFit looks for roots in the intervals \([0, 0.1] \), \([0.1, 0.2] \), etc. In each interval \([a, b] \) it checks if the sign of \( f(a) \) is opposite to the sign of \( f(b) \) (or if one of these values is undefined and the other defined). If this is the case, the corresponding interval is searched for a root.

Enter a value \( Y \) in the field **Look for \( f(x) = 0 \)** to find the roots of the equation \( f(x) – Y = 0 \). Per default, this value is 0. For example, you can use this feature to find all x-values where a function becomes equal to 1.0.

**Table of roots**

By choosing Table of Roots from the Analyze submenu, you can create a table of the roots of your function for different values of one of the function’s parameters:
The top part of the box contains the same entries as the Roots dialog box (see above). In the lower part of the box, you can enter the parameter you want to make the table for, its range and the step width for tabulating.

Note that if you have more than one root for a given parameter value, only the first root will be found and entered in the table for every value of the parameter you vary.

Finding minima and maxima

To find the extrema of a function (i.e. the x-values where f(x) becomes largest or smallest), choose “Extrema” from the Analyze submenu (menu Calc). A dialog box similar to the one for the Roots command appears. You enter the x-range within which extrema must be found and a number of sub-intervals. proFit tries to find one local extremum (minimum, maximum) within each sub-interval.

To tabulate the extrema of a function (i.e. the x-values where f(x) becomes largest or smallest) for different values of one of its parameters, you choose “Table of Extrema” from the Analyze submenu. The dialog box displayed by this command is again the same as for the roots command (see above)

Note: If you want to find the extrema of a function by varying not only its x-value but also its parameters (multi-dimensional optimization), use choose “Optimize” from the menu Calc. This command is described above.

Integration

To calculate the numerical integral of a function, choose Integral from the Analyze submenu (menu Calc). In the dialog box that appears you can enter the limits of the integral as well as the number of iterations
The number of iterations affects the accuracy of the results. A larger number of iterations yields a more accurate result but more time is needed for the calculation.

To **tabulate** the integrals by varying a parameter of the function or one of the integral's limits, choose Tabulate Integral from the Analysis submenu.

### The Spline function

There is one special function in the list of predefined functions: the **Spline** function. You can use this function only when you have a set of data points \((x_i, y_i)\) in a data window (the \(x_i\) column and the \(y_i\) column are identified by small ‘x’ or ‘y’ labels in column head. Change the default x- and y- columns by clicking the header of a column while holding down the command key.). The Spline function is defined as a smooth cubic Spline curve going through all your data points. The Spline function is useful for interpolation, especially when you do not have a mathematical model for your data. This is a simple data set together with its Spline function.

![Graph](image.png)

To use the Spline function for a given data set:

1. **Choose the Spline function from the Func menu.**
2. **Bring its parameters window to the front and click the “Select Data” button.**
   
   A dialog box appears:
Use the popup menus to select the data set to be used by the Spline function.

If you do not use the “Select Data” button in the parameters window, then the Spline function will use the data in the frontmost data window (Select the appropriate x- and y-column by clicking the desired column number while holding down the command key).

If you did use the “Select Data” button, but you close the data with the data set used by Spline, then the Spline functions reverts back to using the data set in the frontmost data window.
6 The Preview Window

There are generally two different approaches that are used by plotting applications for managing graphs and the data used to generate them:

- The first one consists in maintaining a permanent link between the data you plot and the result of the operation (the graph). In this approach whenever you edit the data you used for creating the plot, the plot automatically changes to reflect the new values of the data set. Since the link between data and plot needs to be maintained, it is in generally not possible to save data and graphs separately, and they must be saved in the same document. In applications using this approach, the graph is only a different “view” of the data, but does not lead an independent life.

- In the second approach, graphs and data are independent. Although a graph can be created from data, and data can be recovered from a graph, the two documents lead separate lives. After it has been created, the graph does not know anymore about the origin of the data used to create it, and if you modify that data, the graph remains untouched.

pro Fit uses the second approach. There are data documents, and there are drawing documents. From the data you can create graphs. From the graphs you can recover the data used to plot them. Drawing and data documents can be stored and maintained separately and don’t affect each other. In Chapter 7, “Drawing”, you will see how you can use the Draw menu to plot a function and a data set, obtain graphical representations of your data and functions, and edit the graphs to obtain the precise graph style you are looking for.

There is an ongoing discussion between the supporters of the first approach outlined above and the supporters of the second approach used by pro Fit. A link between data and its graphical representation is in fact also useful. pro Fit’s answer to this dilemma is the Preview Window.

The preview window is a graphical representation of the current function and/or the current data set. It gives you a graphical “view” of the function and the data set. Any change in the data set or in the function is reflected in the preview window. You can even use the preview window to graphically edit the function parameters or the data set.

Use the preview window to have a “quick look” at a function or a data set without actually plotting it. For instance, you can let the Preview Window be a floating window and keep it in front while you load many different data files. The preview window will automatically display all data contained in the current x- and y- columns of the front window.

You can also use the preview window to view functions, graphically edit function parameters, select a range of data points, compare a function to a data set, etc.
Choose **Preview** from the Windows menu to see proFit’s Preview Window. This is how the Preview Window looks like when it has its smallest size and is working as a floating window.

On the left side of the Preview Window there are some check boxes that determine how the window behaves and what it shows. The main part of the window is a rectangular viewport that shows a graphical representation of the current function and data set. On the right of the window there is a tool palette with tools for changing the coordinates displayed by the viewport, for graphically editing the function and the data set, and for determining precise x- and y- coordinates.

Check **Floating** to make the preview window a “floating window” which always stays in front of all document windows. Uncheck this option to transform it into a normal window, which you can be hidden by other windows.

Check or uncheck **Show data** and **Show function** to choose what is shown in the window. When Show data is checked, the window displays the current data set, *i.e.* the x- and y- columns of the current data window. You can select the data set to be shown in the preview window by clicking the **Data** button or by directly setting x- and y- columns in the data window.

The **Fitted params** check box appears whenever a fit was successful, to give you the option of seeing a plot of the function using the parameters obtained in the last fit, instead of seeing the function with the parameters shown in the Parameters window.

Click the **Redraw** button if you want to let proFit redraw the complete function at maximum resolution. proFit automatically decreases the resolution at which it draws the function if it notices that the function is too slow. You can override this by clicking the Redraw button.

The **Undo** button appears only when the Preview Window is floating, and it allows you to undo the last operation. When the Preview Window is not floating, you can undo the last operation as usual, by choosing Undo from the Edit menu.

At the right end of the title bar there is a **zoom box**. Click it if you want to work with a larger window.

At the edges of the rectangular viewport that displays the function and the data set are four edit-fields giving the coordinate range to be displayed. You can edit the values to change the x- or y- range. Between these edit-items there are check boxes labeled **auto** and **log**. Check them to let proFit automatically recalculate the ranges based on the ranges of current function and data set, or to use logarithmic scaling.

There is a **permanent link** between the preview window and the data or function it displays. The preview window always displays an up-to-date representation of the current function and data set.
Change a coordinate in the data window, or add a data point, and the corresponding point will automatically appear in the preview window. Change a function parameter and the representation of the function in the preview window will be updated automatically. Modify a function definition and add it to the menu once again, and the preview window will automatically display the new function.

If you select data points in the preview window, the corresponding rows are selected in the data window. If you select some rows in the data window, the corresponding selection is shown in the preview window. There is even the possibility of clicking and dragging data points in the preview window. Doing so changes their coordinates in the data window.

**Preview Window Tools**

To the right of the preview window there is a palette of five different tools. You can use them to select data points and change their coordinates graphically, to change the ranges of the preview window viewport, to graphically change the value of the function parameters, and to set coordinate markers.

**Selecting data points with the arrow tool**

Use the **arrow tool** to select data points. Simply click a data point to select it. Click and drag to select a range of points with a selection rectangle. Hold down the shift key to add points to the current selection, or to remove points from the current selection. If you hold down the **shift** key while dragging a selection rectangle, the selection state of the data points contained in the rectangle toggles between selected and not-selected. Hold down both **shift** and **option** keys to always add the points inside the selection rectangle to the current selection.

You can set the **color** of the data points and the color used to mark selected data points using the **Preferences...** command in the File menu. If you have a monochrome monitor, proFit will use a dithered pattern to mark the selected points.

Whenever you select a data point in the preview window, the corresponding row is selected in the data window. If you then choose Data Transform... from the Calc menu, you can perform calculations on the data in the selected rows only.

---

Selecting a data point in the preview window always selects the **whole** corresponding row in the data window. If you select a range of data points in the preview and then delete them, you will delete all data in the selected rows and not only in the current x- and y-columns.

---

**Changing the ranges of the preview**

You can change the ranges of the preview either by editing them manually, or by using the **drag tool** or the **zoom tool**.

Click in the viewport area with the drag tool and drag the area of the data set or function curve displayed by the preview. The ranges of the preview will change accordingly. You start dragging inside the viewport, but you can go on dragging also outside, thus changing the coordinates by a large amount.
Click in the viewport area with the zoom tool (the lens) to zoom in and magnify the clicked area. Hold down the option key while clicking to zoom out.

If you hold down the command key you can click and drag with the zoom tool, thus selecting the precise area that will be displayed in the viewport after zooming.

**Dragging the function curve**

Select the fitting tool and click in the viewport. Hold down the mouse button while you move the mouse. The curve of the function follows the position of the mouse while the selected function parameter is adjusted accordingly.

When using the fitting tool, you must specify which parameter you want to vary. You can do this either by clicking it in the parameter window, or by choosing its name from the small popup menu that appears below the tools palette in the preview window. You can only vary one parameter at a time.

When you select the fitting tool and click into the preview, the selected parameter is varied until the function curve goes through the point indicated by the mouse. pro Fit does this by numerically solving the function $f(a,x) = y$, where $a$ is the selected parameter and $(x,y)$ is the point indicated by the fitting tool. If it is mathematically not possible for the function to go through that point, no matter what the value of the selected parameter is, then you will not be able to drag the function curve to that point. The same applies if pro Fit fails to find numerically the correct value for the parameter.

If you use the fitting tool with a slow function, pro Fit will automatically reduce the resolution with which the function is drawn, so the function will not appear to be smooth anymore. The resolution will be increased again once you are finished dragging. Click the Redraw button to achieve the maximum resolution.

**Inspecting and editing coordinates**

The last tool in the tools palette can be used to place coordinate markers on a given data point, or on the function curve. Select the marker tool and click the curve or a data point. pro Fit creates a new marker at the indicated position.

While you move the marker tool around inside the viewport of the drawing window, the corresponding coordinates are displayed in the bottom left corner of the preview window.

When you create a new marker, it becomes the active marker. The active marker is always flashing on and off.

You can create any number of markers. The first marker you create is the reference marker. Subsequently created markers are auxiliary markers and are numbered starting from 1. Their number appears when they are active (when they are flashing).

To set the color of the reference marker and of the auxiliary markers, choose Preferences... from the File menu. If the reference marker cannot be distinguished by its color, pro Fit automatically draws it larger.

Marker coordinates are displayed in the bottom left corner of the preview window. If there is more than one marker, there can be two other coordinates displayed to the right of the marker coordinates. They correspond to the distance between the reference marker and one of the other markers.
What the coordinates mean:

<table>
<thead>
<tr>
<th></th>
<th>( x, y ) are the coordinates of</th>
<th>( \Delta x, \Delta x ) are the distances from</th>
</tr>
</thead>
<tbody>
<tr>
<td>No active markers around</td>
<td>the reference marker</td>
<td>the other marker (if there is only one)</td>
</tr>
<tr>
<td>One active marker</td>
<td>the active marker</td>
<td>the reference marker</td>
</tr>
</tbody>
</table>

If a marker is active, its coordinates are displayed in editable fields. Edit any of these fields to set the coordinate of the marker.

If the marker is a data marker and the preview window is big, the data window row number that corresponds to the marked data point is also displayed. It is found above the \( x \)-coordinates and is labeled \( "i = " \)

The behavior when changing the text in the edit fields containing the marked coordinates varies depending if the marker is on a data point or if it is on a function curve.

- If the marker is on a data point, the coordinates displayed in the edit field correspond to the coordinates of that data point in the data window. Editing them changes the values in the data window.
- If the marker is on a function curve, editing the coordinates sets the position of the marker. If you edit the \( y \)-coordinates, pro Fit numerically inverts the function to find the corresponding \( x \)-value. You can use this feature also as a shortcut to calculate the inverse of a function, or its root.

Coordinate markers can be accessed from pro Fit programs using the predefined functions GetMarkedX, GetMarkedY, and GetMarkedCoords.

Managing coordinate markers

We already saw above how to create markers and look at their coordinates. There are a few other simple operations that can be applied to markers.
- Click a marker to make it active.
- Click a marker while holding down the option key to transform it into the reference marker
- Hit the delete key (backspace) while a marker is active to delete it.
- Click and drag a marker to move it to a new position.
- Move a function marker to the right or left border of the viewport to delete it.

To move a marker, click and drag it, or use the left and right arrow keys. A data marker jumps to the next point to its left or its right, a function marker will move along the function curve. pro Fit makes sure that you don’t move a marker outside the ranges of the viewport. You can override this by holding down the option key while moving the marker with the arrow keys.

When you have markers on the function and you uncheck the show function checkbox, all of them are deleted. The same applies to markers on data points when you uncheck the show data checkbox.
Uncheck and check the show function and/or show data checkboxes if you have many markers around and want to get rid of all of them in one rapid move.

Data markers store their position as the number of the data point they mark. If you have data markers around and you delete or add points to the data set, the data markers might move to a new data point. If no new point corresponding to the old index is found for a given marker, that data marker is destroyed.

If you have function markers and you change the ranges of the display in such a way that their x-coordinates are not visible anymore, those markers are destroyed.

**Tips and tricks**

**Using the preview window during a fit**

If Show function is checked during a fit, the function is redrawn from time to time to show how it changes during the fit. This lets you monitor how well the fit converges. However, drawing the function takes time. You should close the preview window or uncheck Show Function to obtain the fastest fitting.

The same thing happens when you use the Error Analysis feature. To perform error analysis, proFit generates random sets of synthetic data points and fits the function to it. If Show Function is checked in the preview window, you will see how the function curve varies in correspondence to the fitted parameters.

See Chapter 8, “Fitting”, for more details on the fitting process and the Error Analysis algorithm.

**Choosing initial values of function parameters**

You can display the data you want to fit together with the fit-function in the preview window. You can then use the fitting-tool to drag the function in such a way that it follows the data points as closely as possible. Try using the fitting-tool with the various parameters you want to fit.

This is a kind of “hand fitting” that can be a very useful and fast way to set up a reasonable set of starting parameters for a fit.

For special applications, you can also mark certain features of your data set using coordinate markers and write a small program which reads the coordinates of these markers and uses them to calculate the optimal initial values for the parameters of the current function.
7  Drawing and Plotting

Drawing and plotting takes place in a drawing window. This window supports most features of commonly used drawing applications.

We will first describe the drawing window and its general features.

The section “Drawing” discusses standard drawing objects and editing techniques.

The section “Plotting” is devoted to the plotting commands used to produce graphical representations of your data and functions. It discusses how to manage graphs and how to edit them.

The drawing window

A drawing window always contains one single page. You can select its size and orientation by choosing Page Setup... from the File menu. Before choosing Page Setup, make sure that you have selected a printer in the Chooser or, if you are running QuickDraw GX, that you have selected your preferred desktop printer in the Finder.

A dotted rectangle frames the printable area of the page. Objects that lie outside this rectangle do not print. See your printer’s manual for more information on printers and paper sizes.

You can view the page in a drawing window using various zoom factors, which you can set using a popup menu in the drawing window tools palette.

Drawing tools

pro Fit provides various tools for editing drawings. These tools are collected in a “tool box”, which is either placed in the left margin of a drawing window or in a separate floating window.

To place the tools in a separate drawing window, choose “Drawing Tools” from the Windows menu. The floating tools palette appears. To move the tools back to the drawing window, simply close the floating window.

If you will never want to have drawing tools inside the drawing windows, you can disable this option: Choose “Preferences” from the Files menu and check “Always use floating toolbox” in the “Drawing” panel.

The upper part of the tools palette contains tools that are used to select, move or create simple objects, such as rectangles and text. Then there is a tool that can be used to pick up a color and apply it to another graphic object and a tool that lets you draw the individual data points such as those used in graphs. The rest of the tools palette contains popup menus for setting line styles and fill patterns, and for choosing the zooming factor of the current view in the drawing window. The drawing window can be viewed at zoom factors from 25% to 400%. To learn more about these tools, refer to the section “Drawing” later in this chapter.
Coordinates, accuracy and drawing info

proFit uses floating point numbers to store the size and position of the various drawing objects. This provides a positioning precision that is much more accurate than any output device (printer or monitor). This is important because all drawing objects can also be created by a user-program. If you write a program that produces graphical output, then you are likely to need a high precision coordinate system. proFit gives you just this. Any drawing that you generate from a program is produced at very high resolution and it will give optimal results when printed on any output device or when exported to other applications as a picture or a QuickDraw GX shape. The precise coordinates of any drawing objects can also be viewed after it has been created using the proFit Drawing Info window, which will be described later in this chapter.

Although all coordinates are precise floating point numbers, apparent accuracy will obviously suffer when drawing on a low resolution device, such as a normal monitor. In order to represent your drawing at a certain resolution, determined by the zoom popup menu, proFit must round the floating point coordinates describing a drawing object.

When you draw something at a low resolution, proFit must figure out reasonable floating point coordinates. It does this by “extrapolating” from the low resolution appearance in such a way that a high resolution view would give the same symmetry. For example, at the 100% view you can draw three overlapping lines with thicknesses of 0.25, 0.5 and 1.0 pts. All three lines have exactly the same appearance (e.g. they appear 1 pt thick). proFit sets up the floating point coordinates of the lines in such a way that the thinner lines are centered on the 1 pt thick line.

Thanks to this interpretation you get the same result, at 100% view, if you draw a 1 pt line and then make it 0.25 pt thick, or if you draw a 0.25 thick line directly. On the other hand, if you draw a 0.25 pt thick line at 400% view, go to 100% view, and draw another 0.25 pt thick line on top of it, the two lines will not overlap. This is because the first line was positioned with a much larger precision than the first line. Use the Align submenu in the Draw menu to make sure that such lines really overlap, or look at their coordinates using the Drawing Info window (see later).

Likewise, if you have two graphs or rectangles, set their size to be exactly equal, and overlap them at 100% view, one of their borders might be off by one pixel if their position is not exactly the same. This is because roundoff errors must occur when calculating their rounded coordinates at 100% view. If you set their position to be exactly equal (using the Align command or using the Drawing Info window), the roundoff errors are exactly the same for the two objects, and they do overlap exactly in the 100% view, too.

If you are concerned with precise positioning, e.g. when drawing overlapping lines or placing arrows on the axes of a graph, always go to a larger zoom factor (e.g. 400%) or have a look at the underlying floating point coordinates. You can do this using proFit’s Drawing Info window.

Choose “Coords” from the Windows menu to see this floating window.
Whenever a single drawing shape is selected, the Drawing Info window shows its floating point coordinates, i.e. its size and its position in coordinates that make sense for the particular shape which is currently selected.

The first row of the Drawing Info window gives the absolute coordinates on the paper, the second row gives the dimensions of the selected shape, and the third row gives the angle of its diagonal and its length. The last row shows the current coordinates of the mouse. The units used to display the coordinates can be chosen using the “Preferences...” command.

All the coordinate fields are editable. Simply click a coordinate and enter a different number to change the size or the position of the selected shape. For example, you can set the precise length and orientation of a line by entering the corresponding coordinates in the edit fields in the third row.

The Lens check box lets you open a small viewport with an enlarged version of the region around the mouse.

**Drawing objects**

A drawing contains different *objects*. There are four different classes of objects in a drawing window:

- Objects that are created by choosing Plot Function or Plot Data from the Draw menu, such as a graph and its associated legend.
- Objects that are created using the tools in the upper part of the tools palette, such as texts, lines and rectangles.
- Objects that were created in another application and that are imported as pictures to proFit by choosing Paste or Subscribe To in the Edit menu (or by dropping them in a drawing window).
- Publishers created by Create Publisher in the Edit menu. Everything within a Publisher’s rectangle is part of the picture that is made available to other applications.

The first class of this list (graphs and legends) is discussed in the section “Plotting”. The other classes (objects created by using the tools palette, imported pictures, Publishers and Subscribers) are discussed in the following section.

**Drawing**

This section describes the general drawing commands and the use of the tools palette.

**General drawing commands**

General drawing commands apply to all types of drawing objects. These commands are probably already known to you if you ever used any drawing application.

Here we shortly review them one by one.
To select an object in the drawing window:

1. **Choose the arrow tool in the tools palette by clicking the box containing the arrow symbol.**

2. **Click the object you want to select.**

   A selected object has four small black rectangles (selection handles) at the corners of its enclosing rectangle.

   To select multiple objects, you can either click on the desired objects while holding down the shift key, or you click into an empty part and drag the mouse to generate a dotted selection rectangle: every object enclosed by the rectangle will be selected. Click on an object while holding down the shift key to deselect it.

   To move an object:

   1. **Click the object and hold down the mouse button.**
   2. **Drag.**

      If you hold down the shift key while dragging, movement is constrained to horizontal or vertical directions. If you hold down the command key while dragging, movement is constrained to diagonal (45°) directions.

      In MacOS 7.5 and later, or if you have the Drag and Drop extension installed, you have a few more options available:
      - If you hold down the option key while dragging, the object is duplicated, i.e. a copy of the original is created at the destination instead of simply moving the original.
      - You can drag one object from one drawing window to another. If you do this, a copy of the object is created in the destination window.
      - You can drag objects to any other application (supporting drag and drop), or to the Finder’s desktop. In the latter case the Finder will produce a small picture clipping, which you will be able to use later on, either by dragging it back to a pro Fit window, or by using it in another application.
      - You can drag objects into the Trash to delete them.

   To change the size (resize) of an object:

   1. **Select the object.**
   2. **Click into one of the four black selection handles at its corners and drag.**

      While dragging, the new outline of the object is shown.

      If you hold down the shift key when resizing, the proportions of the object are maintained, or the height or width remains constant. If you hold down the option key when resizing, the horizontal and vertical dimensions of the object become equal. If the object is a group of different objects, hold down the command key to tell pro Fit to resize all of the objects of the group, regardless of their type (normally pro Fit would not automatically resize texts or data points).

   To rotate an object:

   1. **Select the object.**
   2. **Choose the desired rotation from the Rotate submenu in the Draw menu.**

      Objects can be rotated by angles multiple of 90°
To flip an object, i.e. to exchange its left and right sides or its top and bottom:

1. **Select the objects to be flipped.**

2. **Choose the desired operation from the Flip submenu in the Draw menu.**

   “Flip Horizontal” exchanges the left and right side of the objects. “Flip Vertical” turns it upside down.

Note that you can only flip lines and polygons. It is not possible to flip graphs, legends, imported pictures, or text. (Flip has no effect on rectangles and ovals).

To change the order in which several objects overlap:

1. **Select the appropriate objects.**

2. **Choose the desired operation from the Send submenu in the Draw menu.**

   You can move objects one position forward or backward (commands “Forward” and “Backward”) or you can bring them to the front or to the back of all other objects in the window (“To Front”, “To Back”).

To align objects:

1. **Select the objects to be aligned.**

2. **Choose the desired operation from the Align submenu.**

   Using this menu, you can align objects to each other, or distribute them regularly. If the objects are a group of text objects, then every object retains its alignment when you edit it.

To group objects:

1. **Select all objects to be grouped.**

2. **Choose Group from the Draw menu.**

Objects that can be double-clicked to change them (e.g. text objects, a graph, or its legend), can also be double-clicked and changed while they are part of a group. You don’t have to ungroup them. If the objects are text objects and you aligned them with the Align command before grouping them, their alignment will be maintained when they are edited.

Choose Ungroup from the Draw menu to ungroup a group.

> If you resize a group containing text objects or data point symbols, the proportions and size of the text and data points remain the same. If you want to resize them proportionally with the group, hold down the **command** key while resizing the group.

---

**Objects created with the tools palette**

The upper part of the tools palette contains the drawing tools needed to create some of the more simple drawing objects.

The lower part contains pop-up menus to select background patterns, line widths and dashing, and arrows. Their use is explained in the section “Editing drawing objects”.

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Drawing and Plotting 7-5
Text objects

Use the text tool to create text objects:

1. Select the text tool from the tools palette.
2. Click inside the drawing window.

The text dialog box appears:

Here you can enter your text and specify font, font size, text styles and the vertical position of each character. proFit uses the command key equivalents “H”, ”T”, and ”S” for the fonts Helvetica, Times, and Symbol, respectively.

The Superscript and Subscript buttons (keyboard equivalents and ) switch to superscript or subscript characters with smaller font size. The Normal button (keyboard equivalent: command key – space bar) restores the vertical position and the font size to their previous settings.

To set the vertical position of the selected characters, click and drag the baseline indicator (black triangle at the right side of the text box). To shift the vertical position, click the white triangles above and below the baseline indicator. Clicking the white triangle above (below) moves the selected text up (down) by three points. If you hold down the option key while clicking the triangle, the offset is only one point.

The size of the selected text can be set by changing the font size in the size field or to use the pop-up menu to its right. To increase or decrease the size of all selected text proportionally, click one of the triangles at the right of the size pop-up menu. Doing so increases or decreases the text size by
approximately 10 – 20%. To increase or decrease it by just one point, hold down the option key while clicking the triangles.

Each text object contains only a single line of text, for multiple lines you must create a text object for each new line.

*Hint:* To write a text having several lines in a drawing window, edit the text in a function window or in the results window. Then copy or drag and drop it into the drawing window – each line is converted to a text object. If your original text contains tabulators, pro Fit will use them as column delimiters to order the text in a table. Ungroup the resulting text group if you want to edit the position of the columns.

You can set the **justification** of a text object (right justified, left justified or centered) by using the align commands in the Draw menu (left, right, center horizontally). The default justification is centered.

If you have several lines of text objects (use distribute in the align menu to make equidistant lines), you can set the justification of these texts and then group them. They will preserve their justification when the group is resized or the texts are changed within the group by double-clicking them.

---

**Kerning and ligatures:** Typesetters often use a special technique called kerning to make text appear more regular. During kerning, letters with a lot of white space between them (such as a ‘o’ following a ‘T’), are moved closer to each other. Furthermore, some characters will be transferred into a single character when following each other (fl will e. g. be turned into fl):

![Trifle example](image)

Text without kerning and ligatures (left) and with (right)

When you have QuickDraw GX installed, you can use kerning when printing and exporting graphics: for this, you must check “Use QuickDraw GX” in the Drawing/General command of the Preferences submenu (and enable the export of QuickDraw GX shapes in the PICT Options panel of the Preferences submenu). For more details see Chapter 12, “Printing”.

**Rectangles and ellipses**

Rectangles and ellipses are created using the corresponding tools of the palette. Select the appropriate tool, click the desired position of one corner of the rectangle (or the enclosing rectangle for an ellipse) and then drag the mouse to the opposite corner.

**Lines and polygons**

Creating lines and polygons is easy as well. Select the appropriate tool, click the start of the line and drag to its end. For polygons, click at the positions corresponding to the corner points of the polygon (release the mouse when moving from one point to the next). Double click when finished.
By holding down the mouse button for a while when you select the polygon tool, you can change the tool to the one for closed polygons.

Hold down the shift key to constrain lines (or polygon sections) to horizontal, vertical, or diagonal directions.

When drawing a polygon, hold down the command key and double-click to create a corner that remains a corner even when the polygon is smoothed.

Lines and polygons can have arrows. To define at which ends of the line (polygon) arrows must be drawn and to select the type and size of the arrow(s), use the arrow pop-up menu in the tools palette.

To smooth polygons:

1. **Select the polygon you want to smooth.**

2. **Choose the appropriate smoothing method in the Smooth submenu in the Draw menu.**

   The two possibilities for smoothing can be seen in the figure below. You can either select a standard Bézier curve that does not touch the corners of the polygon, or you can select a smoothed curve that goes through all the corners of the polygon.

   ![Smooth options](image)

   An unsmoothed polygon and its two smoothed versions.

To reshape polygons:

1. **Select the polygon you want to reshape.**

2. **Make sure it is in reshape mode.**

   If the selection marks of a polygon appear at the corners of its enclosing rectangle, the polygon is not in reshape mode. If the selection marks appear at its corners it is in reshape mode:

   ![Reshape options](image)

3. **If the polygon is not in reshape mode, choose Reshape from the Draw menu, double-click it, or type the Enter key**

   This puts the polygon into reshape mode.

To move one of the corner points of a polygon, click and drag it. To remove one of the corner points, click it while holding down the option key. To add a corner point, click a line of the polygon while holding down the option key. Note that you can only add points to unsmoothed polygons.
Points

When plotting data, the data points are represented by special symbols. You can create such plot symbols manually anywhere in a drawing window. This is useful for creating your own legends or for exporting single point symbols to other applications (e.g. for figure captions).

Since the point symbols can assume a quite large size, they can also be used as parts of standard drawings. Data point symbols can be edited using a particular set of tools that let you achieve effects not easily achieved with other drawing objects (below you will find more details about editing data point symbols).

To create a point object:

1. **Choose the point tool from the tools palette.**
   
   Keep the mouse button down for a little while to select the symbol that you want to use. A pop-up menu with a choice of data points appears. Its top part contains a set of standard, predefined point symbols. The last line contains user-defined symbols, and the Other... field lets you define new point symbols.

2. **Click the desired position within the drawing.**

   A new point symbol drawing object is created.

   1. Choose the point tool from the tools palette.
   
   To change the plot symbol of a point object, select it and choose the desired symbol from the point style pop-up menu in the tools palette (or double-click it to go directly to the custom points dialog box).
   
   If the selected object is a graph or a legend, the new point style is applied to the data plots contained in the graph. See the section ‘Graphs and legends’, later in this chapter, for details.

   On the right you see a selection of the data point styles offered by pro Fit. Choose Other... from the point style menu to create your own data point symbols using the “Custom Points” dialog box:
pro Fit defines a data point symbol as a background shape and a foreground shape. With this dialog box, you can design both of them. pro Fit offers some predefined simple shapes, and lets you edit any closed polygon to define a new data point symbol. In the above example, both foreground and background shapes are defined using a closed polygon. You can use this dialog box simply to change the size of an existing point symbol, or to design more complicated point symbols.

Draw the foreground and background shapes in the preview area at the right of the dialog box. Use the popup menu above it to set the magnification of the preview. The center of the preview area defines the “hot spot” of the data point symbol. When plotting, the “hot spots” of data point symbols are positioned on the correct mathematical coordinate.

Draw a closed polygon by dragging the polygon handles (the little circles or squares at the edges of the polygon). To make your work easier, pro Fit lets you define a rotational symmetry and mirror symmetries. Choosing 5 from the Symmetry popup menu (like in the above example) tells pro Fit to draw the definition points at 5 positions 360/5 degree apart before connecting them with lines. Use the # Pts popup menu to set the number of definition points. Checking the H or V check boxes tells pro Fit to draw the definition points at the 2 positions obtained by mirroring them at a horizontal or vertical axis, respectively. You can achieve quite astonishing effects by combining these symmetry settings and using only one or two definition points.

Hold down the shift key while dragging a polygon handle to constrain the dragging along radial directions. Hold down the command key while dragging a polygon handle to resize and rotate the whole polygon in one single move.

Choose a Symmetry of “1” and no mirror symmetries to draw a polygon free-hand.
Note that if you do this you can draw a polygon that is not centered inside the preview area. This means that if you use such symbols for plotting, the symbols will not be centered on the mathematical coordinates of the data points.

Click the Copy to Menu... button to add the point symbol you just defined to the point symbols menu for later use.

The data point symbols you define are normally used when plotting (see the section “Plotting”, below, for more details on this). However, you might also want to use them to achieve some special effect in a drawing. For example, you can use a triangle or a rectangle to define a point, and you can rotate them by any amount. You can’t do this that easily using the standard drawing tools. You can also define closed polygons with any special symmetry. The data point symbols you define can then be used as drawing objects in the drawing window (their size can be quite big). You will be able to resize them as usual by dragging a selection handle, and you can always modify them by double clicking them.

**Editing drawing objects**

You can change many attributes of drawing objects, such as color, line thickness or background pattern. To do this, first select the desired object(s). Then change the attributes using the Fill, Pen, Dash, and Arrow popup menus.

A fill pattern and a fill color can be specified for all drawing objects, except simple lines. See Chapter 10, “Printing” for a list of limitations on patterns when printing with PostScript.

A line color can be specified for all drawing objects except imported pictures.

The two Pen popup menus are used to select a thickness and a line color. The dash pattern of a line is selected using the Dash popup menu. Choose Other... from this menu to design your own dash pattern and add it to the Dash menu.

The line thickness and dash pattern can be specified for all objects containing lines. If the selected object is a graph, the line styles of the axes, ticks, grid, and frame will be changed. The color also applies to the labels. (More complex options are available for the graph. See section ‘Graphs and legends’ in this chapter.)

If the selected object is a legend, you can change the appearance of the curves and data sets displayed in the legend and the corresponding graph. See the section ‘Graphs and legends’, later in this chapter, for details.
Arrows of various size and shape can be added to polygons and lines using the Arrows pop-up menu.

<table>
<thead>
<tr>
<th>Arrow</th>
<th>Style</th>
<th>Size</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>Other...</td>
<td></td>
<td></td>
</tr>
</tbody>
</table>

Arrows can be added to all lines and polygons, smoothed as well as unsmoothed.

Choose Other... from the Arrows menu to design your own arrows and add your personal arrow styles to the Arrow menu.

You can define a different arrow to be used for the start and the end of a line, use half-sided arrows, define various other types of line caps, etc.

Fill colors and line colors are set using the corresponding popup menus.

To copy the line color from one object to another

1. **Click the color measuring tool (.paint_brush.) in the tool palette.**
2. **Click the color you want to copy to pick it up.**
   The shape of the cursor changes and becomes a paint bucket.
3. **Click the drawing object to which you want to transfer the color.**
The line color of the clicked shape takes the color you picked with the color measuring tool.

To picked up a **fill color** for the target shape, instead of a line color, hold down the shift key while clicking with the color measuring tool.

proFit stores the color that was measured with the color measuring tool inside the standard color popup menu. This opens up an other, even more flexible possibility to copy colors.

1. **Click the color you want to copy with the color measuring tool.**

2. **Select an object and apply the measured color using the standard Fill- or Line-color popup menus.**

On black and white monitors proFit displays a simpler version of the color menus, with a more limited choice of color. To see the standard color menu which is displayed on color monitors, hold down the option key while clicking the popup menu symbol.

**Exporting pictures**

There are five ways to export proFit drawings:

- saving the whole drawing as a PICT file,
- using the Copy or Cut commands in the edit menu,
- dragging them and dropping them to their destination,
- choosing Create Publisher from the Edit menu,
- saving the whole drawing as an EPS file.

In the first four cases the drawing is converted to a picture (a data structure in the so called PICT-format) or a QuickDraw GX shape. A picture can be imported into most other Macintosh applications.

Use the **Preferences...** command, in the File menu to set various options that determine which kind of picture is created. The original definition of the QuickDraw PICT format defined only pictures with the resolution of the original Macintosh screen, i.e. 72 dots per inch. To print a picture on a printer with higher resolution, additional data must be included in the picture. There are several ways of doing this, and the choice of method depends on the printer you are using and the application you are working with. See Chapter 12, “Printing”, for more details on this subject.

**Saving a drawing as a PICT or EPS file**

To save a drawing as a picture to be exported to other programs choose **Save as** from the File menu and click the radio button **PICT** in the dialog box that appears. The current PICT Options will be used for creating the picture. PICT Options are discussed in Chapter 12, “Printing”.

To save a drawing as an **Encapsulated PostScript File**, choose **Save As** from the File menu and click the radio button **EPS file** in the Save As dialog box.

The size of EPS files created in this way is kept as small as possible. This small size is useful when you want to transmit your pictures over e-mail to a publisher. However, keeping a small size introduces some limitations on the number of text formatting options you can use. If a certain text-formatting option is not supported by the PostScript font you plan to use, like “Outline” or “Shadow”, or “Underline”, then these text formats are ignored when storing your document as an EPS file. Typographical formatting styles like Bold Face or Italic are nearly always available in all common PostScript fonts.
There is another point involved in keeping the size of EPS files small, and it is again connected to fonts. ProFit does include information on the fonts used in your document, but does not include the fonts themselves. So make sure that you use fonts that are available to the application to which the ProFit EPS files are imported.

An alternative way to generate an EPS file is to choose Print... from the File menu and select “File” as destination. If you do this, the created EPS file will be much larger, but it includes the whole definition of the fonts you use in your drawing.

A ProFit EPS file contains a PostScript representation of the drawing for printing, and a picture to display on screen (called the *template*). The format of the picture template that is included in EPS files can be selected using the PICT options panel of the Preferences dialog box (File menu). All PICT options can be used except the “embedded PostScript” option (which will automatically be replaced by “normal”). It is advisable to use the high resolution bitmaps only if the high resolution information is really needed. Otherwise use a normal picture or a low resolution bitmap because they require less memory.

PICT Options are discussed in Chapter 12, “Printing”.

A drawing saved as a PICT or EPS file cannot be opened by ProFit anymore.

To be able to modify it later, save a copy in the ProFit format!

**Exporting pictures over the clipboard**

To copy a part of a drawing in order to export it to another application, select the objects you want to copy and choose **Copy** or **Cut** from the Edit menu. Alternatively, you can drag the selected objects directly to their destination. The current PICT Options will be used to create the exported picture. PICT Options are discussed in Chapter 12, “Printing”.

**Exporting pictures using Publishers**

To make a portion of a drawing available to other applications or other users, you can also use the command **Create Publisher** in the Edit menu.

A Publisher creates a picture of a rectangular part of your drawing window, e.g. of a plot of some data. Creating a publisher will create an *Edition Container* – a file containing this picture. When you change something within the Publisher rectangle (e.g. you add some points to your plot), you can tell the Publisher to send this newer Edition of the picture to its Edition Container. In this way, the Edition Container always contains the latest version of the picture. By default, the new edition is always sent to the Edition Container when you save your file.

If you are defining a series of drawings to be included in some publication written by somebody else, it is useful to Publish the drawing using this feature, and load them into their destination using the Subscribe mechanism. Another application can import the picture in the Edition Container by selecting **Subscribe to** from the Edit menu. In this way you can be certain that the publication always contains the latest version of your graphs or drawings. Whenever the contents of the Edition Container are changed, the subscribing application will be informed of the changes and will load the newest version.

To create a Publisher:
1. Select the objects you want to publish.

2. Choose Create Publisher from the Edit menu.

   The following dialog box appears:

   ![Dialog box for creating a publisher]

   Click the button **PICT Options** to choose the PICT options for the publisher you are about to create. (By default the current PICT Options are used.) Find more information about PICT Options in Chapter 12, “Printing”.

3. Select the appropriate name and location for the Edition Container and click Publish to create it.

   In the drawing window a Publisher is enclosed by a gray rectangle. This rectangle can be moved and reshaped like other drawing objects. The publisher contains everything inside its rectangle.

   Double-click the publisher rectangle to see the Publishers Options dialog box (or choose **Publisher Options** from the Edit menu). Apart form the standard items, this dialog box also contains a **PICT Options** button in the bottom left corner. Use it to change the picture format used by the publisher.

**Importing pictures**

Every picture in the standard PICT format can be imported into a drawing window. (Note that you cannot paste QuickDraw GX shapes into proFit 5.0.)

There are two ways of importing pictures: over the clipboard (by choosing **Paste** in the Edit menu) or via an Edition Container (by choosing **Subscribe to** in the Edit menu).

**Importing pictures over the clipboard or using Drag&Drop**

When you create a picture in any application you can transfer it via the clipboard by copying and pasting it or by directly dragging and dropping it into a proFit drawing window.

Note that proFit imports pictures ‘as a whole’ and does not take them apart. If you use a drawing application to create a line and a rectangle and paste these objects together into proFit, they are interpreted as one picture, not as a line and a rectangle.
An imported picture can be resized or rotated, but it cannot be edited in any other way. Rotating and resizing may not work with imported pictures if they contain any non-standard information, such as PostScript commands.

**Importing pictures by subscribing**

Another method to import pictures is to subscribe to an Edition Container by choosing Subscribe To... from the Edit menu.

To open the application that created the Edition container, Click Open Publisher in the Subscriber Options dialog box (Choose Subscriber Options... form the Edit menu to see this box), or double click the Subscriber while holding down the option key.

If you have resized a Subscriber (or rotated it), Go to the Subscriber Options dialog box and check **Original size and orientation** to go back to the original subscriber.

**Plotting**

pro Fit generates graphical representations of functions and data sets inside drawing objects called **graphs**. The coordinates of the data points are stored in the graph with double precision, and can always be recovered from it.

A graph can have various components (read more about this later in this section). The most important of these are its coordinate axes. A graph can have multiple x- and y- coordinate axes, which can have different ranges and scalings.

A graph always maintains two special coordinate axes, which can never be deleted. This are the **main coordinate axes**, and are called **X1** and **Y1**. The other axes are called **X2**, **X3**, **Y2**, **Y3**, and so on.

The axes can have **linear**-scaling, **logarithmic**-scaling, **1/x-scaling**, or **probability**-scaling.

The **linear** scaling type is the standard scaling type. It indicates that there is a linear relationship between the coordinates of the graph and your paper.

A **logarithmic** scaling indicates that there is a logarithmic relationship between the coordinates of the graph and your paper – it expands the lower end of an axis and compresses its upper end. The min and max values for logarithmic axes must both be positive.

The **1/x** scaling type can be used to plot a function whose y-value is expected to be proportional to 1/x. If you plot such a function on a “1/x” scaled x-axis, the function is a straight line. The min and max values for 1/x-axes must both have the same sign.
The probability scaling type can be used for plotting normally distributed data – or, to be more accurate – their integral. If you have a sample of sand, and you determined the percentage of grains having a diameter smaller than \( x \), plot this percentage as a function of \( x \) using probability-scaling for the y-axis. If the size of the grains is normally distributed, your data points will lie on a straight line.

With proFit, you can plot on any one of the coordinate axes contained in a graph, you can add new coordinate axes, and you can change their characteristics.

The next section discusses the general options that are always available when plotting. Then we discuss the procedures for plotting functions and data sets, and finally we describe how to edit and use existing graphs.

**General plotting options**

Whenever you plot a function or a data set, you can choose if you want to plot it into an existing graph, or if you want to create a new one. You can also choose if you want to plot into an existing drawing window or to open a new one. And finally you can choose which coordinates axes you want to use for plotting, their ranges, and their scaling.

To plot a function or a data set, choose Plot Function... or Plot Data... from the Draw menu. The options outlined above are common to function and data plotting and can be set in both the plot function dialog box and the plot data dialog box. Therefore, the upper part of both dialog boxes looks the same:

Check **Plot into current graph** to plot into the current graph. The current graph is usually the one where the last plotting took place. However, you can define any graph to be the current graph by double-clicking it and checking **Current Graph** in the dialog box that appears (Read more about this dialog box later in this chapter.). As a shortcut, you can hold down the command key and double-click the graph.

Check **Open new window** to create a new graph in a new drawing window

If both “Draw into current graph” and “Open new window” are unchecked, a new graph is drawn in the frontmost drawing window.

The fields labeled **X-axis** and **Y-axis** determine which axes will be used, their ranges, and their scaling.

The two popup menus in the top left corner of the fields “X-axis” and “Y-axis” are used to choose the axis to be used for plotting, and to determine its range. The second popup menu determines the **scaling type** of the axis.
Check **Auto range** to let proFit automatically calculate the ranges of the axes, starting from the y-values returned by your function, or from the range of the selected data. If you plot into an existing graph, the ranges of the axes you use for the plot will be extended, if necessary.

**from, to** are the ranges of the axes.

**Plotting a function**

To plot a function:

1. **Choose the function you want to plot from the Func menu.**
2. **Set its parameters in the parameters window.**
3. **Choose Plot Function... from the Draw menu.**

The Plot Function dialog box appears:

![Plot Function Dialog Box](image1)

The top part of this dialog box has already been discussed above. Here we go on to explain the rest of its contents.

The function can be plotted over the whole given range. Alternatively, you can specify start point and end point manually using the **From .. To** edit items at the bottom left of the dialog box.

![Graph Examples](image2)

A graph with its curve from min to max (left) and a graph created using the **From.. To** option.

If **Use fitted parameters** is checked, the function is plotted using the parameter values calculated in the last fit. If Use fitted parameters is not checked, the parameter values in the parameters window are used.
If you are using linear x-axis scaling, the entry in the field **Step** determines the distance (step width) between consecutive calculated x-values. If you are using any other x-axis scaling, the field has the name **#Steps** and determines the number of x-values that will be calculated to plot the function.

The default value for step is “auto”. This invokes a specially designed plotting algorithm that automatically selects the x-values at which the function is calculated. If the curve representing the function is strongly bent in a given interval, then the number of points that are required for drawing the function is large. On the other hand, if the function is a straight line, the number of points needed is smaller. The following figure illustrates this.

![function and calculated points](image)

Note that the number of calculated points is optimized for the range a function is plotted in. If you change the axes range of a graph later (e.g., for “zooming” into a detail), the number of calculated points may not be sufficient anymore for representing the curve accurately. In this case you should redraw the function to create an optimized plot for the new range.

Note that plotting with the “auto”-option results in the smallest number of data points stored to represent a function’s curve. In this way you can create a plot that uses a minimum amount of memory and that is redrawn at maximum speed. However, to create such a curve, the function has to be calculated at a much larger number of points. If you are working with a slow function, you may prefer to use a fixed step to obtain faster plotting, and to go over to auto step only when you want to produce a final graph.

### Plotting a data set

To plot data:

1. **Open a data window with the data you want to plot.**
2. **Choose Plot Data... from the Draw menu.**

The following dialog box appears:
The upper part of this dialog box was discussed above.

Special attention must be paid to the Auto range check boxes, because they also influence which parts of the complete data set are transferred to the graph.

If you do not use **Auto range** but define your own ranges in min and max, all data points outside these ranges are ignored – only data points within the ranges of the graph are plotted and stored together with the graph. If you always want the complete data set to be stored with the graph, check Auto range and resize your graph after plotting.

Use the **Data window** pop-up menu to select the data window that contains the data to be plotted.

Use the **X-column** pop-up menu to select the column that contains the $x$-values of your data. You can only select one $x$-column at a time. Use the **Y-columns** list to select the columns that contain the $y$-values of your data. You can select multiple columns by holding down the shift key while clicking.

To plot only part of the data in the $x$- and $y$-columns, check **Selected rows only**. In this case only the data in the currently selected rows will be used for plotting. To use this feature, first select the rows you want to plot in the data window or with the help of the Preview window and then choose Plot Data... from the Draw menu.

Use the **Point style** pop-up menu to select a plot symbol. If you are plotting multiple data sets, only the first set will be drawn with this symbol. The symbols of subsequent sets are chosen according to the current **graph style**. See section “Styles”, later in this chapter for further information about graph styles.

Check **Connected** if you want to draw connecting lines between your data points. The data points will be connected according to the order in which they appear in the data window – not in ascending order of $x$-values. If necessary, use the command Sort in the Calc menu to sort your data before plotting.
Graphs and legends

When you plot data or functions, you create a graph object and a legend object.

Graphs and legends are the most important drawing objects.

Editing legends

A legend contains a description for each curve or data set of its graph. The description consists of a symbol identifying the plot and a text. You can change the line and point style of a plot as well as the text by double-clicking the respective items in the legend.

- Double-click the text of a legend to change a name of a plot.
- Double-click the plot symbol to choose the color, plot symbol and line styles for a plot.

Find more information on this topic later in this chapter.

To change the space allocated for the plot symbols or the distance between lines in the legend, simply resize the legend by dragging its selection points.

A graph is logically linked to its legend and vice versa. If you change the appearance of a plot, the change is reflected in both the graph and its legend.

To maintain this relationship, pro Fit does not let you duplicate a legend. However, you can select a legend and choose Ungroup from the draw menu. This transforms the legend into a set of simple drawing shapes, which then can be copied.

If you do not need the legend, delete it. You can always create a new legend for a graph by double-clicking the graph and checking “Draw legend” in the dialog box that appears.

Note that you can change the text style, font, and font size of a legend by selecting it and choosing an appropriate setting from the Style, Font, and Size submenu in the Misc menu.

You also can change the line styles and color of curves and lines in a legend by choosing the appropriate setting from the “Pen” and “Dash” pop-up menus in the drawing tools palette:

- To change the line style of the first item in a legend that is drawn using a line (either connected data points or a function curve), select the legend and choose the line style in the “Pen” and/or “Dash” pop-up menus.
- To change the line style of all items in a legend, select the legend and choose the line style in the “Pen” and/or “Dash” pop-up menus while holding down the shift key.
• To add a connecting line to the first data point in a legend, select the legend and choose a line style from the “Pen” or “Dash” menu while holding down the option key.
• To add a connecting line to all data points in a legend, select the legend and choose a line style the “Pen” or “Dash” menu while holding down the shift key.

By default a legend lists every plot of the related graph. You can, however, hide one or more plots from a legend by unchecking “Appears in legend” in the dialog box for editing curve styles. This is explained later in this chapter.

A legend can be ungrouped by selecting the legend and choosing Ungroup from the Draw menu. When an legend is ungrouped, it is transformed into a set of lines, data points and texts.

**Editing graphs**

The nearly unlimited possibilities for changing and editing a graph are one of proFit’s key features. A whole set of specialized options lets you create the graph you need. These options are accessed either by double-clicking the graph or its legend, or by using the Graph submenu in the Draw menu. (This submenu is only available if a single graph is selected or if a drawing window contains only one graph.)

When you double-click a graph or choose “General...” from the Graph submenu, the following dialog box appears:

![Graph Settings dialog box](image-url)
The icons in the list to the left of this dialog box correspond to the items in the **Graph** submenu. Click the icons to access and edit the various parts of a graph. Click the **Apply** button to see the effects of your changes.

Check **Current graph** to make this graph the currently active graph. This is the graph where plotting takes place per default.

The three **Draw** check boxes indicate if **legend**, **frame** and **grid** should be drawn or not. If you uncheck the box named legend, the legend is deleted. If you check it again the legend reappears to the right of the graph.

The **Drawing Sequence** popup menu defines the order in which the various parts of a graph (curves, axes, grid) are drawn. This is especially important if you use color to highlight your curves or if you use very large data points. A grid in front of a curve can then look quite different from a grid behind a curve.

The **Graph width** and **Graph height** edit fields let you enter precise dimensions for the graph. You can also do this by selecting the graph in the drawing window and editing its size using the Drawing Info window.

The button **Styles** lets you save and load the current settings of a graph. A more detailed description of graph styles is given at the end of this chapter.

In the following sections we discuss the various parts of a graph and how to edit them.

**Axes**

When you want to edit an axis, double click it. Alternatively, you can choose Axes... from the Graph submenu in the Menu Draw, or you can reach the axis editing panel using the list of icons in the Graph Settings dialog box.

The axis editing panel for x-axes looks like this:
Use the popup menu in the top left corner to navigate between the various axes, to create a new axis, or to delete the current axis. (The X1 and the Y1 axes are the main axes and cannot be deleted.).

The edit field in the top right corner gives the position of the selected axes in the main axes coordinate system. Use this field to change the position of a horizontal (or vertical) axis with respect to the vertical (horizontal) main axis coordinates. The position is set by default to the minimum and maximum bounds of a plot when it is first created.

If the dialog box does not show the main axis (X1 and Y1 are the main axes) an additional check box is present. It is called Same as X1 (or Same as Y1).

If Same as X1 is checked, most settings of the selected axis (such as the range, scaling, color, line thickness, tick positions) are taken from the main X1 axis.
If you want to use two different axes for the top and for the bottom of your plot, you have to uncheck this box before making any changes.

The radio buttons **General**, **Labels**, and **Lines** let you switch between different sub-panels that are used to edit the general appearance of an axis, the appearance of its labels, and the kind of lines that are used to draw the axis and its tick marks.

If you check General, you can set the following options:

![Graphical representation of the General, Labels, and Lines options]

The **Draw** check boxes determine which parts of an axis are drawn.

The **First**, **Last** fields and the popup menu to their right are used to edit the range of the axis and its scaling type. See the beginning of this section for a discussion of scaling types. Note that First can be larger than Last if you want to reverse the axis.

The **Ticks** field to the right of the Draw check boxes is used to edit the tick marks. Enter the first major tick, the distance between major ticks, and the number of minor ticks between two consecutive major ones.

The edit field **1st major** gives the coordinate of the first major tick on the axis.

For a linear axis the **Distance** field defines the distance between the major ticks. For a logarithmic axis this field changes its name to **Decades** and defines the number of decades between major ticks. For a 1/x-scaling the edit fields work in the same way as for linear scaling. For probability scaling, you can edit the list of tick marks directly using the **Custom** check box.

For a linear axis the **# minor** field gives the number of minor ticks that are drawn between two major ones. For a logarithmic axis this field is replaced by a check box called **small ticks**, which must be checked to draw the minor ticks. If major ticks are drawn for each decade, the minor ticks are drawn for each multiple of ten. If there is more than one decade between major ticks, the minor ticks are drawn at all the powers of ten between the positions of the major ticks.
Instead of automatically calculating the positions of individual ticks, you can set them manually. Check the custom check box. This changes the contents of the ticks field.

A list appears that contains all the ticks of the axis. To add a tick, click a free space in the list (there is always a free space at the bottom of the list) and enter the desired coordinate.

To remove a tick, select it in the list and press the delete key. To change the position of a tick, click it and enter a new value. Check major to create a major tick. Major ticks are written in bold face in the ticks list. Click the Standard button to automatically re-calculate the tick positions according to the present axis settings.

To set the label of a tick mark to some general text instead of a number, double-click the label in the drawing window. The text edit dialog box appears and you can then enter any kind of text you want.

Click Labels in the axis dialog box to edit the format of the labels. The inner part of the dialog box now looks like this:

Use the Format field to set the format of the numbers. Use Decimal to suppress exponential representation, Auto exponent to have all labels in exponential format with varying exponent, Fixed exponent to have all labels in exponential format with a common exponent. The Digits field defines the number of digits to be shown after the decimal point.

Use the Font field to specify the text font, size, and style to be used for the labels of the current axis.

The Location popup menu defines where the labels of an axis are drawn. The edit field to its right defines the distance between the labels and the axis or the frame of the graph. The value in this field is in points (= 1/72 inch or 0.35 mm). Note that it can also be negative.

Click Lines to change the appearance of the lines used for drawing the axis and its tick marks, and to set the position where the tick marks are drawn. The inner part of the dialog box now looks like this:
Use the **Ticks location** popup menu to set the position of the tick marks. In the **Major ticks** and **Minor ticks** fields you can set the line style, length and color of major and minor tick marks. The line style used to draw the axis can be edited using the “Axis line style” popup menus. All the options outlined above for editing axes let you create many different kinds of graphs. Note that you can create new axes and change their scaling, tick marks, etc., also if you don’t use them to plot any curve.

For example, you can uncheck the “Same as X1” check box in the X2 axis panel and edit it to reflect a completely different scaling, labels style, and range than the X1-axis.

A typical application for this is a graph that displays its x-values on its horizontal bottom axis and the reciprocal x-values on its top axis.

As an example, imagine that you have a set of data that was measured for different light wavelengths between 400 and 1000 nm. You would like to plot your data as a function of wavelength, but you would also like to have a reading for the light energy in eV on the top axis. The energy of the light is inversely proportional to the wavelength, so you have to use 1/x scaling for the top axis.

To create such a graph:

1. **Create a graph with an x-axis from 400 to 1000.**
   
   Simply plot your data between these limits. Choose **Plot Data...** from the Draw menu. Make sure that you create a new graph by unchecking ‘Plot into current graph’ in the dialog box that comes up.

2. **Double-click the upper x-axis (“X2”-axis).**

   The axis dialog box (see above) for the top axis appears.

3. **Uncheck “Same as X1”.**

   Do this to make sure you only change the top x-axis, leaving the bottom x-axis alone.

4. **Change the axis scaling to “1/x”.**

   Be sure that the “General” radio button is selected and use the scaling popup menu, found to the right of the edit fields for the axes ranges.

5. **Enter 1.2398 for First and 3.0996 for Last.**
A wavelength of 400 nm corresponds to an energy of 3.0996 eV, while a wavelength of 1000 nm corresponds to an energy of 1.2398 eV.

6. **Edit the tick marks**

Do this by changing the values in the Ticks field. Note how the density of ticks tends to increase for larger values. Go over to custom ticks and edit the ticks list directly if necessary.

The end result could be something like this:

![Graph](image)

Note that the top axis, which has 1/x scaling, has the smallest value to its right and the largest value to its left.

Click **Prefix** in the axis dialog box to set pre- and postfix for the labels, to multiply them with a given factor or to offset them by a given value:

![Prefix and Postfix Dialog](image)

Click **Prefix** or **Postfix** to prepend or append a string to each label.

The value in field **Factor** is multiplied with the value of each label before its string is generated. You may e.g. enter 100 here to display values between 0 and 1 in percent.

The value in the field **Offset** is added before the string of the label is generated.
Curves and data points

You can change the appearance of curves and data points in a graph in many ways. Choose Curves from the Graph submenu (Draw menu) or click the Curves icon in the Graph Settings box. You can also double click a plot symbol in the legend.

The Graph Settings dialog box now displays the curves editing panel.

Here you can select and change or delete all curves and data sets of a graph.

To change the drawing order of the plots, select a plot (by clicking it in the list) and click Forward, To Front, Backward or To Back to move it one position backward or forward or to move it to the back or front of all plots. The first plot symbol at the top of the list is drawn first, so back means top of the list, and front means bottom of the list.

Change the drawing order if you have white data points behind a curve and you do not want the curve to go through the points.

To change the text describing a curve or a data set, click Edit Text.... Instead of doing this you can also double-click the text.

The pop-up menus titled Line style let you edit the line that draws a curve or connects the data points.

The pop-up menu Points lets you select the symbol for data points. Check connected to draw lines between successive data points. The menu Thickness defines the line thickness used to draw the data point symbols. It can be set to auto, in which case the line thickness will be chosen depending on the size of the data points.
You can also fill the region between a curve and one of the axes with a color of your choice. To do this, check **Fill** and select the axis towards which the curve must be filled and the fill color using the two popup menus to its right.

The **Coordinate Axes** popup menu defines the coordinate axes used by the selected curve or data set. With this pop-up menu you can change the reference axis of any given curve.

Doing this for function curves which were drawn with **auto step** is not recommended. If the scaling of the original axis and the one of the destination axis differ considerably, the results can be disappointing. Remember that a function curve is only defined by a set of points. *ProFit* calculated these points in an optimized way when it plotted the function *for the axis scaling and range on which the function was plotted*. If you then change scaling or range, your curve may loose its smoothness. In such a case it is better to redraw the function curve on the new axis.

Check **Appears in legend** to make the curve or data set appear as an entry in the legend. Uncheck this check box to hide the corresponding entry in the legend. When an entry is visible in the legend, you will usually change its style by double-clicking it. When an entry is not visible in the legend, you must choose Curves... from the Graph submenu to access and change the style of the corresponding curve or data points.

Click **Tabulate** to recover the original data points that were used to draw the plot. In this way you can retrieve data points from a drawing when you have lost the original data set, or you can obtain a list of the data points that *proFit* calculated to draw a particular function.

Click **Delete** to delete the curve or data points from the graph. You can use the delete (backspace) key as a keyboard equivalent for this button.

Click the **Error Bars...** button to define error bars for the selected data set (this button is dimmed for a function).
Here you can specify if you want to use error bars for your data points and if you do, what they should be.

You can use symmetric or asymmetric errors. To use asymmetric errors, check **Use asymmetric errors** for horizontal and/or vertical direction, otherwise leave this option unchecked. If you check the option, you can select the errors on the top/bottom (or left/right) of the data points individually.

Using the menus titled **Type** or **Top, Bottom, Right, Left**, you can select the type of errors to add:

- Choose **Individual** if each point should have its own, unique, non-percent error. In this case, you must have stored the error values in a data window. Choose this window from the **Window** pop-up menu. Choose the column that holds your error values from the pop-up menu **Column**. The numbers found in the chosen column are assigned to each point in the plot sequentially. If you don’t check **skip empty data fields**, an error of zero is used for each empty data cell. Otherwise, pro Fit only uses data cells that contain a valid number. Make sure that the column you select contains the correct number of error values and in the right order (i.e. the same order as the data which was plotted originally). In general, you can add error bars months after you plotted the original data set, and pro Fit does not know the origin of the data set anymore. It will simply take the error column you specify and apply the data values sequentially to all data points. Therefore, the order in your error column must be the same as the order of the original data points when they were plotted.
- Choose **Constant** if each data point has the same error. Enter the error value in the edit field that appears.
- Choose **Percent** if the errors are a percentage of the x- or y-values of the data points. Enter the error value (in percent) in the edit field that appears.
- Choose **None** to remove the errors from your data set.
• Choose **Unchanged** if you don’t want to change the error bars in a given direction.

**Frame**

A frame is a rectangular box around your graph:

![An unframed and a framed graph.](image)

To change the appearance of a frame, either double click a graph and click the **Frame** icon, or choose **Frame** from the submenu Graph in the Draw menu.

In the dialog box that appears you can edit the **Line style** of the frame, and determine if tick marks must be drawn on it. The tick positions of the main coordinate axes (X1 and Y1) are used. If you draw a frame with ticks, you usually do not wish to draw the axes ticks as well: Uncheck the corresponding check boxes in the axis dialog box.

**Grid**

Grid lines are horizontal and vertical lines at the positions of the ticks.

![A graph without and with grid lines.](image)

To add grid lines to your graph, double click a graph and check **Draw grid**. This will add horizontal and vertical grid lines. To customize the grid lines click the **Grid** icon in the same dialog box or choose **Grid** from the Graph submenu:

In the Grid editing panel that appears you can define where you want to have horizontal and/or vertical grid lines, and if you want to see them at minor ticks, major ticks, or both. You can also choose which axes must be used as a reference to draw the grid lines. The grid lines are drawn at the tick marks of their reference axis. By default, the ticks of the main axes (X1 and Y1) are used.

**Graph Styles**

The appearance of a graph is defined by many parameters, such as its size, the ranges of its axes, the number of minor ticks, the symbols used for plotting, etc. These settings are called the **style** of a graph. You can save the style of a graph to use it (or parts of it) later for another graph. Styles are saved in the preferences file.
By using styles, you can create graphs with equal formats, e.g. graphs having the same size, the same length of the ticks, the same fonts, etc.

To save the style of a graph you can either double-click the graph and click the button Style in the dialog box that comes up, or you can choose Styles... from the Graph submenu (in the Draw menu) after having selected your graph:

This box shows a list of the styles that are already saved in the current preferences file. You can delete one of these styles by selecting it and clicking Delete. To save a new style, enter its name and click Save. To load a style, select its name in the scrolling list and click Load. The name of the button changes from Save to Load when you move from the Style name edit field to the Saved styles scrolling list.

If you click the Default check box when saving a style, or if you define a style with the name “Normal”, this style becomes proFit’s default style. The next time you start up proFit, the first graph you create will use this style.

When you load a style, a dialog box appears, asking you to choose which parts of the style you want to apply to your graph:
The characteristics of a style are:

- **Bounds**: The ranges of the graph, i.e. the minimum and maximum of all the axes; the positions of the first ticks; the distance between major ticks; the number of minor ticks.
- **Axes and grid styles**: The line thickness, dash and color of the axes, the frame and the grid; the distance of the labels from the axes; the location of the ticks (inside or outside).
- **Curve styles**: The line style of all plots, i.e. curves and data points.
- **Text styles**: The font, size, and text style of the labels.
- **Label styles**: The number format of the labels. The number of digits after the decimal point and the representation (exponential, auto, decimal) of the labels.
- **Tick styles**: The number of minor ticks, the axes scaling (logarithmic or linear) and whether the labels are visible.
- **Graph size**: The horizontal and vertical size of the graph (length of the coordinate axes).

**Graph coordinates and zooming**

Normally you can look at coordinates and analyze data sets and function using the Preview window. However, options similar to the ones available in the preview window, although more limited, can be used when editing graphs.

Hold down the command and option key simultaneously and click and drag over a graph object (the graph must not be part of a group). proFit displays the mouse location in the main axes coordinate system. The coordinates are displayed to the right of the cursor and in the bottom left corner of the drawing window.

If you now press the shift key, you can select a part of the graph. The ranges of the graph will be changed to display only this part. This is useful for zooming in on some part of the plotted data set.

![Graph coordinates and zooming](image)
8 Fitting

This chapter describes what proFit does when you perform a fit.

‘Fitting the parameters of a function to a data set’ roughly means finding those parameters that make the function’s curve follow the data points as closely as possible.

There are various possible definitions of the term ‘as closely as possible’. The correct definition is often determined by the origin and characteristics of the data set to be fitted. For example, a data set might be subject to large errors in the x-coordinate and to smaller errors in the y-coordinates. The probability of incurring in a given measurement error can decrease in some known way when the magnitude of the error increases.

There are also various possible methods of looking for the best parameter set.

proFit provides a choice of different ways for “measuring the distance” of the data points from the function, as well as a choice of different methods to reach the best parameter sets.

The first part of this chapter deals with the definition and mathematical description of deviation functions and fitting algorithms, the second part shows you how to select these options in proFit and how to run a successful fit.

Mathematical background

In order to find the best parameter set describing a given measurement, it is necessary to establish a quantitative method to “measure the distance” between a data set and the function that should describe it.

This requires the introduction of weights for the data points and of probability distribution functions. They are described in the next sections.

Distribution functions and data weights

Consider a function \( f(a_1, a_n, x) \equiv f(x) \) (we won’t write explicitly the function parameters every time) and a measured data set \( \{(x_i, y_i), (x_j, y_j), \ldots, (x_N, y_N)\} \).

Let’s assume that the function, with its “true” parameter set, correctly describes the quantity that was measured. We further assume that, when the data point \((x_i, y_i)\) was determined, the “true” system (the one described by the function \(f(x)\)) was at the coordinates \((\hat{x}_i, f(\hat{x}_i))\). When the x-coordinate was determined, an inevitable experimental error occurred, and \(x_i\) was measured instead of \(\hat{x}_i\). When the y-coordinate was determined, another inevitable experimental error occurred, and the measurement gave \(y_i\) instead of \(f(\hat{x}_i)\).

In real life the true parameter set is not known. One has to measure it by measuring many data points at different coordinates and fit \(f(x)\) to the complete data set. This is the way we usually find a parameter set which best describes the measurement. The parameter set obtained in this way is not the true (unknown) parameter set, but it should be a good approximation for it. (See the section on Error Analysis to find out how to estimate the errors of the fitted parameters.)
The fitted parameter set corresponds to a function \( f(x) \) which maximizes the probability that the measured data set came from the system described by \( f(x) \). To maximize this probability, we have to minimize the deviations between the measured data points and the function curve. This deviation can be defined in different ways, depending on the way in which the experimental errors are distributed, but it is usually a function of the weighted distances

\[
d_{xi} = \frac{\hat{x}_i - x_i}{\sigma_{xi}} \quad \text{(1a)}
\]

\[
d_{yi} = \frac{f(\hat{x}_i) - y_i}{\sigma_{yi}} \quad \text{(1b)}
\]

\( \sigma_{xi} \) and \( \sigma_{yi} \) give the magnitude of the errors expected when measuring the \( x_i \) and \( y_i \), respectively. The role of these x- and y- errors is to define the correct scaling of the x- and y- deviations between a measured data point and the function that should describe it. The errors normalize the deviations, introducing dimension-less numbers \( d_{xi} \) and \( d_{yi} \). Data points are weighted differently (given more or less importance) depending on their errors. A small error will magnify the importance of a given difference, a large error will make the normalized difference less important.

The distances \( d_{xi} \) and \( d_{yi} \) give the difference between measured coordinates and “true” coordinates. Obviously, we don’t know the true coordinates, otherwise there wouldn’t be any need for a fitting program in the first place. But we can estimate the true coordinates by minimizing some function of the distances \( d_{xi} \) and \( d_{yi} \). This function describes the “difference” between the model function and the set of data points, and it is chosen in such a way that its minimization corresponds to the situation with the highest probability of producing the measured data set.

If the x- and y-errors are independent, a fitting algorithm must generally minimize a mean deviation \( \chi_R \) of the type

\[
\chi_R = \sum_i \left[ R_x(d_{xi}) + R_y(d_{yi}) \right], \quad \text{(2)}
\]

where the functions \( R_{x,y} \) are deviation functions that tell us in a quantitative way how bad it is that a certain (normalized) distance \( d \) is found for a data point. They are normally related to the error probability distribution. This is the function that gives the probability that a certain measurement error occurs. For example, \( R_{x,y} \) can be the negative logarithm of the corresponding probability distribution for the distances \( d_{xi} \) and \( d_{yi} \).

Minimization of \( \chi_R \) as defined in Eq. (2) adjusts the function \( f(x) \) in order to maximize the probability that the measured data set corresponds to an underlying “reality” described by the adjusted \( f(x) \).

This is true as long as the following assumption is fulfilled: the measurement errors for each data point must be uncorrelated and described by probability distributions centered around the “true” values \((\hat{x}_i, f(\hat{x}_i))\).

The above assumption might appear harmless, but it is in fact more stringent than one would causally expect. For example, in most cases one tends to assume that the probability distribution is Gaussian, but the actual probability distribution for the measurement errors might be different, with a sizable probability of finding larger errors from time to time, i.e. points that are clearly outside the expected trend (“outliers”).

To allow for an analysis of such cases, proFit provides a set of deviation functions \( R \) which correspond to various error probability distributions.
The most common deviation function provided by proFit is the **squared deviation**

\[ R(d) = d^2. \]  

(3)

When using this deviation function, Eq. (2) becomes the **mean square deviation** between data points and function. Eq. (2) then corresponds to the negative logarithm of the probability of obtaining the data set in the presence of **normally distributed** measurement errors. The deviation function (3) corresponds to a **Gaussian** error distribution. In this case the probability density that a certain error occurs when measuring \( x_i \) or \( y_i \) is given by a Gaussian distribution (or normal distribution).

The next deviation function provided by proFit is

\[ R(d) = |d|, \]  

(4)

and corresponds to a two-sided **exponential** error distribution \( \exp(-|d|) \). It leads to the calculation of a **mean absolute deviation** instead of a mean square deviation.

The deviation function

\[ R(d) = \log(1 + \frac{1}{2}d^2), \]  

(5)

corresponds to a **Lorentzian** error distribution \( 1/(1 + d^2 / 2) \).

The last deviation functions available in proFit are

\[ R(d) = \begin{cases} 
    c[1 - \cos(d/c)] & |d| < c\pi \\
    c & |d| > c\pi
\end{cases} \]  

(6)

with \( c=2.1 \) and

\[ R(d) = \begin{cases} 
    \frac{c}{6} \left[ 1 - \left( \frac{d}{c} \right)^2 \right] & |d| < c \\
    \frac{c}{6} & |d| > c
\end{cases} \]  

(7)

with \( c = 6 \). These deviation functions are called **Andrew’s sine** (the derivative of (6) is \( \sin(z/c) \)) and **Tuckey’s biweight**, respectively. They don’t correspond to a particular probability distribution for the errors. They are designed to decrease the weighting of data points with very big errors (outliers) in order to allow a “robust” fitting through the more “reasonable” data points. It should be obvious that this procedure should only be used if you know your experiment and data set well enough, and we repeat the usual calls for caution!

Note that using the deviation functions (6) and (7) with another constant \( c \) is equivalent to changing all errors of the data points and the resulting mean deviation value by a constant factor.

Each term in the sum (2) describes a deviation between the measured data point \((x_i, y_i)\) and the “nearest” point on the function curve \((\hat{x}_i, f(\hat{x}_i))\). The coordinate \( \hat{x}_i \) must be chosen in such a way that each term in the sum (7) is minimized for each data point.
When the deviation function $R$ is the squared deviation $R(d)=d^2$, then each term in (2) gives the square of the Euclidean distance between $(x_i, y_i)$ and $(\hat{x}_i, f(\hat{x}_i))$. The term is minimized when the line connecting the data point to the function curve is perpendicular to the function curve. A fit-algorithm must thus adjust the function until the sum (2) of the squared perpendicular distances between data points and function curve reaches a minimum.

We refer to the literature for more detailed discussions of the above deviation functions. A short description is also found in the classical book by W.H. Press, B.P. Flannery, S.A. Teukolsky, W.T. Vetterling, *Numerical Recipes - the Art of Scientific Computing*.

**The mean square deviation: Chi-Squared**

When squared deviation functions are used, (2) gives the mean square deviation, which is often called $\chi^2$:

$$\chi^2 = \sum_i \left( \frac{(\hat{x}_i - x_i)^2}{\sigma_{x_i}^2} + \frac{(f(\hat{x}_i) - y_i)^2}{\sigma_{y_i}^2} \right)$$

The mean square deviation (chi-squared) is used when the measurement errors are described by a Gaussian probability distribution, and in this case the errors $\sigma_{x_i}$ and $\sigma_{y_i}$ correspond to the standard deviations of the Gaussian distributions.

The denomination “chi-squared” has become so common that it is often used to indicate the result of (2), and not only to indicate the particular case (8).

For the sake of simplicity, proFit follows this somewhat “dirty” convention and uses the denomination “chi-squared” when referring to the result of (2), even if deviation functions other than square deviations are used. The same is true for the predefined function ChiSquared, which can be used in proFit programs to retrieve the value of (2) obtained in the last fit.

**Zero X-errors**

In most experiments it is possible to determine the x-coordinate much more precisely than the y-coordinate. In such a case the x-errors can be assumed to be very small. The only way to minimize the mean deviation (2) is then to have $\hat{x}_i \equiv x_i$. The mean deviation function becomes much simpler:

$$\chi_R = \sum_i R \left( \frac{f(x_i) - y_i}{\sigma_{y_i}} \right),$$

The function is evaluated at the x-coordinates of the measured points. The function value and measured y-coordinate directly give the normalized distance, when weighted with the measurement error.

**The “usual case”: Chi-squared and zero x-errors**

In many experiments it is not only possible to make the x-errors so small that they can be considered zero. It is also common to have (or hope for) Gaussian distributed measurement errors. In this case we have to minimize a particularly simple expression for chi-squared:
\[ \chi^2 = \sum_i \frac{(f(x_i) - y_i)^2}{\sigma_{yi}^2}, \] (10)

Since this case is easy to handle from an algebraic and numerical point of view, many common fitting algorithms and applications work under the assumption that the mean deviation is the mean square deviation given by Eq. (10). A classical fitting algorithm that works on this basis is the Levenberg-Marquardt algorithm in its unmodified, original form (see below).

**Error analysis and confidence intervals**

Although some fitting algorithms (most notably the Levenberg-Marquardt fitting algorithm) do provide estimates for the error of the parameters, these estimates are often not sufficient or too imprecise.

`pro Fit` provides a general way for estimating the confidence intervals within which the “true” value of a fitted parameter can be assumed to lie with a certain probability level.

The influence of variations in the data points on the fitted parameters is analyzed with the help of a Monte Carlo simulation. For this purpose, synthetic data sets are generated starting from the points \((\hat{x}_i, f(\hat{x}_i))\) that were obtained in the fit (see above). For each of the original data points a simulated data point is generated by random variation around \((\hat{x}_i, f(\hat{x}_i))\) within the specified errors and using the specified error distributions. This produces a synthetic data set that effectively simulates a measurement. The simulation of the measurement is based on the function that was determined in the last fit (which is assumed to correspond to the underlying “reality”) and on the measurement errors that were specified.


For each of the synthetic data sets, a fit is performed. Once that all synthetic data sets have been fitted, the **confidence intervals** are calculated by analyzing the values obtained for each parameter. The confidence interval thereby corresponds to the range enclosing a given percentage of the values.

When error analysis is complete, the results are printed in the Results window and a list of the fitted parameters for each synthetic data set appears in a new data window. You can use the set of simulated parameters for further statistical analysis.

**Fitting algorithms**

In the previous section we gave a short overview of the most important mathematical tools used to establish criteria distinguishing a good fit from a bad one. Once these criteria are established, one can use them to analyze parameter sets, and to find out in which direction the best parameter set can be found.

The search for the best parameter set is the responsibility of a fitting algorithm, and `pro Fit` lets you choose between three different ones: The *Monte Carlo*, *Levenberg-Marquardt*, and *Robust* algorithms.

The algorithms differ by the method they use to orient themselves in parameter space and to find the location of the best parameter set.

The **Monte-Carlo** algorithm minimizes (2) with any definition of \(R\) by randomly varying the parameters and (if the x-errors are not zero) the set of x-coordinates \(\hat{x}_i\) and looking for the smallest value of (2). This algorithm is often useful to scan parameter space and find good initial values for a Levenberg-Marquardt, or Robust fit.
The Levenberg-Marquardt algorithm minimizes the mean square deviations using (8). It finds at the same time the set of x-coordinates \( \hat{x}_i \) and the function parameters that minimize the mean square deviations between the data points \((x_i, y_i)\) and the function values \((\hat{x}_i, f(\hat{x}_i))\). When the x-errors are zero, the Levenberg-Marquardt algorithm minimizes (9).

The Robust fitting algorithm minimizes (2) with any definition of \( R \) by continually moving “downhill” in parameter-space until the bottom of a valley is found.

The Linear Regression and the Polynomial fitting algorithms are specialized for polynomials of 1st and nth degree. While the Linear Regression allows for x-errors (we use a straight forward algorithm if there are no x-errors), the Polynomial fitting algorithm is restricted to y-errors only.

The mathematics used by the various algorithms to perform their job is outlined in the next sections.

The Monte Carlo algorithm

This method randomly varies the parameters of a function within given intervals. When x-errors are defined, the algorithm also varies randomly the set of x-coordinates \( \hat{x}_i \) while observing the given errors and error distributions.

For each random guess, \( \chi_R \) is calculated according to Eq. (2) and the parameter sets corresponding to the smallest values of \( \chi_R \) are remembered.

The strength of this method is also its biggest disadvantage. It looks for the best parameter set by shooting blindly inside the given region of parameter space. Although there is an option of letting this parameter space region follow the position of the currently best parameter set, this algorithm can only converge very slowly towards the best parameter set.

Its main use is to “scan” parameter space in order to find good parameter starting values for one of the deterministic fit algorithms, or to try to “jump out” of a local minimum where a deterministic fitting algorithm is stuck.

Since the algorithm is normally used for a first estimate of fitted parameters, it is not recommended to run it with non-zero x-errors – this merely slows down the algorithm without substantially increasing the accuracy of the estimates.

The Levenberg-Marquardt algorithm

The Levenberg-Marquardt algorithm is derived directly from the mean square deviation expressions (8) or (10) and cannot be used with deviation functions \( R \) other then the square deviation \( R(d) = d^2 \).

The Levenberg-Marquardt algorithm is in principle the fastest fitting algorithm available in pro Fit. Its performance, however, depends strongly on the behavior of the function to be fitted as well as on the selected starting parameters.

The classical version of the Levenberg-Marquardt algorithm does not allow for x-errors and minimizes the mean square deviation (10). The algorithm can be described in words as follows:

Starting from a given set of parameters, the mean square deviation \( \chi^2 \) is calculated. Then the parameters are varied slightly to observe their influence on \( \chi^2 \). From this, the direction in which \( \chi^2 \) decreases most rapidly can be evaluated and a new set of parameters is chosen. This procedure is reiterated with this new set of parameters. When the minimum is near, the algorithm goes over to a more deterministic “guessing” at the position of the minimum and solves some equations to find it. The fitting stops when the value of \( \chi^2 \) does not decrease anymore between successive steps.

When x-errors are specified, the algorithm is modified in such a way that it minimizes (8). It finds at the same time the set of x-coordinates $\hat{x}_i$ and the function parameters that minimize the mean square deviations between the data points $(x_i,y_i)$ and the function values $(\hat{x}_i,f(\hat{x}_i))$.

The extensions to the Levenberg-Marquardt algorithm that allow the interpretation of x-errors are described in P.L. Jolivette, “least-squares fits when there are errors in X,” Computer in Physics, Vol. 7, No. 2, 1993.

**Partial derivatives**

To fit a function of the type $y = f(a_1,\ldots,a_n,x)$ the Levenberg-Marquardt algorithm needs the partial derivatives of the function with respect to its parameters. It uses the partial derivatives when it estimates the influence of the parameter set $\{a_i\}$ on $\chi^2$. The partial derivatives $f_i'$ are given by

$$f_i'(x) = \frac{\partial f(a_1,\ldots,a_n,x)}{\partial a_i}$$

and they are calculated for all x-coordinates $\hat{x}_i$ during every iteration.

More information on how to define functions and their derivatives is given in Chapter 9, “Defining functions and programs”.

**Estimation of parameter errors**

The Levenberg-Marquardt algorithm allows the determination of the standard deviations of the parameters. These are the values that are printed in the results window after a successful fit, under the heading "standard deviations". The standard deviation defines the region that contains 68.3% of the total integral of a Gaussian distribution.

The standard deviation $\sigma_{a_j}$ of the parameter value $a_j$ obtained after a successful fit is found from

$$\sigma_{a_j} = C_{jj}^{1/2}$$

where $C_{jj}$ is the diagonal element of the covariance matrix $C$. The full covariance matrix of the parameters used in the fit is the inverse of a matrix $A$: $C=A^{-1}$.

The matrix $A$ is also called curvature matrix, and it is defined by the errors (standard deviations) of the data points and by the partial derivatives of the function with respect to the parameters. When x-errors are specified the derivative of the function with respect to x must also be calculated and the curvature matrix $A$ is given by
If the x-errors can be considered to be zero, the curvature matrix $A$ has the simpler form:

$$A_{ij} = \sum_k \frac{1}{\sigma_{yk}^2 + \sigma_{xk}^2} \left( \frac{\partial f(x_k)}{\partial a_i} \partial f(x_k) \frac{\partial f(x_k)}{\partial a_j} \right).$$

(13)

If the x-errors can be regarded as zero, proFit lets you specify “unknown” y-errors. In this case, the $y_i$ are assumed to be normally distributed, all with the same standard deviation $\sigma$. For fitting, $\sigma_{yi}$ is taken to be 1 for all $i$. The “real” $\sigma_{yi}^2$ is then estimated from $\sigma^2 = \chi^2 / \nu$ (where $\nu$ is the number of degrees of freedom, i.e. the number of data points minus the number of parameters) and $\sigma_{ai}$ is calculated from the expressions given above.

Loosely speaking, this matrix describes the propagation of the errors from the data points to the parameters. We refer to the specialized literature for more details.

It is interesting to consider the case where a parameter reaches one of its limits during a fit. As you know, proFit lets you specify, for each function parameter, an interval of allowed parameter values. If a parameter is at one of the boundaries of this interval after a fit, its standard deviation cannot be calculated. The parameter is then considered to be constant (i.e. it is not a free parameter anymore). The standard deviations of the other parameters and $\chi^2$ are calculated using the effective number of active parameters at the end of the fit. The results obtained are the same as those that would have been obtained by fitting with the parameter fixed at its limit from the start.

The standard deviations of the parameters (and the covariance matrix) that are obtained in a Levenberg-Marquardt fit have a clear quantitative interpretation only if the errors of the data are normally distributed. If the data errors are not given, the calculations for evaluating the standard deviations of the parameters assume that the $y_i$ are normally distributed and that the function is the correct description of reality.

Interpret the results carefully!

An alternative, more general way to estimate the errors of the fitted parameters is described in the section “Error analysis and confidence intervals”.

The Robust minimization algorithm

This method minimizes $\chi_R$ (2) with any definition of $R$ by continually moving “downhill” in parameter-space. Starting from some initial value, the parameters are varied and the resulting value of $\chi_R$ is calculated. From this, the algorithm finds the direction in which $\chi_R$ decreases and moves that way. Then it samples again the surroundings by varying the parameters. It stops when a minimum is reached.

When the x-errors are not zero, the $\hat{x}_i$ necessary for calculating the “minimal distance” between a data point and the function curve are calculated for each data point by an explicit minimization of the term $\left[ R(d_{xi}) + R(d_{yi}) \right]$ in Eq. (2).

Minimization is performed with limited precision in order to save processing time. The $\hat{x}_i$ will be determined to an accuracy which is a fraction of the x-error specified for each point. proFit will also count the number of function calls it is using to determine one $\hat{x}_i$ and will stop after a maximum of 50
function calls (normally much less function calls (<10) are needed to find the minimum). This procedure introduces a small uncertainty in the determination of $\chi^2_R$. However, the statistical significance of such an uncertainty will be limited, because the precision with which the $\hat{x}_j$ are determined is in any case much better than the errors of the data points.

A robust fit with x-errors larger than zero will be considerably slower than the same fit performed with zero x-errors. When for zero x-errors evaluation of (9) requires a number of function calls equal to the number of data points, evaluation of (8) will require more or less ten times more function calls when x-errors are defined.

### The Linear Regression algorithm

In this case we assume a straight-line model for the measured data with normally distributed errors.

$$y(x) = a + b \cdot x$$  \hspace{1cm} (15)

A) If there are no x-errors and the y-errors are assumed to be known ($\sigma_i$ is the uncertainty of $y_i$) equation (9) can easily be simplified. At its minimum the derivatives after the two parameters $a$ and $b$ vanish. This leads to a set of linear equations that are solved analytically:

$$a = \frac{S_{xx}S_y - S_x S_{yy}}{\Delta}, \quad b = \frac{S_{xy} - S_x S_y}{\Delta} \hspace{1cm} (16)$$

using the following definitions:

$$S = \sum_{i=1}^{N} \frac{1}{\sigma_i}, \quad S_x = \sum_{i=1}^{N} \frac{x_i}{\sigma_i}, \quad S_y = \sum_{i=1}^{N} \frac{y_i}{\sigma_i},$$

$$S_{xx} = \sum_{i=1}^{N} \frac{x_i^2}{\sigma_i}, \quad S_{xy} = \sum_{i=1}^{N} \frac{x_i y_i}{\sigma_i}, \quad \Delta = S S_{xx} - \left(S_x \right)^2 \hspace{1cm} (17)$$

From these we are also able to calculate the variances of $a$ and $b$, and the correlation coefficient between them:

$$\sigma_a^2 = \frac{S_{xx}}{\Delta}, \quad \sigma_b^2 = \frac{S_{xy}}{\Delta}, \quad r_{ab} = \frac{-S_x}{\sqrt{S_{xx} S_{xy}}} \hspace{1cm} (18)$$

B) If the measurement shows errors in the $x_i$ the minimization of (8) becomes more difficult, i.e. the set of equations derived for $a$ and $b$ are not linear any more. However, they are solved with numerical means, i.e. with a standard root finding algorithm.

Together with the fitting parameters and their variances the correlation coefficient $r$ is calculated (Pearson's $r$). It takes a value between -1 and 1 depending on how much the x-values and the corresponding y-values are correlated. $r = +1$ if there is a complete correlation with a positive slope, $r = -1$ if there is a complete correlation with a negative slope, and $r = 0$ if there is no correlation at all.
The significance of the correlation is the "probability that \(|r|\) should be larger than its observed value in the null hypothesis" (\(x\) and \(y\) being uncorrelated). It ranges from 0 (= good correlation) to 100% (= bad correlation).

We refer to the specialized literature for more details.

**The Polynomial fitting algorithm**

Our model is the general linear combination of arbitrary functions

\[ y(x) = \sum_{k=1}^{M} a_k F_k(x) \]  \hspace{1cm} (19)

The functions \(F_k\) can be wildly nonlinear functions of \(x\). "Linear" refers only to the model's dependence on its parameters \(a_k\).

Once again we assume that the measurement errors \(\sigma_i\) of the \(i\)th data point are known. By defining the matrix \(A\) and the vectors \(b\) and \(a\) as

\[ A_{ij} = \frac{F_j(x_i)}{\sigma_i}, \quad b_i = \frac{y_i}{\sigma_i}, \quad a_i \]  \hspace{1cm} (20)

it is possible to describe the minimization equations in matrix form

\[ (A^T \cdot A) \cdot a = A^T \cdot b \]  \hspace{1cm} (21)

The variances of the parameters can be found as the square root of the diagonal elements of the inverse matrix \(A^{-1}\).

To solve equation (21) we use the method of Singular Value Decomposition (SVD). It is a very robust algorithm for overdetermined as well as for underdetermined systems, although it is a little slower and needs more memory resources than solving the normal equations.

For further details see the literature listed below.

**Goodness of fit**

It is very important to know the quality of a fit; otherwise the minimizing parameters found are in general not meaningful. The goodness of fit, which is the probability \(Q\) that a value of chi-square \(\chi^2\) should occur by chance, is calculated by the incomplete Gamma function

\[ Q = \text{gammq} \left( N - M, \frac{\chi^2}{2} \right) \]  \hspace{1cm} (22)

It depends on the degree of freedom, defined as the difference between the number of measured points \(N\) and the number of varied parameters \(M\).

If \(Q\) is large, e.g. > 0.1, the fit seems reasonable. If it is small, e.g. < 0.001, there might be something wrong.

**Literature and suggested reading**


The fitting process

General features
With proFit, fitting is a highly interactive process. You can decide which parameters have to be varied, set their starting values (estimates) and choose a fitting method. You can inspect the fitting process while it is running, and interrupt it if you don’t like it. You can reiterate the process and change fitting algorithms.

The fitting process starts from the parameter values given in the parameters window. You can change these values (click the numbers and edit them). The window also shows which parameters are to be fitted: Only those whose name is shown in bold face will be fitted (for these parameters the check box “Use for fitting”, which appears when you select a parameter, is checked).

The following is the parameters window for the function Polynom. All parameters will be fitted except the parameter named ‘deg’:

To change the fitting mode of a parameter (e.g. from ‘fit’ to ‘not-fit’), click its name. It will switch from bold to normal or from normal to bold. Alternatively, you can click the check box Use for fitting, in the “selected parameter” field.

Some parameters can never be fitted. For example, it does not make sense to fit the degree of a polynomial. The name of such a permanently fixed parameter cannot be made bold by clicking it. The Use for fitting check box is disabled.

Parameters that can never be fitted are called constant parameters, those that are currently not fitted are called inactive parameters, and those that are currently fitted are called active parameters.

Parameter limits
The value of a parameter can be limited to any specified interval by entering the boundaries of the allowed interval in the corresponding edit fields. The edit fields appear in the “active parameter” field once you select a parameter. A parameter is not allowed to leave the specified interval during fitting, optimization of the function, or when you enter a new value in the parameters window.

See Chapter 5, “Working with functions and programs”, and Chapter 8, “Defining functions and programs”, for more information on how to set parameter limits in user-defined functions. If no limits are specified, the default values are -∞ and ∞ (-Inf..Inf).
During fitting, each parameter is constrained to the interval specified by the parameter limits.

**Running a fit**

Running a fit consists basically of three simple steps:

1. **Choose the function to fit in the Func menu.**
   
   Add your own function to the Func menu if it is not already there.

2. **Define which parameters you want to fit and their starting values.**
   
   You can do this in the parameters window as described above. Look at the function and the data set in the Preview Window to see how good your starting values are. Use the **Fitting-tool** in the Preview Window to “push” the function towards the data points.

   The importance of good starting values depends on the function to be fitted. Some functions, like the Gauss function are more difficult to fit. A polynomial can be fitted with almost any starting parameter set.

3. **Choose Fit from the Calc menu.**
   
   The Fitting Setup dialog box appears:

   ![Fitting Setup dialog box](image)

   Using this dialog box, you can set a number of fitting options. Once you are satisfied with them, click **OK** and fitting will start.

   You can switch from one fitting algorithm to the other using the **Algorithm** popup menu. More details about particular options for each algorithm are given below.

   The **Window** menu lets you select a data window (by default the foremost data window).
The **X column** and **Y column** menus define the data set coordinates $x_i$ and $y_i$. If **Selected rows only** is checked, only rows intersecting the current selection are used for fitting. Otherwise, all data in the X- and Y-columns will be used.

The popup menus **X-Errors** and **Y-Errors** let you specify the errors of your data. In the X-Errors menu, choose **zero** to use zero x-errors (the usual case). In the Y-Errors menu, choose **unknown** if you don’t want to specify y-errors – in this case, a value of “1.0” will be used as the error for all data points (regardless of the order of magnitude of the y-values) and all points will have the same weight in the calculation of $\chi R$ (which is calculated with $\sigma_yi \equiv 1$). Choose **Constant** if you want to enter the error as a fraction of the data value in %. If you have the errors stored in a column of your data window, then select **Individual** and choose the appropriate column in the pop-up menu that appears.

> Make sure that the columns you select contain the correct error values in the correct positions. For each row in the table, there must be a one to one relationship between the values in the x-, y-columns and the values in the error columns.

The **Distribution** popup menu, which appears when you define errors, gives the error-probability distribution that will be assumed for the fit. This popup menu is dimmed if the Levenberg-Marquardt algorithm is used, because this algorithm only works with Gaussian error distributions.

The check box **Use last choice** tells proFit to use the data window and error settings of the previous fit. This feature is rarely used, but it makes fitting easier when you have to fit the same data columns several times but want to work with other data windows before and after a fit.

The results of the fit are shown in the results window. Check **Print active parameters only** if you only want to see the values of the parameters that were fitted. Use this option if your function has many parameters that you do not fit and you do not want all the values of inactive or constant parameters to clutter the results window. Check **Print full description** to get, for each fit, a header that describes the settings that were used for fitting.

Check **Error Analysis** if you want to obtain more information on the accuracy of the fitted parameters. Confidence intervals for each fitted parameter will be determined by a Monte Carlo method that simulates a large number of fits with a series of synthetic data sets. More about this in the Error Analysis section, below.

To start fitting, click **OK**. Fitting can run for fractions of a second or for hours, depending on the execution speed of the function you selected, the number of parameters to fit, and the number of data points. The results of the fit appear in the result window. You might want to choose its name from the windows menu and position it in a comfortable place before running a fit. You can let proFit always bring the results window to the front after a fit by using the Preferences... command.

To speed up fitting when you are using one of your functions, you should define the function’s partial derivatives with respect to its parameters. The section “The role of the partial derivatives” below gives more information on this topic.

You can interrupt fitting by holding down the command key (⌘) and the period-key (.) simultaneously.

Note that proFit can run any fit in the background, this means that you can work with another application while proFit is fitting. You may want to place proFit’s progress window in a corner of your screen to watch what is going on.
Inspecting the progress of a fit

During lengthy fits, you can inspect what is going on and see if the fitting algorithm is behaving correctly. proFit displays information on the current fit in its progress window:

This window lists the total number of iterations, the current values of chi squared, and the current values of the best parameter set.

You can see the progress of the fit graphically if you open the Preview Window and check the Show Function check box. During a fit, proFit will periodically draw the function corresponding to the best parameter set. This allows you to see how the function approaches the data set during a successful fit. Because of this previewing feature, you will notice soon enough if the fit is not converging correctly, and will then be able to interrupt it.

If your function performs many lengthy calculations, redrawing the function periodically can slow down the fit. Hide the Preview Window, or uncheck “Show Function” if fitting speed matters.

Error analysis and confidence intervals

Check Error Analysis in the Fit dialog box to get more information on the confidence intervals of the parameters.

When Error analysis is checked, two more edit fields appear in the Fitting Setup dialog box.
The Error Analysis algorithm simulates a number of data sets equal to the value specified in the iterations edit field. For each iteration, the corresponding parameter set will be determined by the fitting algorithm you selected (either the Robust algorithm, or the Levenberg-Marquardt algorithm).

You should always use the Levenberg-Marquardt algorithm when performing error analysis. Using the Robust algorithm is not recommended because this algorithm is inherently slower than the Levenberg-Marquardt algorithm. Since error analysis can need thousands of iterations, the convergence speed of the algorithm is very important.

All parameter sets generated during error analysis will be collected and displayed in a data window once Error Analysis is completed. You can then use them for a more complete analysis of the distribution of each parameter.

Based on the simulated parameter sets, proFit estimates confidence intervals. You must specify which confidence interval you want proFit to calculate by entering the corresponding probability in the confidence intervals field. proFit calculates a confidence interval in such a way that the given percent of the simulated parameter values are contained inside it.

During error analysis, proFit shows the status of the calculation in its progress window:
The window shows the status of the calculation and the confidence interval estimations based on the currently available data. The calculation is a Monte Carlo calculation, so the boundaries of each confidence interval will converge slowly and randomly towards some stable values.

If you want to see what happens during error analysis and your function draws itself fast enough, open the Preview Window and make sure “Show function” is checked. pro Fit will redraw the function periodically during error analysis and you will be able to see how the fitted function changes depending on the simulated data sets which are generated randomly. However, doing so will waste time for drawing the function and slow down the error analysis procedure. Hide the Preview Window, or uncheck “Show function” to make the error analysis procedure as fast as possible.

**Fitting results**

When fitting is completed, a summary of the results of the fit is displayed in the results window. Depending on which fitting algorithm you used, the data printed to the results window can vary slightly.

You may often want to transfer the values of the fitted parameters to the parameters window to use them as starting values for a further fit. Choosing **Params ->>>** from the Calc menu transfers the best set of parameters to the parameters window.

The results of a fit are made available to custom functions and programs through a set of predefined functions used for accessing the fitted parameters, the confidence intervals, the value of chi squared, and, for the Levenberg-Marquardt algorithm, the full covariance matrix. See Appendix A for more details.

If you want to save the parameter sets obtained in every single fit, store them in a dedicated data window. You can copy them from the parameters window and paste them into a single row of the data window, or you can write a small macro (a pro Fit program) that transfers the fitted parameters directly to their data window. See chapter 9 “Defining functions and programs” to see how to do this. An example program for transferring parameter values to a data window is found on the pro Fit distribution disks.

**Using the various fitting algorithms**

pro Fit provides three different fitting algorithms: The *Monte Carlo*, *Robust*, and *Levenberg-Marquardt* algorithms. They are described in the preceding section.
The following sections describe how each of these fitting algorithms is used, and what particular options you can set for each algorithm.

**Using the Levenberg-Marquardt algorithm**

To start a fit with the Levenberg-Marquardt algorithm, choose **Fit** from the Calc menu after having selected the appropriate function from the Func menu. The Fitting Setup dialog box appears with Levenberg-Marquardt pre-selected in the Algorithm popup menu. See the preceding section for a description of this dialog box.

When you define errors, the **Distribution** popup menu is dimmed and set to a Gaussian distribution. The Levenberg-Marquardt algorithm can only work if the errors of the data set are normally distributed.

The Levenberg-Marquardt fit stops running when the chi-squared determined from the current parameter set doesn’t decrease appreciably anymore from one iteration to the next.

When finished, the parameter values and their standard deviations are printed to the results window. If you need to access the complete covariance matrix, you can define a program that uses the predefined function **CovarMatrix**. See Appendix A for more details on how to use this function.

**Using the Robust minimization algorithm**

To run a Robust fit, choose “Robust” in the algorithm popup menu of the fit dialog box. This dialog box appears when selecting “Fit” from the Calc menu, and it was described above.

Using the **Distribution** popup menu, which appears when you define errors, you can select the error distribution that best describes your experiment. Robust fitting will deserve its name if you select a distribution that diminishes the importance of outliers (like Andrew’s sine or Tuckey’s biweight).

When finished, the resulting parameter values are printed to the results window. This algorithm does not determine a “standard deviation” for each parameter, like the Levenberg-Marquardt algorithm does. To obtain error estimations you have to run a Levenberg-Marquardt fit after the Robust fit converged, or you have to check the **Error Analysis** check box and perform a Monte Carlo analysis. See the corresponding section for more details.

**Using the Monte Carlo algorithm**

To run a Monte Carlo fit, choose **Monte Carlo Fit** from the Calc menu or chose **Monte Carlo** in the Algorithm popup menu of the Fitting Setup dialog box.

When you do this, two more items appear to the right of the Algorithm popup menu (Please refer to the beginning of this section for a basic discussion of the Fitting Setup dialog box.)

Clicking **Ranges...** presents another dialog box where you can define the ranges within which the parameters can be varied:
By default, these ranges are the ten percent deviations of the starting value of the parameter (or –1 and 1 if the starting value is 0).

Checking **Auto search** tells pro Fit to make a more flexible search for the best set of parameters. The Auto search check box determines whether the limits within which the parameters are varied will be kept fixed (auto-search unchecked) or if they will be adapted during the fit (auto-search checked). In the latter case, the limits will be shifted after every iteration to keep them around the best parameter set. (Note that the parameters are never allowed to leave the parameter limits defined in the parameters window.)

The Monte Carlo Fit runs until you interrupt it by pressing `Esc-`.’. If you don’t stop the fit yourself, the Monte Carlo Fit runs for ever.

The three best sets of parameters are displayed in the results window after you interrupt the fit.

> The Monte Carlo fit slows down exponentially when the number of parameters to be fitted is increased.

**Using the Linear Regression algorithm**

To run a Linear Regression fit, choose “Linear Regression” in the algorithm popup menu of the fit dialog box. This dialog box appears when selecting “Fit...” from the Calc menu, and it was described above.

As the name indicates, this algorithm forces you to select the Polynomial function of degree 1, with both parameters being fitted. It assumes a Gaussian distribution of errors. X-errors and Y-errors are possible.
When finished, the parameter values and their standard deviations are printed to the results window. Additionally, the correlation coefficient \( r \) is calculated, as well as its significance, which is the probability that \(|r|\) should be larger than its observed value in the null hypothesis (\(x\) and \(y\) being uncorrelated).

**Using the Polynomial fitting algorithm**

To run a Polynomial fit, choose “Polynomial” in the algorithm popup menu of the fit dialog box. This dialog box appears when selecting “Fit...” from the Calc menu, and it was described above.

As the name indicates, this algorithm forces you to select the Polynomial function of any degree. It assumes a Gaussian distribution of errors. Only Y-errors are possible.

When finished, the parameter values and their standard deviations are printed to the results window.

**Fitting multiple functions and x-values**

You may sometimes want to fit *simultaneously* several functions \( (f_1 \ldots f_q) \) with one or more common parameters. Or you may want to fit a function that does not depend on a single \( x \)-value but on a set \( (x_1, x_2 \ldots x_p) \) of \( x \)-values. Or you might even encounter a combination of these two cases.

In the most general case, you have \( q \) functions, each of them depending on one or more \( x \)-variables. Each function has some parameters, some functions can share one or more parameters:

\[
\begin{align*}
y_1 &= f_1(x_1, x_2 \ldots x_{p_1}) \\
y_2 &= f_2(x_1, x_2 \ldots x_{p_2}) \\
&\quad \vdots \\
y_q &= f_q(x_1, x_2 \ldots x_{p_q})
\end{align*}
\]

For each function, you have a set of data points that should be described by it. Now you want to fit all these functions simultaneously.

There are several methods of tackling this kind of problem with proFit. Some of them are described in the following section.

**Functions with multiple \( x \)-values**

Let us first consider the special case of a single function that depends on more than one \( x \)-value:

\[
y = f_1(x_1, x_2 \ldots x_p).
\]

Example: The photoconductivity \( \sigma \) of some light detectors as a function of the incident light intensity \( I \) and the operating temperature \( T \) obeys a relation of the form

\[
\sigma = s I e^{-T_o/T},
\]

where \( I \) is the intensity of the incident light and \( T \) is the absolute temperature (in Kelvin). \( s \) and \( T_o \) are parameters.

In our example, we have a number of measurements of the conductivity \( \sigma \) at different temperatures \( T \) and different intensities \( I \). The values are given in the table below.
Here is a graphical representation of this data set:

<table>
<thead>
<tr>
<th>Temp [K]</th>
<th>Intensity [mW/cm²]</th>
<th>Conductivity [$10^{-8} \ \Omega^{-1} \ \text{cm}^{-1}$]</th>
</tr>
</thead>
<tbody>
<tr>
<td>200</td>
<td>0</td>
<td>0.00</td>
</tr>
<tr>
<td>200</td>
<td>20</td>
<td>8.45</td>
</tr>
<tr>
<td>200</td>
<td>40</td>
<td>16.90</td>
</tr>
<tr>
<td>200</td>
<td>60</td>
<td>25.35</td>
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<td>0</td>
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</tbody>
</table>

In order to fit these points with our function, we must define the function and the data set in such a way that the function can obtain its two x-values from the current data window. We enter the temperature $T$ (which is our $x_1$ value) into column 2 of a data window, the intensity $I$ (which is our $x_2$ value) into column 3, and the conductivity (which is our $y$ value) into column 4. We fill column 1 with numbers from 1 to 12, thus numbering all our measured points.
Conductivity data entered into a data window. Note the auxiliary column 1, providing a unique number for each data point.

Now we define a function $y = F(x)$ that returns the conductivity as its $y$-value (see Chapter 9, “Defining functions and programs”, on how to define your own function) and takes the number of the data point (in column 1) as $x$-value. When this function is called with a given value of $x$, it looks up the values of temperature and intensity (i.e. the values for $y_1$ and $y_2$) from columns 2 and 3 of the current data window. Then it calculates the conductivity according to our model $\sigma = s I \exp(-T_0/T)$:

$$\text{function conductivity; } \begin{array}{l}
y := a[1] \times \text{data}[x,3] \times \exp(-a[2]/\text{data}[x,2]); 
\end{array}$$

Note that data[x,3] is the value of the x-th cell of the third column in the data window that was chosen for fitting, data [x,3] is the intensity and data[x,2] is the temperature.

Now we can fit this function to our data. We use the first column as its $x$-value and the conductivity column as its $y$-value. Before fitting, don’t forget to set reasonable starting values for the parameters (in this case most positive numbers will do). The fit returns $a[1] = 2.2$ and $a[2] = 330$.

The general idea of this method is to replace a function $f(x_1, x_2, \ldots x_p)$ by a single valued function $F(x)$ which takes an index as its $x$-value. From this index, $F$ can find the cells in the current data window where the values $x_1, \ldots x_p$ are stored. Once $x_1, \ldots x_p$ are known, $F$ can calculate $f(x_1, \ldots x_p)$.

**Multiple functions with one x-value**

Another special case that we can easily lead back to the form $y = f(x)$ is the case of multiple functions with one $x$-value. These functions can share one or more common parameters.

$$y_1 = f_1(x),$$
$$y_2 = f_2(x),$$
\[ y_q = f_q(x) \].

One method to transform this problem into a ‘fittable’ form is the following:

Let us assume that we have \( x \)-values ranging between 0 and 1000. We now define a function \( f \) of the form:

\[
y = \begin{cases} 
    f_1(x) & \text{if } x = 0..999 \\
    f_2(x - 1000) & \text{if } x = 1000..1999 \\
    f_3(x - 2000) & \text{if } x = 2000..2999 \\
    \text{etc.} 
\end{cases}
\]

Now we can enter the \( x \)-values of our points in the first column of our data window and all \( y \)-values in the second column. The first \( N_1 \) rows (where \( N_1 \) is the number of data points we have for \( f_1 \)) contain the values of \( x \) in column 1 and the corresponding values of \( y_1 \) in column two. The next \( N_2 \) rows (where \( N_2 \) is the number of data points for \( f_2 \)) contain \( x+1000 \) in the first column and \( y_2 \) in the second column, and so on. In this way we have reduced a set of multiple functions to a single function.

When fitting multiple functions, it is very important to specify the standard deviations of the \( y \)-values of each function. The reason for this lies in the fact that the \( y \)-values for each function may have a different order of magnitude. E.g. \( f_1 \) might return values in the order of \( 10^{10} \) while \( f_2 \) returns values in the order of 1. If you do not specify the error range of the \( y \)-values, the fitting algorithm weights them all equally and a given deviation of a data point from the function \( f_1 \) has the same weight as a deviation from \( f_2 \). For most cases, however, it would be more reasonable to give a stronger weight to deviations from \( f_2 \) than to deviations from \( f_1 \). This can be achieved by specifying percentage errors in the Fitting Setup dialog box.

**Multiple functions with multiple \( x \)-values**

This is the general case as described in the equations

\[
\begin{align*}
    y_1 &= f_1(x_1, x_2, \ldots, x_{p_1}) \\
    y_2 &= f_2(x_1, x_2, \ldots, x_{p_2}) \\
    \vdots \\
    y_q &= f_q(x_1, x_2, \ldots, x_{p_q})
\end{align*}
\]

We have a set of \( q \) functions. Each function has a certain number of \( x \)-values (which do not need to be the same for all functions). The functions share some parameters that you would like to fit.

The solution to this kind of problem is a combination of the two methods explained above. We define a single valued function \( \Phi(x) \) that takes an index as its argument. \( \Phi \) returns the value of one of the functions \( f_1 \ldots f_q \) for given \( x \)-values \((x_1 \ldots x_{pq})\). The \( x \)-value of \( \Phi \) tells

(a) which function of \( f_1 \ldots f_q \) should be evaluated;

(b) for which \( x \)-values it should be evaluated;

The \( x \)-values are found in certain columns in the current data window.

Example:
You have two data sets, which are described by two functions. One of these functions has only one \( x \)-value (called \( t \)), the other has two \( x \)-values (called \( u \) and \( v \)): \( f_1(t), f_2(u, v) \). The functions have some parameters in common.

The data set for \( f_1 \) consists of \( n_1 \) pairs of values \( \{ t_1, y_{11} \} \), the data set of \( f_2 \) consists of \( n_2 \) triplets of values \( \{ u_i, v_i, y_{2i} \} \). You also have error estimates for all \( y \)-values (\( \Delta y_{ji} \)).

In order to fit the parameters of all functions simultaneously, you must first choose a method of arranging the data sets in a data window. We propose to put the \( x \)-values into separate columns. All \( y \)-values must be in one column since you will need them for fitting. As the \( x \)-value for fitting you create an index \( k \) which is constructed from the formula:

\[
k = 1000 \times i + j
\]

where \( i \) is the number of the function and \( j \) the index of the data point in the data set of this function. This works fine as long as we have less than 1000 points in each data set. Note that this scheme of coding can also be used for more than two functions.

A data list for this problem will be filled up like this:

<table>
<thead>
<tr>
<th>col. 1</th>
<th>col. 2</th>
<th>col. 3</th>
<th>col. 4</th>
<th>col. 5</th>
<th>col. 6</th>
</tr>
</thead>
<tbody>
<tr>
<td>1001</td>
<td>( y_{11} )</td>
<td>( \Delta y_{11} )</td>
<td>( t_1 )</td>
<td>( u_1 )</td>
<td>( v_1 )</td>
</tr>
<tr>
<td>1002</td>
<td>( y_{12} )</td>
<td>( \Delta y_{12} )</td>
<td>( t_2 )</td>
<td>.</td>
<td>.</td>
</tr>
<tr>
<td>.</td>
<td>.</td>
<td>.</td>
<td>.</td>
<td>.</td>
<td>.</td>
</tr>
<tr>
<td>1000+n_1</td>
<td>( y_{1n_1} )</td>
<td>( \Delta y_{1n_1} )</td>
<td>( t_{n_1} )</td>
<td>( u_{n_2} )</td>
<td>( v_{n_2} )</td>
</tr>
<tr>
<td>2001</td>
<td>( y_{21} )</td>
<td>( \Delta y_{21} )</td>
<td>.</td>
<td>.</td>
<td>.</td>
</tr>
<tr>
<td>.</td>
<td>.</td>
<td>.</td>
<td>.</td>
<td>.</td>
<td>.</td>
</tr>
<tr>
<td>2001+n_2</td>
<td>( y_{2n_2} )</td>
<td>( \Delta y_{2n_2} )</td>
<td>.</td>
<td></td>
<td></td>
</tr>
</tbody>
</table>

The function you define for fitting first converts the index (which is its \( x \)-value) to the number of the function it has to call (by testing if it is larger or smaller than 2000), then gets the appropriate \( t \) or \( u \) and \( v \) values and calls \( f_1 \) or \( f_2 \):

```pascal
function twoFunctions;
var u,v:real;
begin
  if x < 2000 then begin
    x := data[x-1000,4];
    now calculate \( y := f_1(x) \)
  end
  else begin
    u := data[x-2000,5];
    v := data[x-2000,6];
    now calculate \( y := f_2(u,v) \)
  end;
end;
```

For fitting you use column 1 as the \( x \)-value, column 2 as the \( y \)-value and column 3 as the error value.
If you often have to perform this kind of fitting and for a large number of points, it may be convenient to write a small program that, starting from separate columns for all data sets, creates a data list as shown above by merging all y-values and their errors and by creating an appropriate index column.

**General hints for fitting**

**Starting parameters**

As already pointed out, the success of a fit often depends critically on the choice of a good set of starting parameters. Bad starting parameters can cause convergence to a false (i.e. local) minimum of the mean deviation $\chi_R$. It is good practice to always try to figure out reasonable values for starting parameters.

**Redundancy of parameters**

Sometimes a fit converges slowly or is even stopped with the cryptic error message ‘A singularity occurred’. This can be caused by badly chosen starting values for fitting. However, this error is often a consequence of poorly defined or redundant parameters. For example, consider the exponential function

$$y = A \times \exp\left(\frac{-1}{t_0} (x-x_0)\right) + \text{const}.$$  

This function has four parameters: $A$, $x_0$, $t_0$ and $\text{const}$. However, the parameters $A$, $t_0$ and $x_0$ are not independent, as it is easily seen when writing (5) in factors:

$$y = A \times \exp\left(\frac{x_0}{t_0}\right) \times \exp\left(\frac{-x}{t_0}\right) + \text{const}.$$  

The first two factors ($A$ and $\exp(x_0/t_0)$) both have the same influence on $y$. A change of $x_0$ can be compensated by a change of $A$. These parameters are redundant. When trying to fit them simultaneously, the fit fails.

Another problem often encountered during fitting is caused by the ‘poor’ definition of a parameter. Example: If you are trying to fit the data points $(x_1 = 1, y_1 = 2.01)$, $(2, 3.99)$, $(3, 6.00)$, $(4, 8.02)$, $(5, 9.98)$, $(6, 12.00)$ to a polynomial of second or higher degree

$$y = a_0 + a_1 x + a_2 x^2 + a_3 x^3 + ...,$$

you will get a very poor estimation of the parameters $a_2$, $a_3$, ... because your data points are nearly on a straight line and are sufficiently described by the parameters $a_0$ and $a_1$. The standard deviations of the coefficients $a_2$, $a_3$, ... will be accordingly large.

**The errors of the data set**

When using errors (standard deviations) for your data, it is useful to keep some points in mind:
• Multiplying all errors of your data points with a common factor does not affect the results of fitting, but changes the estimate of the standard deviations or the confidence intervals of the fitted parameters.

• Changing the relative errors of your data points affects the numerical weight of the data points. Example: If you have a large number of points in one area (e.g. between \( x = 1 \) and 2) and just one or two points far out (e.g. at \( x = 50 \)), it is necessary to decrease the error for these ‘lonely’ points if you want to force the function to come close to them.

• When plotting a curve in a graph with a logarithmic \( y \)-axis, a deviation of the curve from a small \( y \)-value appears much larger than the same deviation from a larger \( y \)-value. If this astonishes you, it is probably because your measurement errors are proportional to the measured value. When plotting a fit on a graph with a logarithmic \( y \)-axis, the errors of the \( y_i \) are often given in percent. This results in smaller deviations from points with small \( y \)-values. Here is an example of logarithmically plotted data with fits using percentage errors and constant errors.

A fit with percent errors gives a more satisfying visual agreement between curve and data. Obviously, for serious data fitting you should always specify the real measurement error you expect for every data point.
9 Defining functions and programs

proFit allows you to define functions and programs:

- A function is added to the menu ‘Func’. It behaves like any of proFit’s built-in functions and you can use it for fitting, plotting, etc., see Chapter 5, “Working with functions”.
- A program is added to the menu ‘Prog’. A program performs a sequence of tasks. Programs can be used for scripting proFit.

Both, functions and programs, can be defined in the same syntax, which is based on the Pascal programming language. In addition to this, programs can be written in Apple Script.

All commands that can be given to proFit using its menus, can also be issued through proFit’s program definition language or through AppleScript. You do not need to know much about the syntax of these “programming languages” in order to do this. The command that corresponds to any user-action can be generated automatically by switching on “recording”, either in proFit, or in Apple’s Script Editor, or other equivalent scripting utilities.

Programs can be considered to be “macros” that can be used to automatize tasks. However, a proFit program can do much more than what you would normally expect a macro to do, such as complicated calculations and data transformations.

Here is a small list of what functions or programs can do:

- Calculate any kind of numerical value, even if it cannot be expressed in a closed mathematical formula.
- Access the data in a data window, write results into the results window, use dialog boxes and alert boxes.
- Execute any command from proFit’s menus, open and save files, create and close windows.
- Run fitting operations and predefined numerical algorithms and retrieve their results.
- Create graphs and other drawings in a drawing window using a precise, floating point coordinate system.

Note: All the above can also be done from an external module – a piece of code generated by your favorite compiler. If you are used to programming your own code for data or function analysis, you can consider proFit as a big library offering routines for numeric analysis, data input/output and high resolution graphics. Information on how to define external modules is found in Chapter 10, “Working with External Modules”.

When you are defining your functions and programs within proFit, they are translated (‘compiled’) into native computer code when they are added to proFit’s menus. This code can be executed very quickly by your Macintosh.

Simple programs and functions can be defined very easily and quickly.

Even very complicated programs can be defined without much work by simply recording your activities using proFit’s automatic macro recording feature.

This chapter first gives a short overview on the principles of programming in proFit. It then explains the automatic macro recording feature, and finally it lists the features of proFit’s built-in compiler in detail. At the end, it explains how to save programs and functions as modules for later use.
Simple examples

Defining functions

Imagine you want to analyze a function of the form

\[ y = a \sin(x) \times \ln(x) + b \]  \hspace{1cm} (8.1)

with the parameters \(a\) and \(b\). To define it in pro Fit:

1. **Choose ‘New Function’ from the File menu.**

   This opens a new, empty function window.

2. **Enter the formula of your function in the new window.**

   The formula looks as follows:

   \[ a[1] \cdot \sin(x) \cdot \ln(x) + a[2] \]

   Use \(a[1]\), \(a[2]\) for the parameters \(a\) and \(b\).

3. **Click ‘To Menu in the function window or choose ‘Compile & Add To Menu’ from the Customize menu.**

   pro Fit analyses the contents of the window. Since you have entered a simple mathematical expression using the value \(x\), pro Fit assumes that you want to define a function. Your formula is translated into a Pascal-like function definition, it is compiled and added to the menu ‘Func’.

   The function window now shows the Pascal definition of your function:

---

9-2   Defining functions and programs
The new function appears under the name “User_Function” in the menu ‘Func’. It is automatically selected and the parameters window shows its parameters a[1], a[2].

After adding the function to proFit, you can change its parameters in the parameters window. You can plot the function, use it for fitting, calculate a table of its values, etc. (To view the function in the preview window, make sure that the option “Show function” is checked.)

The above method is an abbreviated way for entering functions: you simply enter the function’s expression and proFit translates it into a Pascal function definition before compiling it. In many situations you will, however, want to write or edit the function definition directly. Therefore, let’s have a closer look at it:

```pascal
function User_Function;
begin
  y := a[1]*sin(x)*ln(x) + a[2];
end;
```

The first word of our example is `function`. It tells proFit that the definition of a function follows. The next word (`User_Function`) gives the name under which the function will appear in the Func menu.

The function’s actual definition is given between the keywords `begin` and `end`. The function’s value is calculated and then assigned (by the `:=` operator) to the variable `y`. The variable `x` contains the function’s x-value and `a[1]`, `a[2]` etc. are the function’s parameters.

`a` is a predefined array that represent the function parameters. The parameters can be accessed by their index, i.e. `a[1]`, `a[2]` etc. Instead of using `a[i]` for the parameters, you can also use parameter names of your own by declaring them (as in standard Pascal) in the header of the function. See the section “Alternative function syntax” later in this chapter.

Our sample function is not defined for x<=0. If you use it in calculations with negative x-values, a runtime error is generated. However, the function converges to y=a[2] for x=0. You may want to expand its definition range by defining y(x) = a[2] for all x <= 0. This can be done easily in a new version of our function:
function LogSine;
begin
  if x <= 0
    then y := a[2]
    else y := a[1]*sin(x)*ln(x) + a[2];
end;

Note that you can insert additional spaces or lines anywhere between keywords.
The new version of the function (which now has the name ‘LogSine’) shows how you can use the if statement for conditional execution. It takes the general form

\[
  \text{if condition then } \text{do this} \text{ else } \text{do that}
\]

‘do this’ is executed if the condition is met, ‘do that’ if it is not met.

If you work with your function more often, you might want to make sure that the Parameter window shows reasonable default values for the parameters and a short description of what the function does. Here is a final and more complex definition implementing this (note that texts between curly brackets (‘{’ and ‘}’) are used as comments and are ignored):

function Myfunction;
  description
    { text to appear in parameters window }
    'x > 0: y = A \sin(x) \ln(x) + B',
    'x <= 0: y = B';
  defaults
    { names and defaults for the parameters }
    a[1] := 1,active,'A';
    a[2] := 0,inactive,'B';
begin
  if x <= 0
    then y := a[2]
    else y := a[1]*sin(x)*ln(x) + a[2];
end;

When you add this function to proFit, its parameters window looks like this:

![User Function Window](image)

In the last version of our sample function two additional elements have been added:

9-4 Defining functions and programs
A keyword description followed by two texts between quotes ('...'), which appear at the bottom left of the parameters window.

- A keyword defaults, which is followed by additional information for each parameter, and takes the form: a[i] := value, mode, name, lowLimit, highLimit, where value is the default value of a parameter, mode its default fitting mode (it can be ‘active’ (i.e. the parameter will be fitted), ‘inactive’ (will not be fitted) or ‘constant’ (cannot be fitted)) and name (its name between quotes ("")) used in the parameters window). Using the keyword defaults, you can also define a range of acceptable values for a parameter given in the optional parameters lowLimit and highLimit. See the detailed description of the defaults keyword, later in this chapter.

Once you have successfully defined a function and you have added it to the Func menu, you can save it as a module. A module is a file that contains the computer code for your function and that can be loaded by pro Fit at start-up, or at any other time. Go to the last section of this chapter for more information on modules.

Defining programs

Programs are generally used to create or transform data in a data window or for scripting pro Fit operations. In the following we give some very simple examples of programs.

In a first step, we will write a program that fills the first column of a data window with the powers of two: 2, 4, 8, 16, etc.

1. Choose New Function from the File menu.

This opens a new, empty function window.

2. Enter the definition of your program in the new window.

Enter the following definition:

```program PowersOf2;
var i: integer;
begin
    NewDataWindow;
    for i := 1 to nrRows do
        data[i,1] := 2 ^ i;
end;
```

Note that a program definition starts with the keyword program followed by its name. After that we first have a variable declaration for the variable i, which is of type integer.

The body of our program between begin and end starts with the call NewDataWindow, which tells pro Fit to open a new, empty data window. Then follows a so-called for-loop, which takes the general form

```for variable := startValue to endValue do statement;
```

A for-loop executes its statement for all integer values of its variable between startValue and endValue. If startValue equals endValue, the for-loop is executed only once. If startValue is larger than endValue, the for-loop is never executed.
The end value in our for-loop is \texttt{nrRows}, \texttt{nrRows} is always equal to the number of rows in the current data window.

The statement in our for-loop is an assignment (\texttt{:=}) to the array element \texttt{data[i,1]} that corresponds to the \texttt{i}th data cell in the first column of the current data window. The expression \texttt{2^i} stands for \texttt{2^i} (you can also use \texttt{2**i} instead of \texttt{2^i}).

3. **Click ‘Add’ in the function window**  
   or choose ‘Compile & Add To Menu’ from the Prog menu.

   The program is transformed into computer executable code (it is compiled) and its name appears in the at the end of the menu ‘Prog’.

4. **Choose PowersOf2 from the menu ‘Prog’**.

   The program is executed. It opens a new data window and fills its first column with the desired values.

Our next example program is somewhat more complex. Imagine you have a data window with some data in the first column. You want to write a program that fills the second column with the square root of the values of the first column. You want to take some special cases into account:
- If a cell in the first column is negative, the corresponding cell in the second column should be 0.
- If a cell in the first column is empty, the corresponding cell in the second column should be empty too.
- If any cell in the first column was empty, the program should give the user a warning when it has finished.

The program which does this task looks like this:

```plaintext
program MakeRoot;
var i: integer; {the row counter}
doAlert: boolean; {true if a cell}
            {was empty}
begin
  doAlert := false;
  for i:=1 to nrRows do
    if DataOK(i,1) then {if cell not empty}
      if data[i,1] \geq 0
      then data[i,2] := sqrt(data[i,1])
      else begin
          data[i,2] := 0;
          doAlert := true;
        end;
    if doAlert then
      Alert('Some data was negative');
end;
```

This program shows some additional features of the definition syntax:
- An additional variable of type \texttt{boolean} has been introduced. A \texttt{boolean} variable can take the values \texttt{true} or \texttt{false} which can be used in \texttt{if} statements.
• Before accessing the data in a cell, we test if there is really a number in this cell. This is done with the function \( \text{DataOK}(r, c) \), which returns true if the cell in row \( r \) and column \( c \) contains a valid number. If the cell is empty or if it contains text, \( \text{DataOK} \) returns false.

• The innermost \( \text{if} \) statement (\( \text{if data}[i,2] >= 0 \)) has two statements in its \( \text{else} \) branch. They are grouped by the keywords \( \text{begin} \) and \( \text{end} \) to make it clear that they both belong to the \( \text{else} \) statement.

• At the end of the program an \( \text{if} \) condition checks whether any data was negative. If there were negative numbers in the input column, the procedure \( \text{Alert} \) is called. \( \text{Alert} \) takes one argument, a string (i.e. a text between quotes). It displays an alert box that shows this string. Here is the alert box that appears in case negative numbers are found when the above program is executed:

This alert box has two buttons: ‘Stop’ and ‘OK’. If you click \( \text{Stop} \), the execution of your program is immediately aborted. If you press \( \text{OK} \), the execution of your program continues. For our sample program, it will not make any difference if you press Stop or OK: when the program calls \( \text{Alert} \), it is at its end anyway.

You can now add the sample program \( \text{MakeRoot} \) to the Prog menu (click \( \text{Add} \) in the function window). Then prepare a data window with some data in its first column and run \( \text{MakeRoot} \) (by choosing \( \text{MakeRoot} \) from the Prog menu).

A shortcut

As mentioned at the beginning of this chapter, you can abbreviate the definition of a function by simply entering its expression (using \( x \) and the parameters \( a[1], a[2], \) etc.) in a function window. When you click the button “To Menu” or choose “Compile & Add to Menu” from the ‘Customize’ menu, pro Fit scans the contents of the text window. Compile & Add to Menu If it encounters a simple expression using \( x \), it assumes that you want to define a function and adds the corresponding Pascal syntax around your expression.

You can use the same mechanism for defining programs. For example, you can simply enter the following lines in an empty text window:

```pascal
NewDataWindow;
for i := 1 to nrRows do
  data[i,1] := 2 ^ i;
```

When you click the button “To Menu” or choose Add to Menu from the 'Customize' menu, pro Fit finds that you have entered the body of a program and that you have used the variable \( i \). It therefore adds the necessary Pascal syntax and then compiles your program. Your complete program will look like this:
On-line help for programming

The help menus

When defining functions and programs, you can use a series of predefined names, functions and procedures. To help you use them, pro Fit provides a popup menu “Help” in the header of all function windows.

The “Help” popup menu lists all predefined routines, names, and syntax elements that you can use. The items are organized hierarchically. It is easy to find an item by moving the mouse over all the different headings.

In addition to this, the function window provides a popup menu called “Const” that provides a list of some of the most important nature constants in science and engineering.

When you move the mouse over an entry in the menus “Help” and “Const”, a help balloon is shown giving a short description. When you choose an entry and release the mouse, its definition is pasted into the function window.

You can enable/disable balloon help for these two menus by choosing the entry “Show Balloons” from the popup menu “Help”. Note that when choosing ‘Show Balloons’ from the Help popup menu, balloons are only enabled for the two popup menus – not for any of the other menus or dialog boxes of proFit. To switch on balloons for other parts of pro Fit, choose Show Balloons from the Apple Help menu (the question mark that appears in the menu bar).

Browsing functions and programs

Navigating a lengthy function or program definition can be difficult. To get a quick overview of your definition, click the popup menu “Browse” at the bottom left of the function window.
The menu shows a list of all functions, procedures and programs defined in the file. Choosing an entry from this list takes you there.

**Finding the definition of a symbol**

If you want to find the definition of a symbol, variable or command that appears in a function window, double-click it while holding down the option key. For example, if a function window looks as follows:

and you want to know how “SelectWindow” is defined, double-clicking it while holding down the option key brings up its definition in an Apple Guide panel:
Automatic Macro Recording

pro Fit 5.1 can “record” most operations that you perform and generate a Pascal program or an Apple Script therefrom. (Open Apple’s script editor to record your activity as an apple script. See chapter 11, Apple Script, for more information.)

If you do not know how to program a certain action with pro Fit’s definition language, switch on recording, perform the action you want to program, and look at the recorded commands.

Each text window has record, play and stop buttons:

The record button is the one with the circle in its center, the stop button is the one with the square, the play button is the one with the triangle.

To record your actions, click the record button. pro Fit will automatically generate a Pascal script for nearly everything you do. When you have finished recording, click the stop button. Then you can replay what you did by clicking the play button.

Alternatively, you can use the commands “Start Recording”, “Stop Recording” and “Run” (or “Run Selection”) from the Customize menu.

If you only want to run a part of a script, first select it and then click the play button (or choose “Run Selection”) from the Customize menu. If you don’t select a part of the script before clicking the play button, then the whole script is run. If there are function or program definitions in the midst of the script, they will be added to pro Fit’s menus.

The recorded commands appear at the current insertion point in the text window. You cannot edit the text window while it is recording.
You can record new commands at any place inside an existing program definition. Simply position the cursor where you want the new commands to appear, and click the “record” button.

**Syntax of function and program definitions**

This section gives a full description of the elements of proFit’s syntax for function and program definitions.

Information on how to define programs is found under “program definition syntax”. Information on how to define functions is found under “program definition syntax” and under “function definition syntax”. You need to look under both headings because the function definition syntax is based on the program definition syntax. Read the sections devoted to programs to obtain an explanation of all the general features that are available to programs as well as functions.

**Program definition syntax**

The structure of a program definition is basically identical to that of a program in standard Pascal. It starts with the keyword `program` followed by the name of the program and a semicolon. Then you can optionally define some variables, constants, procedures or functions for your own use. The main part of the program (where the execution starts) is placed between `begin` and `end` at the end of the program.

```pascal
program myProg;

const c = 3e8;
var u,v: real;
   done:boolean;

procedure MyProc;
begin
    statements...
end;

....

procedure Initialize;
begin
    statements...
end;
begin
    statements...
end;
```

After the title of the program, you can define constants and variables.

The definition of `constants` is preceded by the keyword `const`, which is followed by the name of each constant, the operator `=` (not `:=`), and the value of the constant. Example:
const c = 3e8;
    startValue = 22;

Once you have defined the value of a constant, you cannot change it anymore.

The definition of variables is preceded by the keyword var, which is followed by a list of variables.

    var   u,v: real;
    done:boolean;

Note that you can specify the type of each variable (such as real, boolean). If you omit the type specification, it is assumed that the variable is of type real.

Variables and constants that you define in the head of a program can be accessed by all statements within the program and the program’s procedures and functions.

You can use any name you like for a constant or variable (as long as it is not yet used for any other purpose). It can contain letters and digits but must start with a letter. Examples for names are:

    myFunc, xx, J0          legal names
    2ToX                    illegal (starts with a digit)
    then                    illegal (reserved keyword)

The same rules apply to the names of procedures and functions (see below).

Following the definition of constants and variables, you can (optionally) define local procedures and functions. The general form of their definition is:

... for a procedure:

    procedure MyProc(m,n:real; i: integer);
        variable and constant definitions ...
    begin
        statements, separated by semicolons
    end;

... for a function:

    function MyFunc(m,n:real; i: integer):real;
        variable and constant definitions ...
    begin
        statements, separated by semicolons;
        myFunc := return value
    end;

In this case, MyProc (or MyFunc) is the name of the procedure (function). The name is followed by a list of arguments in brackets. If the procedure or function has no arguments, this list (including the brackets) is omitted. In our examples we have three arguments: m, n and i together with their type definitions. If you define a function, the declaration of its return type follows after the argument list. Then follows a semicolon.
After the line defining the name of the function or procedure you can define constants or variables using the same syntax as described for the program (see above). These items are only known within this procedure or function.

The statements of the procedure or function follow, enclosed by `begin` and `end`;

You can call a procedure or function anywhere after its declaration, like this:

```plaintext
...  
MyProc(1.72, 3.13, 20);  
r := MyFunc(1.71, 3.14, 10);  
...
```

Local functions and procedures can also have var parameters. When you change a var parameter, you change the value of the corresponding variable of the calling function. Example:

```plaintext
program Test;  
procedure Increase(var a: Real);  
{ increases value of a by 1 }  
begin  
a := a + 1;  
end;  
begin  
k := 1;  
Increase(k);  
{ increases k by 1 }  
Writeln(k);  
{ writes 2 }  
end;
```

If you define a procedure having the name `Initialize`, it is called automatically whenever the program is added to the menu. Within `Initialize` you may want to initialize any variables or print some information into the Results window. Here is an example:
program DoMyStuff;
var inputColumn:integer;
    {where our data comes from}

procedure Initialize;
    {prints a description of the program and }
    {sets the default value of inputColumn }
begin
    Writeln('This program converts a data column');
    Writeln('into normalized units.');

    inputColumn:=3; {initialization}
end; {of initialize}

begin {main part of program}

    {ask for an input column, default is the one}
    {that was set in initialize}
    Input('which column?',inputColumn);

    {transform data}
    ....
end; {of main part}

The above program uses the predefined function Writeln to output text to the results window and the function Input to ask the user for a column number. All predefined functions are described in Appendix A.

Example
Let us look at an example of a fully functional program:
You have a data window that contains data in the first two columns. The first column contains positive and negative numbers. You are only interested in the positive numbers and you want to delete all rows which have a negative number in the first column.
Here is the program:
program EliminateNegatives;
var i:integer;

procedure DeleteRow(r:integer);
  (deletes the row r and shifts up)
  (all following rows)
var m,n:integer;
begin
  for n:=1 to 2 do
  begin
    for m:=r to nrRows-1 do
      if DataOK(m+1,n) then
        data[m,n] := data[m+1,n]
      else ClearData(m,n);
    ClearData(nrRows,n);  {clear last row}
  end;  {of for loop}
end;  {of deleteRow}

begin  {main part of program}
  i:=1;
  while i <= nrRows do
  begin
    if DataOK(i,1) then
      if data[i,1] < 0 then begin
        DeleteRow(i);  i:=i-1;
        end;
    i:=i+1;
  end;  {of while loop}
end;  {of main part}

This program tests all numerical values in column 1. This is done in a **while** loop with general form:

```
while condition do statement;
```

Its statement is executed as long as its condition is true. If you have more than one statement in a while-loop, they must be enclosed by begin and end.

Our example program executes the while-loop for all rows in the data window (*while i <= nrRows*). If a data cell in column 1 and row i contains a negative number, the procedure `DeleteRow` is called, which deletes the row i by shifting all following rows up.

The procedure `DeleteRow` calls `ClearData(r,c)`, which is a built-in procedure of proFit. `ClearData(r,c)` removes any number from the cell in column c and row r.

In the examples above, we have used the ‘for’ loop and the ‘while’ loop. Let us summarize their use and introduce the third kind of loop (the ‘repeat’ loop):
Loops

proFit supports three kinds of loops, two of which we have already seen (for-loops and while-loops). The third one is the repeat-loop. The loop statements are:

**The while-loop**

\[
\text{while condition do statement;}
\]

The statement of the while-loop is executed as long as the expression in condition returns true. If more than one statement should be executed in the loop, the statements must be enclosed by `begin` and `end`.

**The for-loop**

\[
\text{for loopVariable := startValue to endValue do statement;}
\]

A for-loop executes its statement for all integer values of its variable between `startValue` and `endValue`. If `startValue` equals `endValue`, the for-loop is executed only once. If the `startValue` is larger than the `endValue`, the for-loop is never executed. If more than one statement should be run in the loop, the statements must be enclosed by `begin` and `end`.

An alternative form of the for-loop is

\[
\text{for loopVariable := startValue downto endValue do statement;}
\]

In this for-loop the value of the loop variable is decreased by one after each execution of the loop statement. The loop is terminated as soon as `loopVariable < endValue`.

**The repeat-loop**

The last kind of loop is the repeat-loop. Its general form is

\[
\text{repeat statement until condition;}
\]

In contrast to the while-loop, the statement of a repeat loop is always executed at least once. After the execution of the statement, the condition is tested. If the condition is true, the loop is terminated, else the loop statement is executed again until the condition becomes true.

**Loop control statements: cycle and leave**

You can place the keyword `leave` into a for-, while- or repeat-loop to exit the loop even if its end-condition is not yet reached. Example:
for i := 1 to NrRows do
begin
  if not DataOK(i,1) then begin
    Writeln('Empty cell - loop aborted');
    leave;  ( exits the for-loop )
  end;
  ....
end;

The above example loops through the first column of a data window and does some calculations (indicated by '....'). If, however, an empty cell is found, the loop is aborted.

You can place the keyword \textbf{cycle} into a for-, while- or repeat-loop to immediately start a new iteration of the loop. Example:

for i := 1 to NrRows do
begin
  if not DataOK(i,1) then begin
    Writeln('Empty cell skipped');
    cycle;  ( goes to next value of i )
  end;
  ....
end;

The above example loops through the first column of a data window and does some calculations (indicated by '....'). If an empty cell is found, the calculations are skipped and the loop is continued with the next value of \textit{i}.

\textbf{Optional parameter lists}

Usually, you pass parameters to procedures and functions using the standard Pascal syntax. For example, you write

\begin{verbatim}
  DrawRect(10, 10, 50, 100);
\end{verbatim}

In other words, you pass a value for each parameter and separate the parameters by commas.

However, some of pro Fit's predefined procedures use an “optional parameter list” for passing values, for instance

\begin{verbatim}
  CloseWindow(window 'Data 1', saveOption dontSave);
\end{verbatim}

In the above example, “window” and “saveOption” are the names and 'Data 1' and dontSave the values of the parameters that are passed to the procedure CloseWindow. In other words, each parameter has a name that must be passed in front of its value.

The advantage of this calling convention is that you can omit some parameters (if you want to use their default values). For example, you can call
CloseWindow(saveOption ask);

In this example, we have omitted the parameter “window” and use its default value (the front window) instead.

The pro Fit Programming Guide and Appendix A of this manual state which of pro Fit's predefined procedures use optional parameter lists.

**Aborting procedures, functions and programs**

Use the keyword `Halt` to immediately end the execution of a function or program. Use the keyword `Exit` for exiting from a local function or procedure to the caller.

The following is an example of a program calculating the sum of the presently selected cells in a data window. The program aborts when the selection contains empty data cells. (Note that it uses the predefined variables `selectLeft`, `selectRight`, `selectTop`, `selectBottom` which return the enclosing rectangle of the currently selected data cells.)

```plaintext
program CalcSum;
var row, col: integer; sum: real;
begin
  sum := 0;
  for col := selectLeft to selectRight do
    for row := selectTop to selectBottom do
      begin
        if not DataOK(row,col) then Halt;
        sum := sum + data[row,col];
      end;
  writeln(sum);
end;
```

The following program does basically the same as the one above, but the sum is calculated in a local function, which is aborted by `Exit`:

```plaintext
program CalcSum;
var row, col: integer; sum: real;
begin
  sum := 0;
  for col := selectLeft to selectRight do
    for row := selectTop to selectBottom do
      begin
        if not DataOK(row,col) then Halt;
        sum := sum + data[row,col];
      end;
  writeln(sum);
end;
```
program CalcSum;

function SumSelection:real;
{sums the selected data, returns}
(-1 if a selected cell is empty)
var row, col: integer; sum: real;
begin
  sum := 0;
  for col := selectLeft to selectRight do
    for row := selectTop to selectBottom do
      begin
        if not DataOK(row,col) then begin
          SumSelection := -1;
          Exit;
        end;
        sum := sum+data[row,col];
      end;
  SumSelection := sum;
end;

begin
  Writeln(SumSelection);
end;

Note: Calling Exit from the main body of a function or program has the same effect as calling Halt.

Predefined constants, functions, procedures, and operators

This section lists the operators and the most important predefined constants that are available in the definition syntax. An alphabetical list of all predefined functions, procedures and constants is found in Appendix A.

The following are the most important predefined constants:

\[ \pi \text{ (or pi)} = 3.141592\ldots \]
\[ \text{true} = 1 \]
\[ \text{false} = 0 \]
\[ \text{INF} \text{ infinity} (1/\text{INF}=0) \]

The operators are identical to those that are defined in standard Pascal. In addition, the power operator (** or ^) has been added. The operators – in ascending order of precedence – are:
= <> <= < > >= comparison, returning true (1) or false (0)
+ - or add, subtract, logical 'or'
* / and multiply, divide, logical 'and'
**, ^ power \(x ** y = x^y\)
not logical 'not'

You can change the order of precedence of the operators in the above list by using brackets: ‘(’ and ‘)’. Note that there are two ways for using the power operator \(x**y\) and \(x^y\). They are equivalent. Use whichever you prefer.

On some machines, \(x**y = x^y\) is calculated as \(\exp(y \ln(x))\). As a consequence of this, the \(x^y\) may not work for negative \(x\) and may be slow. Therefore, you should not use this notation for calculating small integer powers (for example: use \(\text{sqr}(x)\) instead of \(x**2\)).

Note for Pascal programmers: ^ is used for the power operator. proFit does not know anything about pointers and ^ is not used for dereferencing.

The order of precedence for the operators is the same as in standard Pascal. But since the proFit definition language does not distinguish between boolean and real expressions (refer to the next chapter), this order of precedence provides a dangerous pitfall

\[ a>x \text{ and } b>y \text{ will be compiled as } (a > (x \text{ and } b)) > y \]

Use brackets to clarify what you want:

\[(a>x) \text{ and } (b>y)\]

Note: In contrast to some other programming languages, all the expressions in a composite logical expression of the form

\[(condition \ 1) \text{ and } (condition \ 2) \text{ and } (condition \ 3)\]

will be evaluated, even if condition 1 returns false.

**Function definition syntax**

If you want to define a function of your own to use it for fitting or plotting, you must write a function definition. The structure of a function definition is the same as the structure of a program definition, but it can optionally contain additional information about the parameters and the contents of the parameters window. This additional information is placed right at the beginning of the function definition.

A function definition starts with the keyword function instead of program. Then follows (optional) information on the parameters and the parameters window:
function myFunc;

the name of the function, myFunc, will appear in the Func-

menu.

function myFunc(ampl, freq: real);

optional, definition of parameter names that will be used to
access parameters in the function code and as a default
parameter name in the parameters window.

description
'text1','text2';

optional, these two strings will appear in the parameters
window.

parameters 4;

optional, the number of parameters (max. 64)

defaults
a[1] := 1.2, active;
a[2] := 3.0, inactive, 'name';
a[3] := 2.0, constant;
a[4] := 1, active, 'i', 0, INF;

defaults
ampl := 1.2, active;
freq := 3.0, constant;

const
c = 2.997E8;

var
temp: extended;
myVar, t: integer;

After this, you can (optionally) define your own local procedures and functions.

Then follows the “body” of the function definition between `begin` and `end`. In this body, you must
calculate the function’s y-value from its x-value and its parameters. For this, you can use the following
variables:

\[ x \]

The input variable, the independent
variable of the function

\[ y \]

The output variable, the function’s return
value. It must be set by your function.

\[ a[1] \ldots a[n] \]

The parameters of the function. Up to 64
parameters can be used.

It is possible to define your own parameter names in the function header and to use your own names
instead of the `a[1]...a[n]`:

function foo(ampl, freq, phase: real);
begin
    y := ampl*cos(freq * x + phase);
end;

If you do this, parameters retain their numbering, defined by their sequence when you define them (ampl, freq, phase). The a[i] remain available as synonyms (a[1]=ampl, a[2]=freq, a[3]=phase) and the parameter numbers can still be used in predefined function such as SetParamName.

**Example 1:**
You want to define the function:

\[ y = a_1 \ln(a_2 x^2) \]

Your definition looks like this:

function logSquare;
begin
    y := a[1]*sqrt(a[2]*cosh(x));
end;

This is a function in its most simple form. If you work with it often, you may want to assign default values to the parameters. You will also see that \( a_2 \) should not be negative. You might therefore improve the above definition as follows:

function LogSquare;
defaults
    a[1] := 1, active, 'a1';
    a[2] := 1, active, 'a2', 0, INF;
begin
    y := a[1]*sqrt(a[2]*cosh(x));
end;

The first line after the keyword defaults defines the default value, default mode (active means that it will be varied in a fit) and name of \( a_1 \). The second lines defines the default value, mode and name as well as the lower and upper limit of \( a_2 \).

**Example 2:**

You want to define the function

\[ y = a_1 \text{sinc}(x-x_1) + a_2 \text{sinc}(x-x_2), \]

with \( \text{sinc}(x) = \frac{\sin(x)}{x} \).

The value of the function sinc is not defined for \( x=0 \), but it converges to 1 for \( x \to 0 \). When calculating sinc, we must test if its argument is 0 to handle this special case.

Since the sinc function is used twice in our example, it makes sense to put it into a local function.
function DoubleSinc;

defaults a[1] := 1, active, 'a1';
a[2] := -20, active, 'x1';
a[3] := 1, active, 'a2';
a[4] := 20, active, 'x2';

function Sinc(u: real): real; { sin(u)/u }
begin
    if u = 0 then sinc := 1 { 0/0 is illegal }
    else sinc := sin(u)/u;
end;

begin  { "body" }
y := a[1]*sinc(x-a[2]) + a[3]*sinc(x-a[4]);
end;

Alternative function syntax
pro Fit 5.0 provides an alternative method for defining the parameters of a function that allows you to use any desired (legal) name for your parameters. In this syntax, you add the parameters in parenthesis after the name of the function. Example:

function MySine(amplitude, frequency);
begin
    y := amplitude*sin(frequency*x);
end;

The first parameter in the list will correspond to parameter a[1], the second one to a[2], etc. You can then refer to each parameter either by using its name (amplitude, frequency) or by using a[i], where i is its number in the parameter list (i.e. a[1] for amplitude, a[2] for frequency).

Special procedures in a function definition
As in a program, the procedures that you define within a function definition can have any valid name you want. However, there are some reserved names for special procedures (Initialize, Check, First, Derivatives, Last) that you can define to customize and optimize your function definition. These procedures are called to perform special actions. For example, one of them (Derivatives) is called to calculate your function’s partial derivatives. Another (Check) can check a value that was entered into the parameters window.

The following describes these special procedures. A summary is provided at the end of the section.

Function Check
This procedure is only used to include some advanced features in your function. It can make function definitions more user-friendly. Check is called each time the user changes a parameter in the parameters
It can check the parameter that was changed and act accordingly. For example, it can refuse a parameter if its value is not acceptable. It can also recalculate some other parameters and cause the parameters window to be redrawn. Check can use the following predefined variables and constants:

- **pNumber**
  The number of the modified parameter

- **a[1] .. a[n]**
  The parameters as they appear in the parameters window.
  They can be checked and/or changed.

- **mode[1] .. mode[n]**
  The mode of each parameter, which can be active, inactive or constant. You can check and/or change the modes.

- **active, inactive, constant**
  These three constants can be used to be compared to or assigned to `mode[i]`.

- **check**
  The function must store its return value in this variable.

- **ok, bad, update**
  One of these three constants must be returned in the variable `check` to tell proFit if it should accept the new parameter and what it should do with the parameters window:
  - If `check`=ok, proFit accepts the new parameter.
  - If `check`=bad, proFit refuses the new parameter and shows the old one in the parameters window.
  - If `check`=update, proFit accepts the new parameter and redraws (updates) the whole parameters window. Use this feature whenever you have changed a parameter other than `a[PNumber]` in the function `check`, so that the user can see these changes.

For example your function can have two parameters that represent the same value in two different units of measurement. Check can be used to update the value of one parameter when the other parameter is changed.

*Note for advanced users: Check is not called during fitting. It is called once when fitting is complete. Don’t use Check for calculating intermediate results for later use in the evaluation of the function. You won’t notice anything wrong as long as you modify the parameters in the results window, but your function will not work when fitting. Always use the procedure First (see below) for calculating intermediate results.*

**Procedure Initialize**

This procedure is used for advanced programming. It is called exactly once after compilation of your function or program. You can use this procedure to initialize the value of variables or to write some instructions into the Results window.

**Procedure Derivatives**

This procedure is optional. If defined, it is used during fitting with the Levenberg-Marquardt algorithm. This algorithm uses the partial derivatives of the function with respect to its parameters. If you do not define the procedure Derivatives, the derivatives are calculated numerically, but this slows down
the fitting process considerably. If you notice that fitting is particularly slow, you should define this function and at least calculate some derivatives (pro Fit will still calculate numerically any derivative you don’t define). The procedure derivatives can use the following predefined variables:

- $x$ The $x$-variable, the function’s $x$-value
- $dyda[1] .. dyda[n]$ The partial derivatives. Must be set to $dyda[i] := \frac{\partial f(x)}{\partial a[i]}$ for all parameters that are not declared as constant.

Derivatives can set the values $dyda[i]$ for some or all of your function's parameters. If you don’t set a value, it will be calculated numerically. Whenever a function is used by pro Fit, a call to the procedure Derivatives is always preceded by a call to the main part of the function. Therefore you may use temporary results from the main part of the function by storing them into global variables. This decreases the number of calculations your function must perform and makes fitting faster.

Example: You want to fit the function $y = a_1 \cdot \sinh(x)$, the partial derivative of which is $\frac{\partial y}{\partial a_1} = \sinh(x)$. Calculating $\sinh(x)$ can take a lot of time, especially when you are working on a slow computer. To avoid calculating expressions twice, you can save temporary results in the main part of the function to use them later in the procedure Derivatives:

```pascal
function MySinh;
var t: real;

procedure Derivatives;
begin
  dyda[1] := t; { use t calculated in body}
end;

begin {the function’s body}
  t := sinh(x); {save sinh for derivatives}
  y := a[1]* t;
end;
```

**Procedure First**

This procedure is used for advanced programming. It is called whenever the parameters of a function have been changed – before the body (main part) of the function is called. The body of a function will never be called without first having been called beforehand.

The procedure first can use the following variables:


The procedure First is mainly used for accelerating calculations that do not depend on the input value $x$. This can make a fit considerably faster. First should calculate all expressions that appear in a function but that do not depend on $x$:
To calculate the mean deviation $\chi_R$ during fitting, proFit calculates the function for each data point $(x_i, y_i)$. This may involve up to several thousand executions of the body of the function definition. If your function definition contains expressions that do not depend on the value of $x$ (such as $\sin(a[2]-a[3])$), they will still be recalculated for each new value of $x$, wasting a lot of time. You can evaluate these expressions in the procedure `First` and store their values in variables used by the main part of the function.

Another use of the procedure `First` is to perform some task before proFit starts to use a function. This is less common for functions defined inside proFit but it is often used when defining external modules (see Chapter 10) that need to allocate and deallocate memory only used while a function is running. The following is a small example of this particular use of `First` that also demonstrates a possible use of the procedure `Last`:

```plaintext
function Foo;
var
  firstTime: boolean;
  data11: extended;
  sinDiff: extended;
  multiplier: extended;
procedure Initialize;
begin
  firstTime:=true; {initialize to true}
end;

procedure First;
begin
  if firstTime then
  begin {the statements in this block are }
    {executed only once, before any other}
    {function call.}
      firstTime:=false;
      data11:=data[1,1];
      {perform here other calculations that}
      {do not depend on parameter values}
      {and do not depend on x}
    end;
  sinDiff:=sin(a[2]-a[3]);
  multiplier:=data11*a[1];
  {perform here other calculations that do not}
  {depend on x but depend on the parameter}
  {values.}
end;

procedure Last;
begin
  {finished using function.}
  firstTime:=true; {reset firstTime to true }
end;

begin
  {the main part of the function.}
  y := multiplier * sin(x)/sinDiff;
end;
```
The above example uses the procedure Last:

**Procedure Last**

This is also a procedure used for advanced programming. It is called when all calculations, fitting, etc. are completed. It is the last piece of function code called by proFit before returning control to the user. Last can be used to clean up, to make final calculations, or to re-initialize some variables to their starting values, as is shown in the example above. Last can also be used to print some special messages or results in the results window or to alert the user of some event. For example, you can let your machine beep when fitting is finished:

```pascal
procedure Last;
begin
  beep;
end;
```

**Summary**

The following table summarizes the special procedures listed above:

<table>
<thead>
<tr>
<th>name</th>
<th>called when</th>
<th>predefined variables and constants</th>
</tr>
</thead>
<tbody>
<tr>
<td>Check</td>
<td>whenever parameters are changed by user</td>
<td>pNumber, a[1]..a[n], mode[1]..mode[n], active, inactive, constant</td>
</tr>
<tr>
<td></td>
<td></td>
<td>check, ok, bad, update</td>
</tr>
<tr>
<td>Initialize</td>
<td>once after compilation</td>
<td>a[1]..a[n]</td>
</tr>
<tr>
<td>First</td>
<td>whenever parameters are changed (e.g., during calculations)</td>
<td>a[1]..a[n]</td>
</tr>
<tr>
<td>Derivatives</td>
<td>during fitting, after calling the function’s main part</td>
<td>x, a[1]..a[n], dyda[1]..dyda[n]</td>
</tr>
<tr>
<td>Last</td>
<td>when calculations are through</td>
<td>a[1]..a[n]</td>
</tr>
<tr>
<td>function’s main part</td>
<td>during fitting and other calculations</td>
<td>x, y, a[1]..a[n]</td>
</tr>
</tbody>
</table>

Note that in addition to the specially predefined variables and constants, all procedures (as well as the function’s main part) can use the general predefined variables, constants, functions and procedures listed in Appendix A.

**General comments about programming**

**Types**

The proFit definition language supports the following types for variables:
1. Simple numeric types:

real, extended, integer, longint, or boolean. These types are not distinguished by pro Fit and are implemented as floating point numbers.

The boolean value true is represented by the real value 1.0 and false by 0.0. All non-zero values are interpreted as true in a boolean expression.

Most Pascal compilers on the Macintosh distinguish between the floating point types extended, double and real, which have different accuracy. All simple number types of the pro Fit definition language have extended accuracy. The accuracy and range of numerical values in pro Fit is given in Appendix C.

2. Complex type:

The Complex data type is used to represent complex floating point values having a real and an imaginary part. Example:

```pascal
program ComplexTest;
var c: Complex;
begin
  c := -1;
  writeln(sqrt(c));
end;
```

The above program recognizes that sqrt is called with a complex argument. Therefore, a complex version of the square root function is used, which can handle sqrt(-1). The output of the above program is:

```
0.000 + i * 1.000
```

Type conversion from real (or other simple numeric types) to complex is automatic. For converting complex numbers to real, use one of pro Fit's predefined functions, such as abs, phase, re, im (see Appendix A). To define complex numbers, use the predefined function compl or the predefined constant ii, which fulfills \( \text{sqr}(ii) = -1 \).

All predefined functions in pro Fit, such as sin, cos, gamma, erf, etc. automatically become complex valued functions if they notice that their argument is a complex number, and return complex numbers as a result.

3. String and char types:

Use the type Char for representing simple characters, String for representing strings of up to 255 characters. Example:
program StringAndCharTest;
    var c: Char;
        s: String;
begin
    c := 'x';
    s := 'hi there';
    writeln(c); {writes "c"}
    writeln(s); {writes "hi there"}
    s := s + ', Joe'; {s now is "hi there, Joe"}
    c := s[2];  {c now is "i"}
end;

Conversion between Strings and Chars is automatic. For conversion between Char (ASCII values) and
Integer use the functions Ord and Chr. For conversions between Strings and numbers, use
NumberToString and StringToNumber.

To access the n-th character in a string s, use s[n]. In other words, strings are arrays of type char.

The following is a list of the most important functions for working with strings:

- **Length**: Returns the length of a string.
- **Pos, Delete**: Find/delete a sub-pattern in a string
- **UpperString, LowerString**: Convert between upper and lower case strings.

See Appendix A for a complete list.

**Arrays**

pro Fit allows the definition of one-dimensional arrays. The following syntax is used:

```pro Fit
var name: array[minIndex..maxIndex] of type;
```

Where *name* is the name of the array, *minIndex* is its minimum index, *maxIndex* is its maximum index,
*type* its type. Since types are ignored by pro Fit, you can omit "of type" in the declaration.

To access an array, use the syntax:

```pro Fit
name[index]
```

Example:

```pro Fit
var arr1: array[1..10] of real;
    arr2: array[0..100];
    i
... for i := 1 to 10 do arr1[i] := 0;
    arr2[33] := 22.1;
```

Note: the maximum size of all variables in a variable list is limited to 32 kBytes. This limits the size of an
array to about 2700 entries for the FPU version of pro Fit, to about 3200 entries for the non-FPU
version, and to about 4000 entries for the Power Macintosh version.

Multi-dimensional arrays are not supported.
**The compiler**

When adding a definition to the list of functions or programs of proFit, the definition text is translated into machine code that can be executed by your computer. This results in a very fast execution speed of programs and functions.

![Diagram](image)

The translation of your definitions into machine code is carried out when you choose Add to Menu from the Prog menu or if you click the button "Add" in the toolbox of the function window.

Any changes that you make to your definition after compilation will not affect the function or program as it was added to proFit’s menus. To update your changes, you must choose Add to Menu again.

**Debugging**

proFit offers a special debugging facility which helps you track down run time errors in your code. If you check **Debug** in the function menu or click the small check box in the header of the function window and compile your definition (‘Add to Menu’), special instructions are added to its code. They allow to identify the position where a run-time error (such as sqrt(-1)) occurred. These additional instructions make the execution of your program or function slower, so you should uncheck Debug when you have finished correcting the function.

If you check debug and recompile your definition (Add to Menu from the Prog menu), the next time the error occurs, its position in your definition will be highlighted.

Note that a function compiled with debug option on appears **outlined** in the Func menu.

**Comparison to standard Pascal**

The programming language used to define functions and programs in proFit is closely related to the Pascal programming language. However, to keep it simple and to allow the generation of fast code, some restrictions are present. The most important differences to standard Pascal are:

- You cannot define your own **data types**.
• All numeric types (except complex) are interpreted as floating point numbers. Boolean expressions are evaluated as floating point numbers (a 0.0 representing false, any non-zero value representing true). No records, structures, or pointers are supported.
• Arrays are one dimensional.
• Case statements are not supported.
• Nested declarations of functions or procedures are not supported.

External functions and programs
Even though pro Fit’s definition language is very powerful, it does not offer the full versatility of a special purpose programming language. It only supports one dimensional arrays (except data[i, j]), records, pointers, etc. In addition, it does not support access to the Macintosh toolbox routines. If you do need any of these features or if you want to write a large program or function for pro Fit where execution speed is crucial, you should write your definition in any compiler of your choice and add the generated code to pro Fit. This process is called ‘writing an external module’. See Chapter 10, “Working with external modules” for details.

Using pro Fit Modules
After you have added a function or program to the menus, you can save its compiled code as a separate file for later use. This file is called a module because it is a self-contained unit that can be used to customize pro Fit’s menus.

You can also create modules in an external compiler. These modules are called external modules. pro Fit comes with a set of external modules for different tasks. You can use them to add functionality to your copy of pro Fit according to your needs. See Chapter 10, “Working with external modules” for an explanation on how to build external modules.

This section explains how to use such modules.

Saving functions and programs
To save a function or program as a module, choose Save Module from the Customize menu to see a submenu with all the functions and programs that can be saved as modules.

This sub-menu has two sections divided by a horizontal line. The first section lists the functions, the second section the programs. Choose the function or program you want to save as a module, and pro Fit will ask you where you want to save it. Note that you can only save functions and programs that you compiled in pro Fit – you cannot save built-in functions or external modules.

The resulting file is a pro Fit document. You can load it by using the Load Module command or by double clicking it from the Finder.

Loading functions and programs
Choose “Load Module...” from the Customize menu to load a module. You are asked to locate the module.
The command “Load Module...” can also be used to load compiled Apple Scripts. See Chapter 11, “Apple Script” for details.

Removing functions and programs from the menus

To remove a function or a program (or an Apple Script) from pro Fit’s menus, choose “Remove from Menu” from the Customize menu. A submenu lists all the functions and programs that can be removed from the menus. Select the name of the function or of the program you want to remove.

Note: you cannot remove any of pro Fit’s built-in functions (Spline, Polynom, etc.).

Loading modules automatically on startup

Imagine you have one or more modules or Apple Scripts that you use often. You can make them available automatically whenever you start pro Fit.

Put the modules you want to add permanently to pro Fit into a folder named “pro Fit Modules”. This folder must be located in the same folder as pro Fit’s or in the Preferences folder of your System Folder. (When you create the folder “pro Fit Modules”, type the name exactly as given here, otherwise pro Fit will not find it.)

Whenever pro Fit starts up, it checks if a folder named “pro Fit Modules” is located in the same folder as the application itself and tries to load all modules it finds there. Then pro Fit looks for a folder “pro Fit Modules” in the Preferences folder of the System folder and again tries to load all modules it finds there.

If you are running pro Fit directly from a server, the modules found in the “pro Fit Modules” folder in the application folder on the server will be available to all users, the modules in the “pro Fit Modules” folder of your system’s Preferences folder will only be available to you.

Loading a set of modules together with a new preferences file

In multi-user environments different users might want to use the multi-preferences-file mechanism provided by pro Fit.

The pro Fit preferences file holds the default settings and other information for many pro Fit’s options. Different users may want to use different preferences files. pro Fit normally uses the preferences file found in the Preferences folder inside your System folder. It is possible, however, to start pro Fit by double clicking another preferences file, or to switch to a new preferences file while pro Fit is in use by choosing Preferences... from the File menu. This allows each user to use his own set of preferences. See Chapter 13, “Preferences” to learn how to use preferences files.

pro Fit provides a mechanism that allows users to load their favorite modules together with their preferences file: whenever a preferences file is opened, pro Fit looks for a folder named “pro Fit modules” in the same folder as the preferences file and loads all the modules it contains.

To take advantage of this mechanism, simply put your preferences file and pro Fit Modules folder inside a common folder.
Whenever proFit opens the preferences file, it also loads all the modules found in the “pro Fit modules” folder.
10 Working with external modules

This chapter explains how to add external modules to proFit. External modules are documents containing the computer code for a function or program.

proFit comes with a number of ready-to-run external modules containing useful functions or programs. The next section tells you how you add them to proFit.

See the sections “Creating an external module” and “Writing an external module” for a detailed explanation of how to create your own external module.

Loading an external module

To add an external module to proFit:

1. Select Load Module from the Misc menu.

   You are asked to locate your module:

2. Choose the external module you want to load and click “Open”.

   proFit checks if an external module can be found in the file you have selected. If yes, it is loaded. If the module is a function, it is added to the Func menu. If it is a program, it is added to the Misc menu.

Instead of loading a module by choosing Load Module, you can double-click its file. (For this, the ‘file type’ and ‘creator’ of the file must be ‘ftCD’ and ‘NLft’, respectively).

An important note for Power Macintosh users:

If you have loaded a module and you subsequently change it (e.g. by recompiling it) you must remove the loaded module from proFit before loading its new version.

To load your modules automatically at start-up, put them into a folder called “pro Fit Modules” located in the same folder as the application itself or in the Preferences folder of the System folder. See the end of Chapter 9, “Defining functions and programs”, for a more detailed discussion of how to work with proFit modules.

The rest of this chapter explains how you can write external modules using your own compiler.

Creating an external module

You need the following to write an external module:

- Some experience in programming.
- A compiler (such as Think® Pascal, Think C, Symantech® C++, Metrowerks® Pascal, Metrowerks® C/C++, or the Macintosh Programmer Workshop™ (MPW)). Your compiler must support the generation of code resources (for 68k computers) or shared libraries (for Power Macintosh).
To create an external module, proceed as follows:

1. **Choose a stationery file to start from and save it under a name of your choice**

   In your proFit distribution package, you will find a number of stationery (template) files that contain “empty” functions or programs:
   - ProgramTemplate.c for creating an external program in C
   - FunctionTemplate.c for creating an external function in C
   - ProgramTemplate.p for creating an external program in Pascal
   - FunctionTemplate.p for creating an external function in Pascal

   Open the stationery from your programming environment and save it under a name of your own (e.g. “xxx.c”).

   Note: you should never modify the files ProgramTemplate.c/p or FunctionTemplate.c/p directly – always work on a copy.

2. **Complete the code**

   Since the stationery files only contain empty routines, you must fill in your code. The following section “Writing external modules” tells you how to do this.

3. **Build your code**

   Note that in addition to the code defined in your file, you must also compile the file “proFit_interface.c” or “proFit_interface.p”, respectively, which contains glue code for calling proFit’s routines.

   If you are using C, please note that “proFit_interface.c” as well as your own source file xxx.c #include the files “proFit_interface.h” and “proFit_paramBlk.h”. Therefore, these files must be in the “search path” of your compiler (they could e.g. reside in the same folder as the ...c files).

   If you are using Pascal, note that your own source file “uses” the unit proFit_interface defined in proFit_interface.p.

4. **Build the module**

   The module should be created in a file having the type “ftCD” and the creator “NLft”.

   If you are building a module for a **Power Macintosh**:

   Set your compiler/linker to build a “shared library” or “import library”. The entry point of your module is the function “main”, which must be exported from your library. Consult your compiler’s manual on how to export symbols from a library. (The example source files contain compiler options for exporting “main” in one of Metrowerks’ compilers. Note that these compiler options may not work correctly with other compilers.)

   If you are building a module for a **68k Macintosh** (i.e. an “old” non-Power Macintosh):

   Set your compiler/linker to build a code resource of type “NLft”, with a resource ID greater or equal to 128.

   The entry point to your code must be at the beginning of the code resource.
If you are creating a module for the FPU-version of proFit, set your compile options to create code using the FPU with 12 byte ‘extended’ (Pascal) or 'double' (C) variables. If you are creating a module for the non-FPU option of proFit, you must set your compile options to not create code for calling the FPU and to use 10 byte ‘extended’ (Pascal) or 'double' (C) variables.

4. **Link the module to proFit**

To do this, either double-click the file you have built or load it from proFit by choosing Load Module... from the Misc menu.

The following gives some hints for creating modules with some of the most common compilers. Note that there are sample “project” and “make” included with the pro Fit package.

**Metrowerks Code Warrior Pro for Power Macintosh**

If you are using Metrowerks Code Warrior Pro or the Power Macintosh, create a project with the files:

- MathLib
- MSL RuntimePPC.lib
- InterfaceLib
- proFit_interface.c
- xxx.c

MathLib, MSL RuntimePPC.lib and InterfaceLib came with your copy of the Metrowerks C/C++ compiler, proFit_interface.c can be found in your distribution package. “xxx.c” is your source code created from “ProgramTemplate.c” or “FunctionTemplate.c”.

Make sure that the files “proFit_interface.h” and “proFit_paramBlk.h” reside in the same folder as your project.

Many mathematical functions (such as sin(), log()) are not part of the standard C function set. In order to use them, use <fp.h> and <fenv.h> (the header files for the Power Macintosh numerics environment).

**Metrowerks Code Warrior Pro for 68k**

If you are using Metrowerks Code Warrior Pro for 68k, create a project with the files:

- MathLib68K (..).A4.Lib
- MSL C.68K (..).A4.Lib
- MSL Runtime68K.A4.Lib
- MacOS.lib
- proFit_interface.c
- xxx.c

"(..)" stands for:
- "(2i)" if you are building a module for pro Fit (68k)
- "(2i_F)" if you are building a module for pro Fit (fpu)
The library files came with your copy of the Metrowerks C/C++ compiler. proFit_interface.c can be found in your distribution package. “xxx.c” is your source code created from “ProgramTemplate.c” or “FunctionTemplate.c”.

Make sure that the files “proFit_interface.h” and “proFit_paramBlk.h” reside in the same folder as your project.

Many mathematical functions (such as sin(), log()) are not part of the standard C function set. In order to use them, use <fp.h> and <fenv.h> (the header files for the Power Macintosh numerics environment).

Note: If you cannot find some of the libraries (such as “MSL C.68k (2i-F).A4.Lib”), you can rebuild them using the application “Build MSL Libraries”, which you will find in the folder “(Build Scripts)” of the Metrowerks Standard Library.

In the target settings “68K Target” of your project, you must set the Project Type to “Code Resource”, Creator to “NLft”, Type to “ftCD”, ResType to “NLft”, ResID to any value larger than 127. Leave SegType empty. Check “Extended Resource”. Set Header Type to “Standard”.

In the target settings “68K Processor” you must uncheck “4-Byte Ints” and “8-Byte Doubles”. Set Floating Point to “SANE” if you are building a non-FPU module or to “68881” if you are building an FPU module.

**Think C or Symantec C++ (for 68k)**

If you are using Think C or Symantec C++ (Version 7.0.x for 68k), create a project containing the files:

- MacTraps: Glue for many Macintosh system routines
- proFit_interface.c: Glue for interfacing pro Fit.
- xxx.c: your code

“MacTraps” came with your copy of Think C and proFit_interface.c can be found in your distribution package. “xxx.c” is your source code created from “ProgramTemplate.c” or “FunctionTemplate.c”.

Make sure that the files “proFit_interface.h” and “proFit_paramBlk.h” reside in the same folder as your project.

Many mathematical functions (such as sin(), log()) are not part of the standard C function set. In order to use them, add the files math.c and errno.c (that came with Think C/C++) to your project and #include the file <math.h> in your source file xxx.c.

Set the project type to "Code Resource" to create a code resource of type 'NLft' with an ID ≥ 128. Set the file type to “ftCD”, the creator to “NLft”.

**Think Pascal (for 68k)**

If you are using Think Pascal 4.0, create a project with the files:

- DRVRRuntime.lib: Glue for many Macintosh system routines
- Interface.lib: Glue for many Macintosh system routines
- proFit_interface.p: Glue for interfacing with pro Fit.
- xxx.p: your code
“DRVRRuntime.lib” and “Interface.lib” came with your copy of Think Pascal, “proFit_interface.p” can be found in your distribution package. “xxx.p” is your source code created from “ProgramTemplate.p” or “FunctionTemplate.p”.

In addition, you may want to add the SANE numerical environment because it defines many mathematical functions not available in standard Pascal. To do so, add the following files to your project:

\[
\begin{align*}
\text{SANELib881.lib} & \text{ or } \text{SANELib.lib} \\
& \text{(with FPU)} \\
& \text{(without FPU)} \\
\text{SANE.p} & \text{ Interface for the SANE routines}
\end{align*}
\]

All these files come with your compiler.

Set the project type to “Code Resource” to create a code resource of type 'NLft' with an ID $\geq 128$. Set the file type to “ftCD”, the creator to “NLft”.

If you are creating a module for the non-FPU version of proFit, you must set your compile options so that they do not create code for the FPU. If you are creating a module for the FPU-version of proFit, set your compile options to create code calling the FPU (and to generate 12 byte extended (or ‘double’ in C) variables).

**MPW C/C++ or Pascal for 68k**

If you are using the Macintosh Programmers Workshop MPW for compilation on a 68k CPU, you must make sure that the function main (which is defined in proFit_interface.c for C modules and in your own file xxx.p for Pascal modules) is the first function in your build order. This is important, because when calling your code, proFit starts executing your code resource from its beginning. Therefore, your code resource should start with the function main or with a jump to this function. Most development environments add such a jump automatically – MPW doesn’t. Therefore:

- If you are writing an external module in C, make sure that proFit_interface.o is the first file being linked.
- If you are writing an external module in Pascal, make sure that your own file xxx.o (which you have created from ProgramTemplate.p or FunctionTemplate.p) is the first file to be linked, because it defines main.

**MPW C/C++ for Power Macintosh**

If you are using the MPW compiler for the Power Macintosh from the RISC SDK, you will find an example for a “make” file on your distribution disks.

**Other compilers**

The distribution disks contain several examples of external modules for other compilers.
Writing an external module

The following comments apply to Power Macintosh as well as 68k modules.

Note once again that the size of the floating point type ‘extended’ (or double in C) must be the correct one for the version of pro Fit you are working with. For the FPU version it is 12 bytes, for the non-FPU version 10 bytes, and for the Power Macintosh version 8 bytes.

To write your external modules, start from a stationery file (ProgramTemplate or FunctionTemplate) as shown above. These files contain some routines that you will have to modify.

Routines to be modified

The following table lists the routines defined in ProgramTemplate.c/p and FunctionTemplate.c/p that can or should be modified by the user. Functions or procedures that are only used by advanced programmers are marked with a †:

<table>
<thead>
<tr>
<th>function name</th>
<th>modify if defining a</th>
</tr>
</thead>
<tbody>
<tr>
<td>SetUp</td>
<td>program or function</td>
</tr>
<tr>
<td>CleanUp †</td>
<td>program or function</td>
</tr>
<tr>
<td>InitializeProg †</td>
<td>program</td>
</tr>
<tr>
<td>Run</td>
<td>program</td>
</tr>
<tr>
<td>InitializeFunc †</td>
<td>function</td>
</tr>
<tr>
<td>Func</td>
<td>function</td>
</tr>
<tr>
<td>Derivatives</td>
<td>function</td>
</tr>
<tr>
<td>First †</td>
<td>function</td>
</tr>
<tr>
<td>Check †</td>
<td>function</td>
</tr>
<tr>
<td>Last †</td>
<td>function</td>
</tr>
</tbody>
</table>

In the following section, we will first describe the routines SetUp and CleanUp that are used for both types of modules. Then we discuss the routines only used in external programs, then the routines only used in external functions.

Note for Pascal programmers:
In ProgramTemplate.p and FunctionTemplate.p you will find a procedure with the name main. Leave this procedure unchanged – it provides the glue between pro Fit and your routines.

Note for C programmers:
The following function definitions are given in Pascal. If you are programming in C, you should keep in mind that wherever a var parameter is passed in Pascal, the corresponding pointer is passed in C. If the description text e.g. says that “a value of 1.0 must be returned in the variable y”, the C code should assign 1.0 to *y, i.e. *y = 1.0. Further differences between the definitions in C and Pascal will be highlighted along the way.

All the following routines have a parameter called pb. It is a pointer to a record (struct in C) of type ExtModulesParamBlock. Most users won’t need the information stored in it. Advanced programmers can refer to the section “Global variables” for more information about data to be accessed through pb.
Routines to be defined in functions and programs

**SetUp**

```pascal
procedure SetUp(var moduleKind: integer; var name: Str255;
                var requiredGlobals: longint; pb: ExtModulesParamBlockPtr);
```

This routine is called when your module is linked to proFit. It must return the following values:
- **moduleKind** must be set to the constant `isProgram` if your module is an external program, and to `isFunction` if your module is an external function.
- **name** must be set to the name of your module. If you are programming in Pascal, you can simply assign a string to it:
  ```pascal
  name := 'myName'
  ```
  If you are programming in C, you must make sure that you return a Pascal string. For this purpose, you can use the function `SetPascalStr` that is defined in `proFit_interface.c`:
  ```c
  SetPascalStr(name, "\pmyName", 255);
  ```
  (The last parameter is the maximum length of the resulting string.)
- **requiredGlobals** should usually be set to 0. Advanced programmers can set it to the size (in bytes) of a global data buffer they want to have allocated. If `requiredGlobals` is returned with a value > 0, proFit allocates a block with the corresponding number of bytes and stores a pointer to it in `pb^.globals` (in C: `pb->globals`). `pb` is a pointer to a record called `ExtModulesParamBlock` and is passed to all routines called by proFit.
  Note that memory allocated in this way is deallocated automatically when your module is unlinked from proFit – you must not deallocate this memory yourself!

**CleanUp**

```pascal
procedure CleanUp(pb: ExtModulesParamBlockPtr);
```

CleanUp is called when proFit is quitting or when your module is removed from proFit. In most cases, you won’t have to do anything here. Advanced programmers may wish to deallocate some special memory, to close a port or to clean up other stuff here.

Routines to be modified in external programs only

**InitializeProg**

```pascal
procedure InitializeProg(pb: ExtModulesParamBlockPtr)
```

This routine is called before a program is run for the first time. Most users can leave it empty. Advanced programmers may wish to allocate some memory, open a port, initialize global (static) variables, etc. here.

**Run**

```pascal
procedure Run (pb: ExtModulesParamBlockPtr)
```

This routine is called when your program is executed. It should hold your program’s main code.

Routines to be modified in external functions only

An important note about parameter indices: When accessing arrays that hold values, names, etc. of the parameters, such as `a[i]`, `a0.names^[i]`, `mode[i]`, `dyda[i]`, the index i ranges from 1 to 64 in Pascal, but from 0 to 63 in C.
This routine is called once after your external function has been linked to proFit. It must return some default values and information about the function. Advanced programmers may also use it for initialization of global (static) variables, memory allocation, etc.

InitializeFunc should return the following data in its parameters:

- **hasDerivatives** must be set to `true` if you want to calculate some derivatives of your function with respect to its parameters yourself (in the function Derivatives described below). Any derivative you don’t calculate will have to be calculated numerically by proFit. If you set `hasDerivatives` to `false`, all derivatives will be calculated numerically and the function Derivatives will be ignored. (The derivatives are used for nonlinear fitting.)
- **descr1stLine, descr2ndLine**: These two strings are displayed in the parameters window and should give a short description of your function. (C programmers should use the function SetPascalStr described under SetUp, above, for setting these strings.)
- **numberOfParams**: Here you should return the number of parameters of your function (up to 64).
- **a0**: This is a record (in C: a pointer to a struct) that defines the default values, modes, names and limits of your parameters. You can leave this record unchanged if you want to use the default values. The following table lists the values that can be set in a0 for each parameter i:

<table>
<thead>
<tr>
<th>Pascal notation 1)</th>
<th>C notation 2)</th>
<th>contains</th>
</tr>
</thead>
<tbody>
<tr>
<td>a0.value^[i]</td>
<td>(*a0-&gt;value)[i]</td>
<td>Default value</td>
</tr>
<tr>
<td>a0.mode^[i]</td>
<td>(*a0-&gt;mode)[i]</td>
<td>Default mode, set to active (varied during fitting), inactive (not varied during fitting), or constant (cannot be fitted)</td>
</tr>
<tr>
<td>a0.name^[i]</td>
<td>(*a0-&gt;name)[i]</td>
<td>Parameter name, a Pascal string of length <code>maxParamLength</code>. 3)</td>
</tr>
<tr>
<td>a0.lowest^[i]</td>
<td>(*a0-&gt;lowest)[i]</td>
<td>The lower limit for a parameter. By default, this value is <code>-INF</code>.</td>
</tr>
<tr>
<td>a0.highest^[i]</td>
<td>(*a0-&gt;highest)[i]</td>
<td>The upper limit for a parameter. By default, this value is <code>INF</code>.</td>
</tr>
</tbody>
</table>

1) In Pascal, indices for these arrays run from 1 to 64
2) In C, indices for these arrays run from 0 to 63
3) C programmers should set the name by calling the function SetPascalStr with a maximum string length of `maxParamNameLength`. Example:

```
SetPascalStr(((*a0->name)[0],"\pname", maxParamNameLength);
```

This procedure is called to calculate the return value of your function. It has the following parameters:

- **x**: The function’s independent variable.
- **a**: The function’s parameters `a[i]`. Note that the index `i` ranges from 1 in Pascal but from 0 in C.
- **y**: The function’s return value to be calculated from `x` and `a`.

---

10-8 Working with external modules
**Derivatives**

```
procedure Derivatives (x: extended; a: ParamArray; var dyda: ParamArray; pb: ExtModulesParamBlockPtr);
```

This routine calculates the partial derivatives of your function with respect to its parameters. You can leave this routine empty if you don’t need it, or you can calculate only some derivatives. You don’t need to calculate all of them. proFit will check if you did not calculate a derivative and will calculate it numerically. Set `hasDerivatives` to false in `InitializeFunc` if you are sure that you will never want to calculate any derivatives yourself. (Note that a call of `Derivatives` with a given x-value is always preceded by a call of `Func` with the same x-value – therefore, you might save a temporary result in `Func` for later use in `Derivatives`. See also Chapter 9, “Defining functions and Programs”.)

Parameters:
- `x`: The function’s independent variable.
- `a`: The function’s parameters `a[i]`. Note that the index `i` ranges from 1 in Pascal but from 0 in C.
- `dyda[i]`: The partial derivatives to be returned.

**First**

```
procedure First (a: ParamArray; pb: ExtModulesParamBlockPtr);
```

This routine is called whenever the parameters `a` have changed before `Func` is called. In most cases, you can leave it empty. Advanced programmers can use `First` for speeding up your function by evaluating temporary results that only depend on your function’s parameters but not on its x-value (for more information: see the description of `First` in Chapter 9, “Defining functions and Programs”).

Parameters:
- `a`: The function’s parameters `a[i]`. Note that the index `i` ranges from 1 in Pascal but from 0 in C.

**Check**

```
function Check (ParamNo: integer; var a0: DefaultParamInfo; pb: ExtModulesParamBlockPtr):CheckPAnswer;
```

Check is called whenever the user has entered a value in the Parameters window. In most cases, you can leave Check empty, returning the value `good`. Advanced programmers can use it for improving the parameters window’s user interface. Applications of Check are described in Chapter 9, “Defining functions and Programs”).

Parameters:
- `paramNo`: This is the index of the parameter that the user has changed (1..64 in Pascal, 0..63 in C).
- `a0`: This is a record (in C: a pointer to a struct) that defines the default values, modes, names and limits of your parameters as they appear in the parameters window. The values that you can access or change in this data structure are listed under the routine `InitializeFunc` above.

Check should return one of the following values:
- `good` if the new parameter is to be accepted
- `update` if the new parameter is to be accepted but the parameters window must be redrawn (because Check changed some values in `a0`)
- `bad` if the new parameter cannot be accepted.

**Last**

```
procedure Last (pb: ExtModulesParamBlockPtr);
```

This routine is called whenever an operation that has used your function (such as a command for fitting) is done. In most cases, you can leave this procedure empty. Applications of `Last` are given in Chapter 9, “Defining functions and Programs”.

---

Working with external modules 10-9
Predefined constants and types

When writing an external module, you can (and must) use several predefined constants, types and procedures (or functions). In Pascal, they are defined in the interface of the file profiFile_interface.p. In C, they are defined in profiFile_interface.h and profiFile_paramBlk.h. This section describes some of the most important things defined in these files.

The definitions in these files should not be changed. Doing so might cause incompatibilities with the present or future versions of proFit.

General remarks:

- **Strings** passed between proFit and an external module are always Pascal strings (and not C strings). If you are programming in Pascal, you won’t have any problems with this. If you are programming in C, you must remember that a Pascal string must be introduced by "\p" (example: "\pMyString"). For assignments, you can use the function SetPascalString described earlier in this chapter.

- **Records (structs)** passed between proFit and an external module always use “68k-alignment”. Therefore, for compatibility with Power Macintosh compilers, definitions for C structs are always preceded by

  ```c
  #if defined(powerc) || defined (__powerc)
  #pragma options align=mac68k
  #endif
  ```

  and followed by

  ```c
  #if defined(powerc) || defined (__powerc)
  #pragma options align=reset
  #endif
  ```

- **Parameter indices** under Pascal always run from 1 to maxNrParams, in C they run from 0 to maxNrParams-1.

The following lists the most important constants and types.

(The numbers in curly brackets give the offset and size of some records and their components. Pascal or C programmers won’t need this information. It is provided for porting the records to another programming language. Numbers followed by (N) give the length for the non-FPU 68k version, numbers followed by (F) for the FPU 68k version, and numbers followed by (P) for the PowerPC version.)

```c
const
  versionNumber = 1;
  maxNrParams = 64;
  maxParamNameLength = 31;
  maxNrInputValues = 6;
  isFunction = 1;
  isProgram = 2;

type
```

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inputRec = packed array[1..maxNrInputValues] {size 48}
  of record
    x: ^extended; {offset 0, size 4}
    s: ^str255; {offset 4, size 4}
  end; {field size 8, offset 8, #fields 6}

checkPAnswer = (update, good, bad); {size 1}
  {update=0, ok=1, bad=2}

ModeType = (active, inactive, constant); {size 1}
  {active=0, inactive=1, constant=2}

ParamName = string[maxParamNameLength]; {size 32}

ParamArray = array[1..maxNrParams] of extended;
  {size 640(N)/768(F)/512(P)}
    {field size 10(N)/12(F)/8(P)}
    {offset 10(N)/12(F)/8(P)}
    {#fields 64}

ParamNameArray = array[1..maxNrParams] of ParamName;
  {size 2048}
    {field 32, offset 32, #fields 64}

ParamModeArray = array[1..maxNrParams] of ModeType;
  {size 64}
    {field size 1, offset 1, #fields 64}

DefaultParamInfo = record
  value: ^ParamArray; {offset 0, size 4}
  lowest: ^ParamArray; {offset 4, size 4}
  highest: ^ParamArray; {offset 8, size 4}
  mode: ^ParamModeArray; {offset 12, size 4}
  name: ^ParamNameArray; {offset 16, size 4}
end;
DefaultParamInfoPtr = ^DefaultParamInfo; {size 4}

type
  {parameters for all functions calling pro Fit}
ExtModulesParamBlock = record
  RunTimeProcPtr: Ptr; {offset 0, size 4}
  globals: Ptr; {offset 4, size 4}
  versionNumber: integer; {offset 8, size 2}
  moduleKind: integer; {offset 10, size 2}
  codeType: integer; {offset 12, size 2}
  name: Str255; {offset 14, size 256}
  requiredGlobals: longint;
  v: array[1..30] of extended; {offset 270, size 4}
end;
The most important constants and types are the following:

- **versionNumber** is the current version of the proFit interface.
- **maxNrParams** is the maximum allowed number of parameters, **maxParamNameLength** is the maximum length of a parameter name for a function.
- **isFunction**, **isProgram** are possible types of a module to be returned by SetUp described above.
- **maxNrInputValues** is the maximum number of input variables for the function **InputBox** described below.
- **inputRec** is the parameter to the function **InputBox** described below.
- **checkPAnswer** is the type of the return value of the function **check** described above.
- **ModeType** describes the mode of a parameter, as explained in Chapter 9, “Defining functions and programs”.
- **ParamName** holds the name of a parameter as it appears in the parameters window.
- **ParamArray**, **ParamModeArray** and **ParamNameArray** are the arrays with the parameters’ values, modes and names.
- **DefaultParamInfo** contains all the arrays with the initial values, limits, modes, and names of the parameters.
- **ExtModulesParamBlock**: This record contains low-level parameters to be passed between an external module and proFit. In most cases, you will not need the information stored here. There are only two fields that you might find useful: **v** and **globals**. These are described in the following section “Global variables”.
- **globalScratch**: A pointer to a data area shared by all modules, internally defined functions and programs, as well as external modules. From programs and functions defined within proFit, you can access this area through the predefined array **globalData[0..99]**.
- **moduleFile**: A file specifier for the file that the module is in. You can e.g. use this specifier for accessing a resource stored in your module.

### Global variables

Global variables (or static variables, as they are often called by C programmers) are variables that remain statically in memory. Their values are preserved between individual calls to your module.
If you are programming for the Power Macintosh, you can define global variables in the way you are used to: In Pascal, you declare them globally within your unit – in C, you declare them outside your functions or, if you declare them inside a function, you declare them as static.

If you are programming for a 68k Macintosh, there is no easy, compiler-independent way for declaring static data. Some compilers (such as Think C) provide support for using global data in code resources. Some others don’t.

The record `ExtModulesParamBlock` provides a method for storing global, static data that works on all compilers:

Each external module has its own record (struct) of type `ExtModulesParamBlock`. A pointer to this record is passed to your procedures and functions in the parameter `pb`. There are some fields in this record that you can use for your own purposes. Data stored there is preserved between individual calls to your functions:

- One of these fields is the array of extended values `pb^.v[1..30]` (under C, this is an array of double values, `pb->v[0..29]`). You can use this array for your own purposes – it is not used by proFit.
- The second such field is the pointer `pb^.globals` (under C, `pb->globals`). If your procedure `SetUp` returns a non-zero value in the parameter `requiredGlobals`, proFit will initialize `pb^.globals` to point to a memory block of corresponding block size (for more information, see the description of the procedure `SetUp` given above). You need to set `requiredGlobals` if you want to use the `pb->globals` pointer.

For examples on how to use global or static data, please refer to the sample code provided on your distribution disks.

**Procedures provided by proFit**

proFit offers a list of functions and procedures that can be called by your external modules. If you are programming in Pascal, they are defined in the interface of the file `proFit_interface.p`. If you are programming in C, they are defined in the header file `proFit_interface.h`. Their implementation can be found in the files `proFit_interface.p` or `proFit_interface.c`, respectively.

Most of the functions and procedures provided by proFit for external modules are the 1:1 equivalents of the ones that can be used when defining a function or program with proFit’s definition language. Refer to Appendix A, “Predefined Functions, Procedures and Arrays” for more information on the individual routines.
11 Apple Script

Introduction

Apple Script is a language for scripting applications on the Macintosh. It provides a common technique for automating tasks, exchanging data, and process remote control.

You can use Apple Script with pro Fit. Note, however, that pro Fit cannot create (i.e. compile) an Apple Script. To use Apple Script with pro Fit, you need an Apple Script compiler, such as Apple’s Script Editor (installed together with your system software). You enter the script in the script editor and compile it there.

Once the script is compiled, you can either run it from your script editor, or you can save it in its compiled form. (When using Apple’s Script Editor, choose “Save As...” from the “File” menu, choose the type “Compiled script” and save the script.) Such a compiled script can be loaded into pro Fit: Choose “Load Module...” from the Customize menu and select the compiled script. It is added to the Prog menu.

In the following, we give some examples for scripting pro Fit through Apple Script. Then we discuss the differences between programs and scripts. Finally we give a list of the Apple Script commands and objects that you can use with pro Fit.

Apple Script is a very powerful programming language. However, it may be confusing for the beginner. The easiest way to get started is using Apple Script’s “recording” capabilities. Just open the Script Editor and click the Record button. Now go into pro Fit and do (by hand) what your script is supposed to do. Script Editor records all your actions as Apple Script commands. Once you are through, go back to Script Editor and click the Stop button. Your script is now complete.

Note that this chapter is not intended to give a beginner’s introduction to the Apple Script language. We will, however, explain some its aspects as we use them. To learn more about Apple Script, consult the dedicated literature, such as the “Apple Script Language Guide” distributed by Apple.

Examples

Opening and closing a single file

The following is a very simple Apple Script for opening and closing a single file:

```
tell application "pro Fit"
    open file "measured data" -- open a file
    run program "Analyze" -- analyze it
    close window "measured data" -- close it
end tell
```

The script starts with the statement `tell application "pro Fit"` which indicates that all subsequent statements (until `end tell`) are to be sent to pro Fit. The following lines tell pro Fit to open a file called “measured data”, run the program “Analyze” from the Prog menu, and then close the file again.
To use this script, you must enter it in a script editor, such as Apple’s Script Editor:

```
-- bring up a dialog for selecting the folder of the files to analyze
set myFolder to choose folder with prompt "Choose a folder with data files:"

-- create a list with all files in the folder
set myFiles to list folder myFolder -- a list of files in myFolder
set myFileCount to count myFiles -- the number of files in myFolder

-- now start working with pro Fit
tell application "pro Fit"
    set oldErrorAlerts to error alerts -- save error alert status
    set error alerts to false -- pro Fit should not show alerts
    activate -- bring pro Fit to front
    repeat with i from 1 to myFileCount -- go through all files
        set theFile to item i of myFiles -- get the i-th file
        try
            -- open the file for processing as data file:
            open file ((myFolder as string) & theFile) as table
            write line "found: " & theFile   -- write comment to Results window
            close window "measured data" -- close the file
        on error errText
            write line "cannot open: " & theFile & " (" & errText & ")"
        end try
    end repeat
    set error alerts to oldErrorAlerts -- restore
end tell
```

When you click Run, the script is compiled and then executed. When compiling the script, the statements are converted into Apple Events, data packets that can be exchanged between applications. When running the script, they are sent to pro Fit.

As mentioned above, you can save the script as a “Compiled Script” and then load the compiled script from pro Fit by choosing “Load Module...” from the “Customize” menu. The script is added to the Prog menu from where it can be run.

**Batch processing**

Imagine you have a large number of data files in a folder. You want to open each of these files from pro Fit and analyze its data. Without scripting, you would have to open each file by hand, run your analysis, then close it again – boring work if you have to do it often. The following script does it all for you:

```
-- bring up a dialog for selecting the folder of the files to analyze
set myFolder to choose folder with prompt "Choose a folder with data files:"

-- create a list with all files in the folder
set myFiles to list folder myFolder -- a list of files in myFolder
set myFileCount to count myFiles -- the number of files in myFolder

-- now start working with pro Fit
tell application "pro Fit"
    set oldErrorAlerts to error alerts -- save error alert status
    set error alerts to false -- pro Fit should not show alerts
    activate -- bring pro Fit to front
    repeat with i from 1 to myFileCount -- go through all files
        set theFile to item i of myFiles -- get the i-th file
        try
            -- open the file for processing as data file:
            open file ((myFolder as string) & theFile) as table
            write line "found: " & theFile   -- write comment to Results window
            close window "measured data" -- close without saving
        on error errText
            write line "cannot open: " & theFile & " (" & errText & ")"
        end try
    end repeat
    set error alerts to oldErrorAlerts -- restore
end tell
```

11-2 Apple Script
This script first brings up a dialog box for selecting a folder by using the Apple Script extension choose folder with prompt. Then it goes through all the files in this folder and uses the command open file name as table for opening the file as a data window. It also uses the command write line text for writing a text into the results window. Then it closes the file.

The open file and close window commands are enclosed by the statements try and on error. If any of these commands fails and returns an error, the write line statement between on error and end try is executed.

Note that we are setting a property called error alert to false before opening the files. This tells pro Fit that it should not show any error alerts of its own when it cannot open a file.

The above example simply opens each file in the folder and closes it again. In practice, you may e.g. want to run a program on each opened file. For this purpose, simply insert

    run program "MyProg" -- analyze it

after the command open file, where “MyProg” is the name of the program you want to run.

The following is a more complete version of the above script. It not only runs a program on each opened file, it also defines the program, adds it to pro Fit’s Prog menu, and then exchanges data with it:

```apple_script
-- the following defines the pro Fit program run for each data file:
set scriptProgram to ¬
"program ScriptProgram;
    var sum, i;
    begin
        sum := 0;
        for i := 1 to nrRows do
            if DataOK(i,1) then sum := sum+data[i,1];
        globalData[1] := sum;    { store result }
    end;
"

-- bring up a dialog for selecting the folder of the files to analyze
set myFolder to choose folder with prompt "Choose a folder with data files:"

-- create a list with all files in the folder
set myFiles to list folder myFolder  -- a list of files in myFolder
set myFileCount to count myFiles  -- the number of files in myFolder

-- now start working with pro Fit
tell application "pro Fit (ppc)"
    set oldErrorAlerts to error alerts  -- save error alert status
    set error alerts to false  -- pro Fit should not show alerts
    activate  -- bring pro Fit to front
    compile scriptProgram  -- add the above program to Prog menu
    set myTable to make new table  -- open new data window
    set k to 1  -- a counter for opened files
    repeat with i from 1 to myFileCount
        set theFile to item i of myFiles  -- get the i-th file
        try
            open file ((myFolder as string) & theFile) as table  -- open the file
            write line "processing: " & theFile
            run program "ScriptProgram"  -- run the program in pro Fit
            close window theFile saving no  -- close without saving
        set sum to globalData 1  -- get result
    end try
end tell
```

Apple Script 11-3
The above script starts with the definition of the program to be run by pro Fit. Then it opens a new data window and stores its reference in “myTable”. Now it opens each data file in the designated folder, calculates the sum of the values in its column 1 and stores these sums in column 1 of the data window myTable.

The script starts with

```plaintext
set scriptProgram to ¬
```

This statement sets the symbol scriptProgram to the text following it. The symbol ¬ at the end of the line tells the script editor that more lines follow (to generate this symbol, type the return key while holding the shift key down).

The statement

```plaintext
compile scriptProgram -- add the above program to Prog menu
```

sends this text to pro Fit and tells pro Fit to compile it, i.e. to add it to the Prog menu.

Then, the script creates a new data window using the command

```plaintext
set myTable to make new table -- open new data window
```

The symbol myTable becomes a reference to the new data window.

Now, the files of the designated folder are opened one by one. After a file is opened, the ScriptProgram is run and the file is closed again. Then the script retrieves the result of the program from globalData[1]. The values in the array globalData can be accessed from scripts by using the object globalData and an index, such as

```plaintext
set sum to globalData 1 -- get result
```

The result retrieved in this way is transferred to the k-th row of column 1 of the data window myTable:

```plaintext
set cell k of column 1 of myTable to sum -- store it in the table
```

As you can see, scripts can exchange data with pro Fit, either through globalData or by accessing values in a data window.

There are other ways of interaction between scripts and pro Fit. They are explained in the last section of this chapter, which lists all Apple Script commands and objects supported by pro Fit.

**When to program, when to script**

As you may have realized, there are various things you can do through Apple Scripts as well as from a program defined within pro Fit. For example, you could define the following program for writing the sum of the two first cells of a data window into the results window:
program Sum;
begin
    Writeln(data[1,1]+data[1,2]);
end;

Alternatively, you could do the same from an Apple Script:
tell application "pro Fit"
    set sum to value of cell 1 of column 1 + value of cell 1 of column 2
    write line sum
end tell

Even though the above examples do the same, you will prefer the program, because defining programs is usually more convenient and faster.

In practice, you probably use programs more often than Apple Scripts. Programs can be defined within pro Fit, they are much faster, and they are better suited for numerical applications. However, there are some things that you simply cannot do from a program, such as exchanging data with other applications, communicating with the Finder, batch processing a large number of files, etc. For these tasks, you can use Apple Scripts.

You can combine the advantages of Apple Scripts and programs: To call an Apple Script from a program, first add it to the Prog menu (choose Load Module... from the Customize menu), then call it with CallProgram(...). To call a program from an Apple Script, compile it and use the command run program.

Apple Script commands and classes

The following is a list of the Apple Script commands and classes (objects) supported by pro Fit. Keywords are shown in **bold**, arguments are listed in *italics*, optional arguments and keywords are enclosed in square brackets, alternatives are separated by /

**Required Suite: Events that every application should support.**

**open**: Open the specified object(s)
- open file -- list of objects to open
  - [as data window/drawing window/funcProg window/text window]
  
  If the file is a file of type text, you can indicate if it is to be opened as text (i.e. in a new function window) or as table (i.e. in a new data window).

  Examples:
  - open file "HD:myData" -- opens the file "myData" on the disk HD
  - open file "data" as table -- opens the (text) file "data" as data file
  - open file "Drawing1" -- opens the file called "Drawing" in pro Fit folder

**print**: Print the specified object(s)
- print reference -- object(s) to print
  - [dialog boolean] -- indicates if we should show print dialog (default is true)

**quit**: Quit an application program
- quit
**run:** Sent to an application when it is double-clicked

**pro Fit suite: Special commands for pro Fit**

**add parameter set:** Adds the current parameters to the parameter set menu

```plaintext
add parameter set
    as string -- the name for the set
    [option for all boolean] -- true if added set should be available for all functions
```

**calculate statistics:** performs statistical calculations on the given window

```plaintext
calculate statistics reference -- the data window for the statistical analysis
    [column integer] -- the column for the statistical analysis. 0 to use all columns.
    median boolean -- set to true to calculate median, minimum, maximum.
    basic boolean -- set to true to calculate basic statistical information.
    skewness boolean -- set to true to calculate Skewness and Kurtosis.
    [selected cells boolean] -- true if statistical analysis of the current selection
    [selected rows boolean] -- true if statistical analysis must be applied
                           -- only to the data contained in the selected rows.
```

To retrieve the results, use e.g.

```plaintext
get statMean of results -- returns the mean value
(Available selectors of results are listed for class "calculation results" below)
```

**capture:** Switches capturing on and off

```plaintext
capture constant -- to file | enabled | disabled | done
    [to alias] -- the file to capture into (not used for options on | off | done)
```

Example:

```plaintext
tell application "pro Fit PPC"
    capture to file "HD:logFile" -- start capturing to logFile
    write line "hi there" -- will be captured
    capture disabled -- disable capturing temporarily
    write line "some text" -- will not be captured
    capture enabled -- enable capturing
    write line "add this to log file" -- will be captured
    capture done -- close the capture file
end tell
```

**clear:** Clears the current selection

```plaintext
clear
```

**close:** Close a window

```plaintext
close reference -- the window to close
    [saving yes/no/ask] -- Specifies whether or not changes should be saved
```

Windows can be specified by name or index (1 is the frontmost window, 2 is the window behind the frontmost window).
If you append the specification saving yes then all changes are saved – if the window has not yet been saved to a file, you are asked to specify where you want to save the changes. If you append saving no, changes are not saved. If you append saving ask or if you do not append a saving specification and the window contains unsaved changes, pro Fit will ask if you want to save the changes.

Examples:
close front window  -- prompts for saving unsaved changes
close window "Table1" saving no  -- closes the window without saving

**compile**: Compile a function or program written in pro Fit's definition language.

compile reference  -- text or file to compile

Examples:
compile file "HD:myProg"  -- compiles the given file
compile "function lin; begin y:=a[1]*x; end;"  -- compiles a text

the following is a more realistic way to define and compile a larger program from a script: (note that you can create the character "¬" by hitting option-return – this character specifies that the line is continued on the next one):

set myProg to ¬

"program test;
var i, sum;
begin
  sum := 0;
  for i := 1 to nrRows do
    if dataOK(i, 1) then sum := sum + data[i,1];
    writeln('sum of col 1: ', sum);
  end;
"

tell application "pro Fit"
  compile myProg  -- compiles the above definition
  run program "test"  -- and runs it
end tell

**copy**: Copies the current selection to the clipboard.

copy

cut: Cuts the current selection to the clipboard.

cut

Note: To get the clipboard of pro Fit, use "get clipboard"

data export options: Sets the options for exporting data as text files

Data export options

mode withtitles/withouttitles/custom -- Base format
[titles boolean] -- Write column titles
[copyInfo boolean] -- Write info as header lines
[optimize boolean] -- Optimize text length
[delimiter string] -- Column delimiter
[terminator string] -- Line terminator
[firstLine string] -- First header line
**data import options**: Sets the options for importing data from text files

- **mode** with titles/without titles/custom -- Base format
- [headerLines integer] -- Number of header lines
- [titles boolean] -- Read column titles
- [copyInfo boolean] -- Read header lines as info
- [delimiter string] -- Column delimiter
- [terminator string] -- Line terminator

**delete**: Removes a function or program from pro Fit's menus

- delete reference -- The function or program to delete
- delete program "FitFrontWindow" -- deletes the specified program
- delete function "linear" -- deletes the specified function

**delete parameter set**: Deletes a saved parameter set

- delete parameter set string -- the name of the parameter set.
  - Omit to delete all parameter sets of the given function
- [for string] -- the name of the function the parameter set belongs to
- [in alias] -- the file in which to save the object
- [fromMenu boolean] -- set to true to delete the parameter set from
  - the alternate parameter sets menu (default = true)
- [fromFile boolean] -- set to true to delete the parameter set from
  - the file specified in the "file" parameter (default = true).

**do script**: Compile and execute one or more Pascal statements

- do script reference -- the window or the statements to execute

Examples:
- do script "Writeln('Hello world');" -- executes the pascal statement

**FFT**: Fourier transform from real to complex numbers (see also "inverse FFT")

- FFT window -- the data window
  - inputCol integer -- input column (data in time domain)
  - outputCol1 integer -- output column 1 (real part or amplitude in frequency domain)
  - outputCol2 integer -- output column 2 (imaginary part or phase in frequency domain)
  - realImaginary boolean -- true if output columns contain real and imaginary parts,
    -- false if amplitude and phase
  - [outFrequencyCol integer] -- frequency output column (calculated from timeInterval)
  - timeInterval real -- time interval between input data points
  - [print results boolean] -- true if comments are to be printed in Results window

**find extrema of**: finds maxima and minima of the given function

- find extrema of reference -- the function to be used
  - xMin real -- lower bound of the interval where extrema must be found
  - xMax real -- upper bound of the interval where extrema must be found
  - subintervals integer -- number of subdivisions where to look for a result
  - [print results boolean] -- true if comments are to be printed in Results window
**find roots of**: finds the solutions of the equation \( f(x) = yVal \)

- `find roots of` reference -- the function to be used
- `xMin` real -- lower bound of the interval where roots must be found
- `xMax` real -- upper bound of the interval where roots must be found
- `subintervals` integer -- number of subdivisions where to look for a result
- `[value real]` -- the function value `yVal` in the equation \( f(x)=yVal \), default is zero
- `[print results boolean]` -- true if comments are to be printed in Results window

**fit**: fits the given function to the given data

- `fit` reference -- the function to use for fitting
- `algorithm` levenberg/monte carlo/robust/linear/polynomial -- fit algorithm to be used
- using reference -- the data window with the data to be used for the fit
- `xColumn` integer -- the x-coordinates of the data to be used for the fit
- `yColumn` integer -- the y-coordinates of the data to be used for the fit
- `[xErrorKind individualErr/constantErr/percentErr/unknownErr/zeroErr]` -- how the x-errors are specified
- `[yErrorKind individualErr/constantErr/percentErr/unknownErr/zeroErr]` -- how the y-errors are specified
- `[xErrorColumn integer]` -- the column with the x-errors, if xErrorKind is individual
- `[yErrorColumn integer]` -- the column with the y-errors, if xErrorKind is individual
- `[xError real]` -- the magnitude of the x-error, interpretation depends on xErrorKind
- `[yError real]` -- the magnitude of the y-error, interpretation depends on yErrorKind
- `[xDistribution gaussianDistribution/lorentzianDistribution/exponentialDistribution/tukeyDistribution/andrewDistribution]` -- the error distribution for the x-errors
- `[yDistribution gaussianDistribution/lorentzianDistribution/exponentialDistribution/tukeyDistribution/andrewDistribution]` -- the error distribution for the y-errors
- `[auto search boolean]` -- used when algorithm is montecarlo.
- `[selected only boolean]` -- true if fitting using selected rows only
- `[full description boolean]` -- true to print a full description of the fit parameters
- `[active parameters boolean]` -- true to print only the active parameters
- `[error analysis boolean]` -- true to perform an error analysis after the fit
- `[stopCounter integer]` -- tells Monte Carlo fitting when it must stop
- `[iterations integer]` -- the number of iterations to be used for error analysis
- `[confidence interval real]` -- confidence interval (in %) to be used for error analysis
- `[print results boolean]` -- true if comments are to be printed in Results window

**get data**: Gets the data of an object

- `get data` reference -- the object
- Result: anything -- the data of the object

**evaluate**: Return the value of a regular Pascal expression

- `evaluate` string -- the expression
- Result: real -- the result of the expression

**integrate**: finds the integral of the given function

- `integrate` reference -- the function to be used
- `xMin` real -- lower bound of the integration interval
xMax real -- upper bound of the integration interval
iterations integer -- number of iterations used
[print results boolean] -- true if comments are to be printed in Results window

**inverse FFT:** inverse Fourier transform from complex to real numbers (see also "FFT")
inverse FFT window -- the data window
  inputCol1 integer -- input column 1 (real part or amplitude in frequency domain)
  inputCol2 integer -- input column 2 (imaginary part or phase in frequency domain)
  outputCol integer -- output column (data in time domain)
  realImaginary boolean -- true if input columns contain real and imaginary parts,
  -- false if amplitude and phase
  [outTimeCol integer] -- time output column (calculated from frequencyInterval)
  frequencyInterval real -- frequency interval between input data points
  [print results boolean] -- true if comments are to be printed in Results window

**load parameter set:** Loads a saved parameter set
load parameter set string -- the name of the parameter set. Omit to load all parameter
  -- sets of the given function.
  [for string] -- name of the function the parameter set belongs to (omit for global sets)
  [from alias] -- the file from which to load the parameter set

**make:** Make a new window.
make
  new: type class -- the class of the new element: 'table', 'drawingWindow',
  -- 'textWindow'
  [with properties: record] -- the initial values for the properties of the element
Result: reference -- to the new object(s)

The keyword “new” is optional in Apple Script.

**what** specifies the type of window to be opened. Specify table for a data window, drawingWindow for a drawing window, textWindow for a function window.

The **with properties** parameter specifies the properties of the window in an Apple Script record. All types of pro Fit windows have the property name holding the name of the window as a string. In addition to this, data windows have the properties nrRows and nrCols with the numbers of rows and columns.

Examples:
make table with properties {name:"myTable"}
  -- creates a new data window having the name "myTable"
make drawingWindow with properties {name: "lookatthis"}
  -- creates a new drawing window having the name lookatthis
make textWindow -- creates a new function window
make table with properties {name:"small", nrCols:10, nrRows:20}
  -- creates a data window with name "small", 10 columns and
  -- 20 rows

-- the following creates a new data window and then closes it using a
-- temporary reference to the window
set myRef to make new table
close myRef

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**page setup:** Brings up the page setup dialog box.

**optimize:** Find the parameters and x value that maximize or minimize a function

**paste:** Pastes the clipboard into the front window.

**plot data:** Plot one or more data columns.
plot: Plots a function.
    plot reference -- the function to plot - omit for current function
    [xFrom real] -- x range: beginning
    [xTo real] -- x range: end
    [new window boolean] -- true if plotting into new window
    [new graph boolean] -- true if creating new graph
    [yFrom real] -- y range: beginning
    [yTo real] -- y range: end
    [autoY boolean] -- true if automatic y-range
    [xScaling lin/log/reciprocal/probability] -- x scaling
    [yScaling lin/log/reciprocal/probability] -- y scaling
    [xAxis small integer] -- x axis to be used (1 ...
    [yAxis small integer] -- y axis to be used (1 ...
    [step real] -- step width or number of steps (0 for automatic)
    [subrange start real] -- start of subrange to plot
    [subrange end real] -- end of subrange to plot
    [fitted parameters boolean] -- true if using fitted parameters
    [curve thickness real] -- if connected, thickness of line
    [curve dash small integer] -- if connected, line dash id
    [curve red integer] -- color: red component
    [curve green integer] -- color: green component
    [curve blue integer] -- color: blue component

reduce data: applies various data reduction algorithm do the data
    reduce data reference -- the window containing the data to be reduced
        using keep/remove/average/smooth/keepSelected/removeSelected -- algorithm
        [points integer] -- number of points over which to average, etc.
        [selection only boolean] -- true if reduction is applied only to the current selection

run program: Run a program from the User submenu.
    run program string -- The name of the program
    Example:
    run program "FitFrontWindow" -- run the specified program

    For a more elaborate example, see the command “compile”, above.

save: Save a window
    save reference -- the window to save
        [in alias] -- the file in which to save the object
        [as data file/drawing file/EPS file/function file/PICT file/text file]
            -- file type for data export

    Windows can be specified by name or index (1 is the frontmost window, 2 is the window behind it, etc). Note that Apple Script allows you to specify indexed objects in various ways (such as window 1, front window, 3rd window, last window)

    Optionally, you can specify the file where the window is to be saved after in. If you do not specify the file where to save the window and the window has never been saved before, you are prompted
to enter a file name. If you don’t specify the file where to save the window and the window has been saved before, the window is saved to the same file as before.

If the specified window is a data window, it is saved as a regular pro Fit file by default (this is equivalent to specifying “as table”). If you want the data window to be saved as text file for exporting it, specify “as text”.

Examples:
save window 1 to file "HD:data" -- saves front window to file
save window "data" to file "data.txt" as text -- saves as a text file

save parameter set: Saves a parameter set
save parameter set string -- the name of the parameter set.
  -- Omit to save all parameter sets of the given function
  [for string] -- the name of the function the parameter set belongs to
  -- (omit for global sets)
  [in alias] -- the file in which to save the parameter set. Omit to save as permanent set

select: Select the specified object
select reference -- the object to select (window, function, row, column, cell)
  options add discontinuously/add continuously/deselect/forget old
  -- omit for deleting the old selection

select all: Selects everything within the front window
select all

set data: Set the data of an object
set data reference -- the object to set
to anything -- the new value

set fit range of parameter: sets the fitting range of a parameter for Monte Carlo fits
set fit range of parameter integer -- the parameter number
  minimum real -- lower range limit
  maximum real -- upper range limit
  percent boolean -- true if the range is defined as percentage deviation
  -- from the parameters value

set legend properties: sets the visibility, position and size of the legend of the current graph
set legend properties
  [visible boolean] -- show or hide the legend
  [offsetx real] -- offset between left of legend and right of graph
  [offsety real] -- offset between top of legend and top of graph
  [width real] -- width of legend item (left part)
  [height real] -- height of a legend item

sort: Sort the numbers in a data window
sort reference -- the data window to be sorted
  using column integer -- the data is sorted with respect to this column
  [order sortAscending/sortDescending] -- the sorting order (ascending | descending)
  [selection only boolean] -- true if only the current selection must be sorted
undo: Undoes the last action.
undo

tabulate: tabulate a function
   tabulate reference -- the function to tabulate
      [parameter integer] -- the parameter to be varied (0 for x)
      from real -- the starting x-value
      to real -- the maximum x-value
      step value real -- the step between successive calculations
      [step numeric/auto/points] -- stepping option (auto | points)
      [x value real] -- the x-value used when tabulating by changing a parameter
      [fittedParams boolean] -- true to use fitted parameters instead
         -- of the current function parameters

tabulate roots of: tabulates the roots of a given function
   tabulate roots of reference -- the function to tabulate
      [parameter integer] -- the parameter to be varied (-2 for xMin, -1 for xMax)
      from real -- the starting parameter value
      to real -- the maximum parameter value
      step value real -- the step between successive calculations
      xMin real -- lower bound of the interval where roots must be found
      xMax real -- upper bound of the interval where roots must be found
      subintervals integer -- number of subdivisions where to look for a result
      [value real] -- the function value yVal in the equation "f(x)=yVal", default is zero

tabulate extrema of: tabulates the extrema of a given function
   tabulate extrema of reference -- the function to tabulate
      [parameter integer] -- the parameter to be varied (-2 for xMin, -1 for xMax)
      from real -- the starting parameter value
      to real -- the maximum parameter value
      step value real -- the step between successive calculations
      xMin real -- lower bound of the interval where extrema must be found
      xMax real -- upper bound of the interval where extrema must be found
      subintervals integer -- number of subdivisions where to look for a result

   iterations integer -- number of iterations used for the numerical computation of
      -- the integral

transform: performs data transformations in a data window
transform reference -- the window containing the data to transform
arcoshOp/tanhOp/... -- the operation used for the transformation calculations
[using reference] -- the function (from the Func Menu) to be used
[xColumn integer] -- the x-column to be used in column transformations
[yColumn integer] -- the y-column to be used in column transformations
[argumentColumn integer] -- the argument-column to be used with
  -- transformation functions that need another argument
  -- besides x. Set this parameter to zero to use a constant
  -- numeric value.
[argumentValue real] -- the argument-value to be used with transformation
  -- functions that need another argument besides x.
  -- Used when the argument column is set to zero.
[expression string] -- the pascal expression to be used as a transformation function
[selected cells boolean] -- true if the transformation must be applied only
  -- to the current selection
[selected rows boolean] -- true if fitting using selected rows only

transpose: Exchanges columns and rows in a data window
  transpose reference -- the data window to transpose

use parameter set: Moves a parameter set found in the alternate parameter set menu to the parameters window
  use parameter set string -- the name of the parameter set or "fitted parameters"
    [for string] -- name of the function the parameter set belongs to
    -- (omit for the current function)
    [option for all boolean] -- true to use one of the sets available for all functions

write: Write a text into the results window
  write string -- the text to be written

write line: Write a text into the results window and advance to a new line
  write line string -- the text to be written

Classes of the pro Fit suite

Many of the classes (windows, columns, etc) that can be accessed within pro Fit have properties or elements. For instance, each window has a property called name, each column has the properties name and default type. A data window (table) has columns as elements, each column has cells as elements.

You can access properties and elements by using the following standard Apple Script commands "get data" or "set data". Abbreviated, they are used as "get", "set" and "copy".

Examples:
  get name of front window -- returns the name of the front window
  if nrRows of window 2 < 10 then error -- "get" is not necessary
set myVar to cell 1 of column 2 of window "Table"
set name of front window to "myData" -- sets front window name
set nrRows of window "Table" to 200 -- resize a data window
set default type of column 2 of front window to string -- set col. type
set myvar to value of every cell of column 4 of front window -- myvar becomes an list of numbers

Note: a list of the properties and elements that can be accessed is given below

The following lists the properties and elements of pro Fit's classes and gives some examples on their use. If a property or element is marked as [r/o], it is “read-only” and cannot be changed.

Class **application**: The pro Fit application

Properties:
- default column type: type class -- real, single
- current function: function -- the currently selected function
- clipboard: a list of record [r/o] -- contains elements of type PICT and TEXT
- decimals: integer -- the number of decimals for numeric output
- error alerts: boolean -- true if alert is to be shown when Apple Event failed
- results: calculation results [r/o] -- Results of preceding calculations
- script debugging: boolean -- true if script debugging enabled, false if disabled
- version: version [r/o] -- the version of the application

<Inheritance> base class properties [r/o]

Notes:
- error alerts indicates if pro Fit should show alerts when handling Apple Events (i.e. when executing an Apple Script). By default, this property is true. When your script does its own error handling, you should set it to false. If you do so, reset it at the end of your script – if you don’t, pro Fit will not show any errors when handling Apple Events from the Finder later.

Setting script debugging to true causes pro Fit to write a list of all Apple Events it receives to the results window. This feature does not work for scripts started from within pro Fit.

Class **calculation results**: The result of the last calculations

Properties:
- chiSquared: real [r/o] -- fitting: chi squared
- fittedParameters: a list of real [r/o] -- fitting, optimization: the fitted parameters
- nrFittedParameters: integer [r/o] -- fitting: the number of fitted parameters
- sumOfDeviations: real [r/o] -- fitting: sum of the error deviations (Robust algorithm)
- correlation: real [r/o] -- fitting: linear correlation between x- and y-values (linear regression)
- probCorrelation: real [r/o] -- fitting: significance of correlation (linear regression)
- covariance: a list of real [r/o] -- fitting: covariance matrix
- nrIterations: integer [r/o] -- fitting: number of iterations
- goodnessOfFit: real [r/o] -- fitting: goodness of fit
- confidenceMin: a list of real [r/o] -- fitting low boundaries of confidence intervals
- confidenceMax: a list of real [r/o] -- fitting high boundaries of confidence intervals
- standardDeviations: a list of real [r/o] -- fitting: standard deviations of the parameters
- optimizedX: real [r/o] -- optimization: x value
- optimizedY: real [r/o] -- optimization: y value
- rootsCount: integer [r/o] -- roots: number of roots
- rootsXValues: a list of real [r/o] -- roots: x values

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rootsYValues: a list of real [r/o] -- roots: y values
extremaCount: integer [r/o] -- extrema: number of extrema
extremaXValues: a list of real [r/o] -- extrema: x values
extremaYValues: a list of real [r/o] -- extrema: y values
extremaSigns: a list of real [r/o] -- extrema: signs (1 for maxima, -1 for minima)
integralValue: a list of real [r/o] -- integral: value of the integral
integralAccuracy: a list of real [r/o] -- integral: last correction
statCount: integer [r/o] -- statistics: the number of evaluated values
statSum: integer [r/o] -- statistics: the sum of all values
statMean: real [r/o] -- statistics: mean
statMedian: real [r/o] -- statistics: median
statStdDeviation: real [r/o] -- statistics: standard deviation
statMeanAbsDeviation: real [r/o] -- statistics: mean absolute deviation
statMinimum: real [r/o] -- statistics: minimum
statMaximum: real [r/o] -- statistics: maximum
statVariance: real [r/o] -- statistics: variance
statSkewness: real [r/o] -- statistics: skewness
statKurtosis: real [r/o] -- statistics: kurtosis

Class cell: A cell in a data window (access by index)
Properties:
  value: real -- the value of the cell
<br/>&lt;Inheritance&gt; base class properties [r/o]
Examples:
get value of cells 1 thru 8 of columns 4 thru 12 of front window
  -- returns a list of lists
set value of cell 2 of column 2 to 22
set value of cells 1 thru 5 of column 1 to {2, 4, 6, 8, 10}
set value of cell 5 of column 8 to "there" -- cell in a text column
set value of every cell of column 1 to 0 -- set all cells of column 1 to 0

Note: You can access cells by giving an index or a range of indices.
If you get the value of an empty cell, a so-called “NAN”-value is returned. Note that the
present version of Apple Script will cause an error when being forced to display such a
value.

Class column: A column in a data window (access by index)
Properties:
  name: string -- the name of the column
  default type: type class -- string, real, single
  decimals: integer -- the number of decimals, -1 for automatic
  format: scientificForm/floatingForm -- display format for numbers
  width: integer -- the width of the column, 0 for default width
<br/>&lt;Inheritance&gt; base class properties [r/o]
Note:
  • You can access columns by giving an index or a range of indices.
  • You can set the type of a column by setting default type to string (text column), real
    (double precision column with approximate range of 1e300) or single (single precision
    column with approximate range of 1e30)
Class **function**: A function (access by name or index)

Elements:
- parameter

Properties:
- name: string [r/o] -- the name of the column
- nrParams: integer [r/o] -- The number of parameters
- shown: boolean [r/o] -- True if the function is shown in the preview window

Class **globalData**: an array of double values (access by index 0..99)

Elements:
- real

Note:
The entries in the list `globalData` can be accessed by index (0 to 99) but not by range.

`globalData` can also be accessed by functions and programs. It provides a mechanism for exchanging data between scripts and pro Fit programs. Example:

```plaintext
set myProg to "program SumOneColumn; { calculates the sum of a column }
var i,j, sum;
begin
  sum := 0;
  j := globalData[1];
  for i := 1 to nrRows do
    if dataOK(i, j) then sum := sum + data[i,j];
  globalData[2] := sum;
end;

tell application "pro Fit"
  compile myProg -- compiles the above definition
  set globalData 1 to 2 -- the column we want to sum
  run program "SumOneColumn" -- runs the program
  delete program "SumOneColumn" -- clean up pro Fit's menus
  get globalData 2 -- get the result
end tell
```

Class **single**: a real value with small accuracy

Class **table**: a data window (access by index or name)

Elements:
- column

Properties:
- name: string -- the title of the window
- nrCols: integer -- the number of columns
- nrRows: integer -- the number of rows

Note:
In most cases, you can use the classes “window” or “table” equivalently, you can write

---

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pro Fit will automatically cast one class type into the other. Note however, that there are some situations where the words are not equivalent, e.g.

```
set name of front window to "data"
set name of front table to "data"
```

The first example sets the name of the front window, the second the name of the front most data window.

Class **drawingWindow**: a drawing window (access by index or name)

Properties:
- name: string -- the title of the window
  <Inheritance> base class properties [r/o]

Class **parameter**: a parameter of a function

Properties:
- name: string -- the name of the parameter
- value: real -- the value of the parameter
- min: real -- the minimum value of the parameter (or none)
- max: real -- the maximum value of the parameter (or none)
- mode: inactive/active/constant -- the mode of the parameter
  <Inheritance> base class properties [r/o]

Class **program**: A program or apple script (access by name or index)

Properties:
- name: string [r/o] -- the name of the column
  <Inheritance> base class properties [r/o]

Class **row**: A row in a data window (access by index)

Plural form:
- rows

Class **textWindow**: a function or program window (access by index or name)

Properties:
- name: string -- the title of the window
  <Inheritance> base class properties [r/o]

Class **window**: a window (access by index or name)

Plural form:
- windows

Properties:
- name: string -- the title of the window
- bounds: bounding rectangle -- the boundary rectangle for the window
- floating: boolean [r/o] -- Does the window float?
- info: string -- the info text
- font: string -- the name of the default font for text
- size: fixed -- the default size for text
- style: 'tsty' -- the default text style for text
  <Inheritance> base class properties [r/o]
Note:
You cannot access floating windows. You cannot change the name of the parameter window or the results windows. To specify a window, you can either use its name or its index. The index ranges from 1 to the number of windows, where 1 designates the front window.

Class **base class properties**: Properties inherited by all objects.
Properties:
- properties: record -- a record containing all properties of the element
12 Printing

There is a wide range of different printers that can be connected to a Mac OS machine, and each of these printers have different capabilities, resolutions and command languages. proFit allows you to get the best out of most of the commonly used printers if you follow the guidelines described in this chapter.

Basically, there are two possibilities for printing proFit drawings. You can print from proFit directly (using the **Print** command from the File menu) or you can export a drawing to another application, such as a word processor (using the **Copy** or the **Create Publisher** commands or by dragging it to the other application), and print it from there. The next two sections discuss these two possibilities separately.

**Printing from proFit**

Before printing, you should choose **Page Setup** from the File menu.

You can print the active window by selecting the **Print** command from the File menu.

proFit offers three different modes of printing: *printing through QuickDraw GX, printing with PostScript* and *printing at the printer’s resolution*. You can select the desired method by choosing **Preferences...** from the File menu. In the dialog box that comes up, click the icon “Printing” in the list at the left. The dialog box now looks as follows:

If you check **Use QuickDraw GX**, proFit uses the features of Apple’s graphics environment QuickDraw GX. This option is disabled if you don’t have QuickDraw GX installed on your computer, and it only works on Operating Systems prior to Mac OS 8. Once you have checked ‘Use QuickDraw
printing with PostScript is disabled. Note that you must restart proFit when you have changed this option.

For best results on any printer, you should check ‘Use QuickDraw GX’ if you have QuickDraw GX installed on your computer and you are using an older system software.

If you check **Print drawings using PostScript**, proFit sends PostScript commands to the printer together with a simple picture describing your drawing. You should check this option if you are printing to a PostScript printer. When you check “Print drawings using PostScript”, you should also check “Use QuickDraw for text”. More information on this option is given below.

If neither ‘Use QuickDraw GX’ nor ‘Print drawings using PostScript’ are checked, proFit prints the drawing “at the printer’s resolution”. No PostScript commands are sent in this case. You should use this setting if you are printing to a non-PostScript printer.

The default setting on a “fresh” installation of proFit is the last one. I.e. no PostScript is sent to the printer. The reason for this is that this default setting gives good results on most printers, PostScript or not PostScript.

If you have a PostScript printer, you will get better results if you check the “Print Drawings using PostScript” option.

### Printing with QuickDraw GX

QuickDraw GX is Apple’s improved printing and graphics environment shipping with System version 7.5. Note, however, that Quickdraw GX printing is not supported anymore under MacOS 8.

You must check the Use QuickDraw GX option in the “Printing” preference panel if you want to export QuickDraw GX shapes through the clipboard or by drag and drop (see next chapter, “Printing a drawing from another application”).

When printing with QuickDraw GX, texts will be kerned and ligatures will be used. For more information on kerning and ligatures see Chapter 7 “Drawing”, section “Text objects”.

### Printing with PostScript

PostScript® is a language for defining graphical objects. It is used by many high quality printers. When an application prints to such a printer, it can use the built-in graphics language of the Macintosh (QuickDraw), which is automatically translated to PostScript by the printer driver before it is sent to the printer. However, some information may be lost during this translation. To get better results, an application can generate the PostScript directly and send it to the printer, obviating the need for any translation.

Check ‘Print drawings using PostScript’ after choosing the “Printing” panel of the preferences dialog box, to let proFit generate PostScript during printing. To print drawings with PostScript, you must disable QuickDraw GX by unchecking the option ‘Use QuickDraw GX’.

When printing with PostScript, you should usually check the option “Use QuickDraw for text” for best compatibility with most printer drivers and printers. If “Use QuickDraw for text” is checked, proFit first creates PostScript code for all items of the drawing window except text items and sends this code to the
Then it draws the texts — without using PostScript. This ensures the correct setting of the font and supports all text styles. If you uncheck ‘Use QuickDraw for text’, text will be sent as PostScript code — this option is not recommended as it can lead to compatibility problems with some printer drivers.

Not all printers support PostScript. Don’t use the ‘Print drawings using PostScript’ option on non-PostScript printers. A non-PostScript printer will ignore the PostScript commands and will print a non-optimized picture (with the resolution of the screen). Switch off the option ‘Print drawings using PostScript’ to get optimal results on a non-PostScript printer (see the next section, below).

Drawings will generally look better when printed with PostScript than when they are printed at the printer’s resolution. However, there are some minor problems when using special patterns or characters:

- When using patterns, only the gray patterns will print. All other patterns will be replaced by a 50% gray pattern.
- If “Use QuickDraw for text” is not checked, outlined, shadowed and underlined fonts are not supported.
- If “Use QuickDraw for text” is checked, text is printed above all other items in a drawing.

**Printing at full printer resolution**

If your printer does not support PostScript, do not check ‘Print drawings using PostScript’. In this case, pro Fit determines the resolution (the number of distinguishable dots per inch that can be printed) of your printer when it is printing a drawing window. Using this information, pro Fit can optimize the picture it sends to the printer in order to take full advantage of the resolution available on your printer.

**Printing a pro Fit drawing from another application**

When you copy or drag a drawing into another application (or when you create a Publisher that you subscribe to from another application), pro Fit creates a picture (often called PICT) that contains all the information required for drawing the copied objects on the screen. However, when it comes to printing on a high quality printer (with better resolution than the screen), more information is needed. This additional information must be packed into the picture. Since there is no standard method of doing this in a way that works for all printers, you should give pro Fit some information about your printer before creating a picture.

You can give this information by choosing Preferences from the File menu and selecting “PICT Options” from the list of icons to the left. This brings up the following dialog box:
You can choose between six picture formats:

- **Normal PICT**: Use this option when you don’t plan to print your pictures at a high quality. Pictures generated with this option look fine on the screen and use a minimum amount of memory.

- **Embedded PostScript**: Use this option when you are planning to print your pictures on a printer that understands PostScript, such as a printer of the LaserWriter® family. The pictures generated with this option still look nice on screen, but they also have PostScript information included. When you select “Embedded PostScript”, you can specify if you want to “Use QuickDraw for Text”. For best compatibility with the widest range of printers and printer drivers, “Use QuickDraw for Text” should be checked.

  For more information on printing with PostScript, see the section ‘Printing with PostScript’ earlier in this chapter.

- **High resolution PICT**: This option generates pictures that print well on most printers if the printing application supports “printing at the printer’s resolution” and does not change any information in the pictures it imports. However, few applications presently support these features. When generating a high resolution picture, you must enter the desired resolution in a text field appearing at the bottom of the dialog box.

  High resolution pictures may not look perfect on screen but they use a minimum amount of memory.

- **Enlarged PICT**: Pictures generated under this option are enlarged by a zoom factor $z$ given by the specified resolution $r$. You can enter the resolution $r$ in an edit field appearing at the bottom of the dialog box. The zoom factor is given by the formula $z = r / 72$ dots per inch.

  You can obtain high quality prints of an enlarged picture on many printers by choosing a reduction factor $1/z$ in the Page Setup dialog box before printing.

- **Bitmap**: This is presently the recommended picture format for printing on any high resolution printer that does not support PostScript if you don’t have QuickDraw GX installed. In a bitmap every pixel of the picture is stored at the printer’s resolution. You can enter the desired resolution in a text field appearing at the bottom of the dialog box.
Bitmaps print well on most high resolution printers. However, a bitmap uses a large amount of memory and often looks unsatisfactory on screen. Also, printing a bitmap can be very slow, especially when printing to a PostScript device.

When you select ‘Bitmap’, you can specify if your bitmap should be black and white or if it should contain color information. Don’t check ‘with Color’ unless you really need a color bitmap – black and white bitmaps use considerably less memory.

- **QuickDraw GX shape**: This option is only available if you have QuickDraw GX installed and if you have checked ‘Use QuickDraw GX’ in the “Printing” panel of the Preferences dialog box.
  If ‘QuickDraw GX shape’ is checked, pictures are exported as “shapes” (the data exchange format of QuickDraw GX). Shapes print fine from all applications that allow importing them. If you are unable to paste a shape into an application, then this application does not yet fully support QuickDraw GX.
  Note: You can also append a QuickDraw GX shape to normal pictures using the “Add QuickDraw GX” option, described below.

The options “Normal PICT”, “Embedded PostScript”, “Enlarged PICT” and “Bitmap” all generate a classic QuickDraw picture. It can be pasted into nearly all applications that support graphics. The option “QuickDraw GX shape” generates a QuickDraw GX shape, which can only be pasted into applications that support this data type.

You also can combine a classic QuickDraw picture and a QuickDraw GX shape to get the best of both worlds. If you select one of the types “Normal PICT”, “Embedded PostScript”, “Enlarged PICT” or “Bitmap” and if you have QuickDraw GX and QuickTime™ installed, there appears a checkbox and a pop-up menu titled “Add QuickDraw GX”:

- Add QuickDraw GX
  - for printer only
  - for screen & printer

Check this option if you want to add a QuickDraw GX shape to your classic QuickDraw picture. When you print such a picture, the QuickDraw GX shape is used when printing through a QuickDraw GX printer driver, while the classic QuickDraw picture is used otherwise.

If you choose **for printer only** from the pop-up menu, the QuickDraw GX shape is ignored when the picture is drawn on screen. If you choose **for screen & printer**, the QuickDraw GX shape is also used for on-screen display when QuickDraw GX is installed.

At the bottom of the “Printing” panel in the Preferences dialog box, there is a button called “Standards”:

- Standards...

Clicking this button brings up another dialog box that lets you store your settings in the preferences file or load previously stored settings:
The upper part of the box lists all styles saved in the preferences file. To load a style, double-click its name. To delete one or more styles, select their names (shift click for multiple selections) and click **Delete**.

To save your current picture settings as a PICT style, type a name in the edit item and click **Save**.

If you save a style with the name **Normal**, it becomes the **default style** and it is loaded whenever you start pro Fit.
13 Preferences

proFit offers many possibilities to customize its features: You can choose the format for exporting pictures, the preferred method for printing, you can save your preferred user interface options, etc. All of these settings are saved in proFit’s preferences file. During start-up proFit looks in the Preferences folder of the System folder for its preferences file. If the file is there, proFit reads its standard settings from it. If the file is not there, proFit creates a new preferences file. You can switch to another preferences file or create a new preferences file anytime later.

If you do not want to load the standard preferences file in the system folder, hold down the option and the shift key while starting up proFit.

Most of proFit’s settings are controlled by choosing Preferences... from the File menu. Doing so brings up a dialog box with several panels. Each panel controls a set of options. To choose a panel, select its icon from the list in the left of the dialog box.

The panels Printing and PICT Options are discussed in Chapter 12, “Printing”. In the following, we discuss the panels General, Drawing, Preview, Interface and Prefs File.

Panel “General”

This panel controls some general options for output, scrolling and data windows.

The first item in this panel defines the # digits after the decimal point used when displaying numerical results. Enter a negative number if you want to set the total number of digits, a positive number for setting the number of digits after the decimal points.
The radio buttons under the title **Default data window range** control the default range and precision of the numeric columns in new data windows. See the section “Data Types” of Chapter 4 for details.

**Show hints** controls if pro Fit should show some hints to guide an unexperienced user. Uncheck this option if you don't want any hints to be shown.

Note that each hint also has an individual checkbox that can be used to disable it. If you uncheck and later check again “Show hints” in the Preferences dialog, all hints (also those that have been disabled individually) will be shown again.

**Panel “Printing”**
This panel is discussed in Chapter 12, “Printing”

**Panel “PICT Options”**
This panel is discussed in Chapter 12, “Printing”

**Panel “Drawing”**
This panel controls some options used by the drawing window:

Check **Typographical minus** if you want to use a longer dash (–) instead of the hyphen (–) as a minus sign for numbers in the labels of a graph. Note that the typographical minus may not be available on non-roman fonts.

Check **Comma instead of decimal point** to use a comma as the decimal marker (12,345) instead of a point (12.345).

**Exponentials** controls the style for drawing exponential labels.
Note that changing the settings under “Format of labels in graph axes” does not affect the labels of existing graphs. When you have changed the settings and want to use them for an existing graph, redraw the axis, e.g. by double-clicking it and clicking the button “Apply”.

**Default units** controls the default units used for measuring and entering distances in the drawing window and the Drawing Info window.

Check **Automatic grouping of new graphs**, if you want to automatically group a graph, the names of its axes, and its legend when it is created. Uncheck this option if these items should not be grouped.

Check **Always use floating toolbox** if you never want the drawing tools to appear inside the drawing window.

**Panel “Preview”**

This panel controls some options for the preview window:

![Preferences Panel](image)

The first two pop-up menus define the colors of the **data points** (the points used for showing your current data). The menu **Color** sets the color of the data points which are not part of the current selection. The menu **Selection color** sets the color of selected data points.

The second two pop-up menus define the colors of markers (for more information on markers, see Chapter 6). The menu **Color** sets the color of all markers except the reference marker, the menu **Reference color** sets the color of the reference marker.

The **Coordinate Lines** are drawn in a light grey color in the preview window, behind the data points and the function curve. They are two perpendicular lines that cross the x- and y- coordinate axes of the preview at the coordinates given in the two edit fields.
Check the option **Allow dragging of data points** if you want to be able to change coordinates in a data window by dragging the corresponding data points in the preview window. Uncheck this option to disable this potentially dangerous option.

**Panel “Interface”**

Using this panel you can control some aspects of pro Fit's user interface.

![Preferences dialog box](image)

Check the box under **Use Appearance services for** to enable the new “three dimensional” look introduced with MacOS 8. This makes the background of all dialog boxes gray, adds shadows to most controls, etc. Drawing these elements takes more time than drawing plain black and white elements. Therefore, if you have a slow computer, you may want to uncheck this option.

The check boxes under **Enable dynamic scrolling for** control what happens if you click and drag the indicator of a scroll bar. If the corresponding checkbox is checked, the contents of the window will be scrolled *while* you drag the scroll bar. This provides a more accurate control of scrolling, but may be sluggish on slower computers.

**Panel “Prefs file”**

Using this panel you can switch between preferences files or create a new preferences file:
Click **New Preferences file** to create a new preferences file. All the settings and extensions stored in the current preferences file are copied to the new preferences file.

Click **Use Preferences file** to switch to another existing preferences file. pro Fit will scan the folder of the selected preferences file for a folder called “pro Fit modules”. If it finds such a folder, any modules stored in this folder are loaded into pro Fit. (For a more complete discussion of the pro Fit modules folder, see Chapter 5, “Working with Functions”).
14 General features

Getting help

proFit offers a powerful on-line help based on Apple Guide. The proFit Guide can be accessed by choosing proFit Guide from the help menu, or by clicking one of the question marks that are present everywhere in proFit windows and dialog boxes. Balloon help is also supported.

When defining functions and programs there is a special feature based on a dedicated help menu which is always present in the header of function windows. See chapter 9, “Defining functions and programs”, for more information on this help menu.

Help balloons

Switch on balloon help by choosing the Show Balloons command from the Help menu.

Once you have switched on balloon help, helpful comments show up whenever you move the mouse over some interesting item. Choose Hide Balloons from the Help menu to switch balloon help off.

Help Balloons can be switched on locally for the Help menus in function windows. They show helpful information on the keyword currently selected in the menu.

The proFit Guide

The proFit on-line help system comes in a separate files called proFit Guide and proFit Programming. These files are found on your distribution disks and must reside in the same folder as proFit. If proFit cannot find one of these file, then the corresponding on-line help is not available.

The main proFit Guide can be accessed using the Help menu to the right of the menu bar.

As an alternative to this, there are lots of question marks everywhere in proFit dialog boxes and windows. Click any of these question marks if you need help in a particular situation. proFit will immediately display a floating window that can guide you through the operation at hand.

The proFit Programming guide provides help on all features of proFit’s function and program definition language. This Guide contains a detailed description of every predefined function or keyword. The programming Guide can be opened directly at the page describing a given keyword, by selecting that keyword in the function window Help menu, or by option-double-clicking a keyword in the text of a function definition.

On-line evaluation of mathematical expressions

Wherever proFit expects a numerical input, such as in spreadsheets or dialog boxes, you can enter a mathematical expression. For example, instead of typing a number directly, you can use a mathematical expression like “exp(1)” or “6+sin(pi/4)”. proFit reads the mathematical expression you typed or pasted and calculates the numerical result.
Text windows, such as the result window, can be used as a calculator by typing an expression on a new line, positioning the insertion point on that line, and hitting the Enter key. The result is displayed on the next line.

You can also use mathematical expressions in all proFit dialog boxes. As an example, if you want to tabulate a function between 0 and two times $\pi$ at intervals of $\pi/5$, type command-T and enter the following:

When typing a mathematical expression, you use the same syntax elements that are available when writing a function definition. In on-line mathematical expressions, $x$ is equal to the last result that was evaluated, and $a[i]$ is equal to the parameter values shown in the current parameters window. You can use all the predefined functions available when writing the definition of a function. As an example, after a successful fit you can type 'ChiSquared' in a data window cell. This tells pro Fit to set the value of that cell to the mean deviation obtained in the last fit (see Chapters 9 and 10, together with Appendix A, for more information on predefined functions).

Let’s look at a simple example that illustrates how you can use proFit’s understanding of mathematical expressions when you are pasting into a data window. Write the following text and copy it to the clipboard:

\[ \text{a}[2] \rightarrow \text{fittedParams}(2) \rightarrow \text{a}[2] - \text{fittedParams}(2) \rightarrow \text{paramSD}(2) \]
\[ \text{a}[3] \rightarrow \text{fittedParams}(3) \rightarrow \text{a}[3] - \text{fittedParams}(3) \rightarrow \text{paramSD}(3) \]
\[ \text{a}[4] \rightarrow \text{fittedParams}(4) \rightarrow \text{a}[4] - \text{fittedParams}(4) \rightarrow \text{paramSD}(4) \]
Where the ‘→’ stands for a tabulator character and each line is terminated with a carriage return (¶). If you paste the above text into a data window after a successful fit, you automatically obtain a table containing the parameter values before the fit, the values after the fit, their difference, and the resulting standard deviations.

**File info**

proFit lets you save a comment with every one of its files. You can edit this comment with the Get Info command from the File menu. Choosing Get Info presents a dialog box with a large field for editing text.

![Dialog box for editing file info](image)

You can add an info comment to data windows, drawing windows and functions or programs.

The data windows let you view and edit this information directly, without using the Get Info command. For this you drag down the info hook (a black area on top of the right scroll bar) of a data window to create an info field of the desired size. See Chapter 4, “Working with data” for more information on data windows.

![Data window with info](image)
Note that the info comments are in general only saved in files that have proFit’s standard formats. If you save a function definition as normal text files (TEXT format) or if you save a drawing window as a picture or EPS file (PICT format, EPSF format), the info comments are not saved. If you save a data file as TEXT, you have the option of placing the info comments right at the beginning of the text file, as a header. To set this option, you have to choose “Custom format” in the dialog box that comes up when saving text files.

**Find and Replace**

proFit provides Find & Replace features to help you navigate through text. This feature is available for the results window and all function windows. You will find it most useful when you are editing the definition of a function or a program inside a function window.

The Find & Replace commands are found in the Edit menu:

When you choose **Find...** the Find/Replace dialog box appears:

![Find/Replace dialog box](image)

Type the text you are searching for and the replacement text in the **Find** and **Replace** edit fields. Use the radio buttons **Forward/Backward** to start the search by moving down from the current insertion point towards the end of your text, or up towards the beginning. Click the **Find** button to start a search, click **Done** if you don’t want to start a search yet. Click **Replace All** to replace all the occurrences of the text appearing in the Find item with the text appearing in the Replace item.

Use the menu command **Enter Selection** to enter the currently selected text in the Find field of the Find&Replace dialog box. Choose **Find Again** to restart a search (the fastest way to find all occurrences of a text is to select it and choose Enter Selection and Find Again in rapid succession). Use **Replace** to replace the current selection with the text in the Replace field of the Find&Replace dialog box.

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14-4  General features
box. **Replace and Find Again** combines the last two commands. **Replace All** is equivalent to the Replace All button in the Find dialog box.

Note that by using the Enter Selection command, or by copying some text and pasting it into the Find and the Replace field, you can enter text that you cannot enter by typing in the dialog box, such as carriage returns (¶) and tabs (→).

These commands can be accessed by using the following key combinations:

<table>
<thead>
<tr>
<th>Action</th>
<th>Modifier Keys</th>
</tr>
</thead>
<tbody>
<tr>
<td>Find...</td>
<td>shift + command + F</td>
</tr>
<tr>
<td>Find Again</td>
<td>shift + command + G</td>
</tr>
<tr>
<td>Enter Selection</td>
<td>shift + command + E</td>
</tr>
<tr>
<td>Replace</td>
<td>shift + command + R</td>
</tr>
<tr>
<td>Replace &amp; Find Again</td>
<td>shift + command + H</td>
</tr>
</tbody>
</table>

These command key equivalents are displayed in the Help Balloons for the corresponding menu items.

### Shortcuts and other options

Although most of proFit’s features and commands are readily accessed through its menus, there are some more advanced or rarely used features that require the use of modifier keys like the option key, the command key, or the shift key.

This is a short list of these features:

<table>
<thead>
<tr>
<th>Action</th>
<th>Modifier Keys</th>
</tr>
</thead>
<tbody>
<tr>
<td>Pressing ‘F’</td>
<td>shift &amp; command to select ‘Find...’ from the Edit menu.</td>
</tr>
<tr>
<td>Pressing ‘G’</td>
<td>shift &amp; command to select ‘Find Again’ from the Edit menu.</td>
</tr>
<tr>
<td>Pressing ‘E’</td>
<td>shift &amp; command to select ‘Enter Selection’ from the Edit menu.</td>
</tr>
<tr>
<td>Pressing ‘R’</td>
<td>shift &amp; command to select ‘Replace’ from the Edit menu.</td>
</tr>
<tr>
<td>Pressing ‘H’</td>
<td>command to select ‘Replace &amp; Find Again’ from the Edit menu.</td>
</tr>
<tr>
<td>Pressing ‘D’</td>
<td>command to dismiss the “Do you want to save changes to...” dialog box. Keyboard equivalent of typing the “Don’t Save” button.</td>
</tr>
<tr>
<td>Selecting a tool in the tools palette of drawing windows</td>
<td>option to keep the tool selected after drawing the corresponding object.</td>
</tr>
<tr>
<td>Dragging objects in drawing windows</td>
<td>command to constrain the movement along 45° lines. shift to constrain the movement to horizontal and vertical directions. option to duplicate an object instead of simply moving it.</td>
</tr>
<tr>
<td>Drawings objects in drawing windows</td>
<td>option or shift to get a square bounding box.</td>
</tr>
</tbody>
</table>
• Drawing lines in drawing windows
  - `shift` to make the line horizontal, vertical or diagonal (at 45°)
  - `option` to make a diagonal line

• Drawing polygons in drawing windows
  - `option`, `shift` same as for lines
  - `command` double-click to produce a corner that remains a corner even when the polygon is smoothed.

• Resizing objects in drawing windows
  - `option` to keep the bounding box of the object square (height=width).
  - `shift` to maintain the horizontal and vertical proportions of the object, its height, or its width.
  - `command` to resize the size of texts in a group.

• Resizing lines in drawing windows
  - `option` to get a line constrained to 45° directions.
  - `shift` to maintain the direction of the original line, or to make the line vertical or horizontal

• Clicking objects in drawing windows
  - `shift` to select an object without de-selecting other already selected objects.

• Clicking graphs in drawing windows
  - `option & command` + click to see the plot coordinates of the point you are indicating with the cursor.
  - `option & command` click, and then press `shift` to select an area of the graph to be enlarged.
  - `command` double-click to make a graph the ‘current graph’.
  - `command & shift` double-click to remove the ‘current graph’ setting.

• Reshaping polygons in drawing windows
  - `option` click (a connecting line) to insert a new polygon point.
  - `option` click (a point ) to delete it.
  - hold down the `command` key while dragging a single point to let the selected point coincide with the nearest neighboring point.
• Using the line style pop-up menu in a drawing window to change the line styles in a legend
  
  - press \textbf{shift} to change the line styles of all the lines in the legend.
  - press \textbf{option} to change the line style and set the attribute ‘points connected’ for the data plot in the first row of the legend.
  - press \textbf{shift \& option} to change the line styles of all the lines in the legend and set ‘points connected’ for all data plots.

• Using the point style pop-up menu in a drawing window to change the point styles in a legend
  
  - press \textbf{shift} to change the point style of all the data plots in the legend.

• Clicking a cell in a data window
  
  - press \textbf{option} to select the whole column above the clicked cell.
  - press \textbf{shift} to enlarge a selection.

• Clicking the column number cell in a data window

• Clicking on the ‘larger font size’ controls in the text-edit dialog box
  
  - press \textbf{option} to set the default columns (x, y, Δx, Δy) using a pop-up menu.
  - press \textbf{option} to increase the font size by 1 pt only.

• Clicking on the ‘subscript/superscript position’ controls in the text-edit dialog box
  
  - press \textbf{option} to change the vertical position of the selected text by 1 pt only.

• Choosing ‘New Function’ from the file menu
  
  - press \textbf{option} to open a new definition window containing a sample function definition.
  - press \textbf{option/shift} to open a new definition window containing a sample program definition.

• Importing text files
  
  - press \textbf{option} to tell proFit not to ask for information and to open the text files as data files using the current settings.

• Saving a drawing as an EPS file.

• Using lists in dialog boxes (e.g. the y-column list in the plot data dialog box).
  
  - press \textbf{shift click, shift \& drag} to select more than one item.
  - press \textbf{shift click} to de-select an item.

• Clicking with the lens tool in the Preview Window
  
  - press \textbf{command} to drag a selection rectangle specifying the region to enlarge.
  - press \textbf{option} to zoom out instead of zooming in.
• Selecting an item from the Help menu in a Function window
  option to paste the template with a ';' and a carriage return
  command to enable pasting templates and disable help panels
  shift to enable help panels and disable pasting templates

• Clicking a marker in the Preview window
  option to transform the clicked marker into the reference marker

• Moving a marker with the arrow keys in the Preview window
  option to let the marker go outside the ranges of the preview.

• Using the left and right arrow keys in a data window
  option to move the insertion point by one character within the active data cell.

• Clicking in the data window
  command to create a discontinuous selection

• Starting proFit
  option and shift in order not to load the standard preferences file

Another commonly used shortcut is typing a period (‘.’) while holding down the command key. This is equivalent to typing the escape key and it interrupts most of the calculations. Use it to stop the plotting of a function, to stop fitting, to cancel printing, or to interrupt lengthy calculations.

The combination Command-key/period is also interpreted as typing ‘Cancel’ in dialog boxes. The escape character is also interpreted as ‘Cancel’. Return or Enter are always interpreted as clicking the outlined button.
Appendix A: Predefined functions, procedures and arrays

When programming in proFit, you can use a large number of predefined functions and procedures. The first part of this appendix gives a short list of these functions and procedures ordered in functional groups. The second part of this appendix provides a full description of each function or procedure in alphabetical order.

Note that the proFit compiler ignores upper/lower case, i.e. SetColumnName is identical to setcolumnnamE. An exception to the above rule applies when you call other functions or want to execute menu commands. In that case the strings you specify for the names of the functions or menu commands are case-sensitive.

All the predefined functions and procedures described here are also available to external modules. In some cases, to avoid conflicts with the names of Mac OS routines, the names used in the external modules interface files (proFit_interface.h and proFit_interface.p) can be slightly different from the names used in proFit’s function windows. Unless the difference between the names is very small and obvious, external modules names are also found in the alphabetical listing at the end of this chapter.

Some predefined functions provide advanced features and are only available for external modules.

Routines only available for external modules are marked with a '*' in the following functional groups descriptions.

To get a fast look at what you can do in a proFit program, go through the following functional group descriptions. To get details on a certain function, see the alphabetical list which follows.

Functional groups

Operators

<table>
<thead>
<tr>
<th>Operator</th>
<th>Description</th>
</tr>
</thead>
<tbody>
<tr>
<td>+ - * /</td>
<td>addition, subtraction, multiplication, division</td>
</tr>
<tr>
<td>** ^</td>
<td>power</td>
</tr>
<tr>
<td>= &lt;&gt; &gt;= &gt;</td>
<td>equal, not equal, larger or equal, larger, smaller or equal, smaller</td>
</tr>
<tr>
<td>&lt;= &lt;</td>
<td>logical and, logical or</td>
</tr>
<tr>
<td>not</td>
<td>logical not</td>
</tr>
</tbody>
</table>

Note that the power operator ‘**’ (‘^’ is a synonym) is evaluated as
\[ x \ ^\ y = \ exp(y*ln(x)) \]

Therefore, x must be positive.

The evaluation of this expression can be rather slow. If you want to calculate simple integer powers, e.g. \( x^2 \) or \( x^3 \), use expressions such as \( \text{sqr}(x) \) or \( \text{sqr}(x) \times x \).
Mathematical functions and constants

- sin, cos, tan, arcsin, arccos, arctan
- sinh, cosh, tanh, arsinh, arcosh, artanh
- erf, erfc
- ln
- log
- exp
tento
- sqr, sqrt
- Gamma, GammaI, GammaLn, GammaP
- π (or pi), true, false, INF, -INF
- invalidNum

Trigonometric functions, (arguments or results in rad)
Hyperbolic functions
Error function
\( \text{erfc} \) is the complementary error function: \( \text{erfc} = 1 - \text{erf} \)
Natural logarithm
Base 10 logarithm
Exponential function, \( e^x \)
Power of ten, \( 10^x \)
Square, square root (\( x^2 \sqrt{x} \))
Gamma function and incomplete gamma function
Constants
An invalid number. Used to mark empty data cells in a data window.

Data processing

- Statistics
- Sort, ReduceData
- FFT, InverseFFT
- DataTransform
- Transpose

Run statistical analysis, get results
Sort, smooth or reduce data
FFT and inverse FFT
General data transformations
Transposing rows and columns

Accessing the data window

- data[i,j], DataOK, ClearData, TestData*, SetData*, GetData*
- GetCell, SetCell
- SetDefaultCols, SetDataWindowProperties
- xColumn, yColumn, xErrColumn, yErrColumn

An array and some routines for accessing the data in the current data window
Setting and reading cell contents, including text-cells.
Set the default x, y, Δx, and Δy columns and the number of columns and rows in the current drawing window.
The column numbers of the x, y, Δx, and Δy columns in the current data window
Appendix A: Predefined functions, procedures and arrays

**NrCols, NrRows**, SelectLeft, SelectTop, SelectRight, SelectBottom, GetSelection*

- **SelectCell, SelectRow, SelectColumn, RowSelected, CellSelected**
  - set the selection and check if a single cell or a row is part of a (possibly discontinuous) selection.

- **GetColName, SetColName, GetColType, SetColType, SetColWidth, ColEmpty**
  - obtain and write titles of single columns and other column characteristics.

- **GetDefaultData*, GetColHandle*, SetColHandle***
  - obtain column data in a single step from external modules.

All the above calls access the current data window. By default, the current data window is the frontmost data window. You can make another data window the current data window by calling `SetCurrentWindow(windowID)` with `windowID` being the window ID of the desired data window.

**Input and output**

ting information on the selection area and the size of the current data window

- **Input, SetBoxTitle**
  - displays a dialog for entering numerical values

- **Ask, Alert**
  - show alert boxes

- **Write, Writeln**
  - these procedures write into the results window

- **CreateTextFile, CloseTextFile, WriteToTextFile**
  - open and close text files, and redirect the output of the write, writeln functions to a text file.

**Drawing**

- **SetLineStyle, SetLineColor, SetFillColor, SetFillPattern, SetDataPointStyle, SetBGDataPointStyle, SetArrowStyle, SetTextStyle**
  - set the style of future drawing calls

- **MoveTo, LineTo, Move, Line, DrawLine**
  - produce line drawings in the drawing window.

- **OpenPoly, ClosePoly**
  - collect line-drawing calls to define a polygon
DrawLine, DrawDataPoint, DrawPICT*, DrawRect, DrawEllipse, DrawArc, DrawText, DrawNumber
GroupBegin, GroupEnd
DisableDrawingUpdates
GetSelectionBounds
GetClickedCoord

create single drawing objects in the current drawing window.
group drawing objects.
inhibit updates in the current drawing window until a program is finished.
find the rectangle corresponding to the boundaries of the current selection in the current drawing window
find the last clicked point in the current drawing window.

All the above calls access the current drawing window. By default, the current drawing window is the frontmost drawing window. You can make another drawing window the current drawing window by calling SetCurrentWindow(windowID) with windowID being the window ID of the desired drawing window.

The drawing routines work on a coordinate system that has its origin on the top left of the paper. Units are 1/72 inch.

The following program creates a “bull’s eye” at the point where you last clicked in the drawing window:

```
program BullsEye;
  const radius = 40; step = 8;
  var x0, y0, t: real;
    begin
    GetClickedCoord(x0, y0);
    GroupBegin;
    t := step;
    while t<=radius do
    begin
      DrawEllipse(x0-t,y0-t,x0+t,y0+t);
      t := t+step;
    end;
    MoveTo(x0-radius*1.1, y0);
    LineTo(x0+radius*1.1, y0);
    MoveTo(x0, y0-radius*1.1);
    LineTo(x0, y0+radius*1.1);
    GroupEnd;
    end;
```

The drawing routines accept floating point numbers as parameters. proFit uses a precise floating point coordinate system for drawings, and drawings created from a program will print at the highest resolution on all output devices.
Plotting in a graph

PlotData, PlotFunction  plot a data set or a function.
SetLineStyle,           set the line style (line thickness, color...) of future line-plots and the
SetLineColor,          style of future data points.
SetFillColor,
SetFillPattern,
SetDataPointStyle,
SetBGDataPointStyle
SetCurveFill,
SetEBarStyle
OpenCurve,
CloseCurve, OpenDataSet,
CloseDataSet
AddDataPoint,
DrawDataPoint
MoveTo, LineTo, Move,
Line

set the filling options of plots and the appearance of error bars for
the next curve or data set added to the current graph.
start/end the definition of curves or data sets for the current graph
add a data point (possibly including error bars) to the current data
set.
define a curve in the current graph.

All the above calls access the current graph. To make a graph the current graph, double-click it while
holding the command key down. From a program, you can use the call SetCurrentGraph to make a
graph the current graph.

The following is a small example program drawing a Lissajous figure in the drawing window:

```plaintext
plot a data set or a function.
set the line style (line thickness, color...) of future line-plots and the
style of future data points.
set the filling options of plots and the appearance of error bars for
the next curve or data set added to the current graph.
start/end the definition of curves or data sets for the current graph
add a data point (possibly including error bars) to the current data
set.
define a curve in the current graph.
```
program Lissajous;
var xmin, xmax, ymin, ymax;
    centerH, centerV, {center of the figure}
    radiusH, radiusV; {and its radius}
    angle;
begin
    xmin:=1;xmax:=3;
    ymin:=2;ymax:=5;
    CreateNewGraph(xmin,xmax, ymin,ymax, false,false);
    centerH := (xmin+xmax) / 2;
    centerV := (ymin+ymax) / 2;
    radiusH := (xmax-xmin) * 0.4;
    radiusV := (ymax-ymin) * 0.4;
    SetLineStyle(1,2);
    OpenCurve('Circle');
    MoveTo(radiusH+centerH, centerV);
    angle := 0;
    while (angle <= 2*pi) do
    begin
        LineTo(radiusH*cos(3*angle)+centerH, radiusV*sin(2*angle)+centerV);
        angle := angle + pi/40;
    end;
    CloseCurve;
    SetLineStyle(1,1);
end;

Creating and accessing graphs

SetNewGraphRect sets the default size and position of graphs created with CreateNewGraph.
CreateNewGraph creates a new graph in a drawing window.
GetCurrentGraph, SetCurrentGraph, GetNextGraph obtain a unique identification number for a graph and use it to access different graphs.

Editing the current graph

SetGraphAttributes set various options that determine the appearance of the current graph.
SetLegendProperties set visibility, position and size of the legend of the current graph.
GetGraphFrame, SetGraphFrame get/set the position and size of the current graph.
GetGraphCoordinates returns the ranges of the main axes in the current graph.
SetRange, MakeTicks, SetLabelsFormat, SetAxisPosition, SetAxisAttributes change the range, ticks, position, labels format, and various drawing options for the current axis.
MakeNewAxis, GetCurrentAxis, SetCurrentAxis, DeleteAxis create/kill coordinate axes in the current graph and change the current axis used to define a new curve or data set.
ClearTicks, ClearLables, AddTick, SetLabel, SetLabelText define a custom list of tick marks and/or labels.

All the above calls access the current graph. To make a graph the current graph, double-click it while holding the command key down. From a program, you can use the call SetCurrentGraph to make a graph the current graph.

Some of the above routines use or change the axes of a graph. They access the current x-axis or the current y-axis. To make an axis the current x-axis, call SetCurrentAxis(xAxis,i), where i is the number of the axis (SetCurrentAxis(xAxis,2) sets the current x-axis to X2). To make an axis the current y-axis, call SetCurrentAxis(yAxis,i).

Calls that work on the current axes are SetAxisPosition, SetLabelsFormat, etc. The following code changes the position of the X2 axis of the current graph:

```
SetCurrentAxis(xAxis,2);  %2nd x-axis
SetAxisPosition(xAxis,0.5);
```

**Setting default parameters**

SetParameterProperties Sets the value, name, limit and mode of a parameter

This routine is usually called in the procedure Initialize of a function. It allows to set the settings of a parameter that are given in the Parameter window.

Example: SetParameterProperties provides an alternative to the defaults statements (for external modules, it provides an alternative to setting the various default values and names by hand).
function foo;
  procedure Initialize;
  begin {initialization of param values, etc. }
    SetParameterProperties(param 1,
      value sin(pi/4), mode paramActive,
      name 'pi', min 0, max inf);
  end;
begin {function definition}
  y:=a[1]-sin(x);
end;

Using other functions or programs

CallFunction,
  CallProgram
SetFunctionParam,
GetFunctionParam,
GetFunctionParamMode,
GetFunctionParamName
GetNumFunctionParams
SetFunctionProperites
GetFunctionName
SelectFunction,
DeleteFunction,
DeleteProgram
GetGlobalData,
SetGlobalData
LoadParameterSet,
SaveParameterSet,
UseParameterSet,
DeleteParameterSet,
AddParameterSet

The following example program copies the active parameters of the current function to the first column of the current data window. It also calls a function called ChangeUnit to calculate new parameter values that it stores in the second column. Before using ChangeUnit, it sets the value of its first parameter to zero.
program CopyParams;
var i:integer;
   pa:extended;
begin
SetFunctionParam('changeUnit',1,0.0);
for i:=1 to GetNumFunctionParams('') do
   if GetFunctionParamMode('',i)=active then
      begin
         pa:=GetFunctionParam('',i);
         data[i,1]:=pa;
         data[i,2]:=CallFunction('ChangeUnit',pa);
      end;
end;

**Numerics on functions**

- **Integrate**, **TabulateIntegral**, **Derivative**
  calculate the integral and the derivative of a function

- **Root**, **TabulateRoots**
  calculate roots

- **Fit**
  set fitting, below.

- **Optimize**, **Extrema**, **TabulateExtrema**
  find extrema of a function by varying its x-value and/or its parameters

- **Tabulate**
  tabulate functions

**Fitting**

- **Fit**
  runs a fit.

- **GetResult**
  retrieves the results.

The following example runs a fit and prints some of the results:
program DoFit;
  var i, nrParams:Longint;

begin
  Fit(function Sin, algorithm levenberg, xColumn 1,
      yColumn 2);
  Writeln('chi squared: ', GetResult(chiSquared));
  nrParams := GetResult(chiSquared);
  Writeln('number of parameters: ', nrParams);
  for i := 1 to nrParams do
    writeln('     ', GetResult(fittedParameter, i));
end;

Using Windows and Documents

NewDataWindow, NewFunctionWindow, NewDrawingWindow
open a new data, function, or drawing window

getWindowID
obtain a unique identification number for a window from its title

FrontWindow, FrontmostWindow
obtain the ID of the document window in front of all others

getWindowType,
check if a window is a drawing window, a data window, or a function window.

setCurrentWindow, GetCurrentWindow, NextWindow
change the window currently used for program input/output.

getWindowTitle,
access the title of a window.

SelectWindow
Bring window in front of all other windows

OpenFile
open a document and put it inside a new window

SaveWindow
save a window's contents into an existing or a new pro Fit document

GetFileDirectory
Get the directory where a given file resides. Set the default directory used to save files without a full path name.

SetDefaultDirectory
close a window.

DataImportOptions, DataExportOptions
set the format for loading and exporting text files

SetWindowProperties
Set the info-text, size, title, position, etc. of a window.

Compile, DoScript
compile/run the contents of a function window

PageSetup, Print
specify document format and print
Note: Windows are usually accessed by window ID. A window ID is a unique long integer number assigned to each window. You can obtain a window ID by calling GetWindowID, FrontWindow, FrontmostWindow, GetCurrentWindow. The following example sets the name of the frontmost data window to "favourite data":

```pascal
program SetWindowName;
    var windowID: longint;
begin
    windowID := FrontmostWindow(dataType);
    SetWindowProperties(window windowID, name 'favourite data');
end;
```

Note: The Results, Parameter and Preview windows always have the same window ID:

- Results: window ID = −1
- Parameters: window ID = −2
- Preview: window ID = −4

The window IDs of data, text and drawing windows are always larger than 0.

**String and character manipulation**

- **Ord, Chr** convert between (extended) ASCII codes and characters.
- **Length** returns the length of a string.
- **Delete** deletes parts of a string.
- **Pos** finds a pattern in a string.
- **UpperString, LowerString** converts between upper- and lower case strings.
- **NumberToString, StringToNumber** convert between numbers and strings.
Miscellaneous auxiliary routines

Random
returns a random number between 0 and 1.

Invalid
checks if the result of a calculation is a valid number.

TickCount, DataString, TimeString
return the number of ticks (1/60 seconds) since start-up and today's date and time

Beep
lets your computer emit an alert sound.

SpeakString
lets your computer speak out loud a text string.

Button, KeyPressed
check the mouse button and the keyboard

GetClickedCoord
find the last clicked point in the current drawing window.

MarkedX, MarkedY, GetMarkedCoord
find the position of coordinate markers in the preview window

Undo, Cut, Copy, Paste, Clear, SelectAll
execute edit menus

DoMenu
execute a menu command

Capture
redirect output of results window to file

SetWaitTitle, SetWaitText
set the text displayed in pro Fit's progress window, shown during lengthy operations.

Advanced routines for external modules only

NumberToStr255*, Str255ToNumber*
conversion

GetModuleFile*
find a module's file

DeactivateProFitWindows*, ActivateProFitWindows*
tell pro Fit that a module is opening a window of its own.

GetDefaultData*
Get the current x- and y- data

GetColHandle*, SetColHandle*
Get and set in one step all the data contained in a column

HandleEvent*, CancelEvent*
event processing
### Alphabetical list

<table>
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<tr>
<th>Function/Procedure/Array</th>
<th>Description</th>
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</thead>
<tbody>
<tr>
<td><strong>Abs</strong></td>
<td>Returns the absolute value of x.</td>
</tr>
<tr>
<td><strong>ActivateProFitWindows</strong></td>
<td>External modules only. Activates pro Fit's frontmost window and enables the menus. Call this routine after closing a window or a dialog that you created from an external module. Each call to <strong>ActivateProFitWindows</strong> must be preceded by a call to <strong>DeactivateProFitWindows</strong>.</td>
</tr>
<tr>
<td><strong>AddDataPoint</strong></td>
<td>Adds a new data point to the current data set in the current graph. ( x ) and ( y ) are the coordinates of the new data point, ( xErr1 ) and ( yErr1 ), ( (xErr2 ) and ( yErr2 ) the lengths of the (asymmetric) error bars. Depending on the parameters passed to <strong>OpenDataSet</strong>, the parameters ( xErr1 ) through ( yErr2 ) may be ignored. Call <strong>OpenDataSet</strong> before calling <strong>AddDataPoint</strong>. The style and size of the data points can be set using the routine <strong>SetPointStyle</strong>. See also <strong>DrawDataPoint</strong>.</td>
</tr>
<tr>
<td><strong>AddParameterSet</strong></td>
<td>Adds the parameters that currently appear in the Parameter window to the parameter set menu. Parameters: ( \text{set} ) (String)The name of the set. ( forAll ) (Boolean)True if the parameter set is to be available for all functions, false if the parameter set is only to be available for the current function. (Default: false) ( permanent ) (Boolean)true if the parameter set must be added permanently to the menu, i.e. if it will be still available after a quit and restart. (Default: true) See also: <strong>UseParameterSet</strong>, <strong>SaveParameterSet</strong>, <strong>LoadParameterSet</strong>, <strong>DeleteParameterSet</strong></td>
</tr>
<tr>
<td><strong>AddTick</strong></td>
<td>Adds a tick at the position ( \text{tickPos} ) to the current axis, makes it a major tick if ( \text{isMajor} ) is true. ( \text{whichAxis} ) is either ( \text{xAxis} ) or ( \text{yAxis} ).</td>
</tr>
<tr>
<td><strong>Alert</strong></td>
<td>Presents a dialog box displaying the string s. Example: Calling <strong>Alert('Incomplete data.')</strong> opens the following window:</td>
</tr>
</tbody>
</table>
If you click ‘OK’ the program continues, if you click ‘Stop’ the program will be stopped.
In external modules, this routine is called **AlertBox**.

---

**AlertBox**

function AlertBox(s:Str255):Boolean;

External module name. See **Alert**. In external modules **AlertBox** is a function, and it returns **true** if the Stop button was clicked.

---

**arccos**

function arccos(x:extended):extended;

arccos returns the arcus cosine (the inverse cosine) of x. Causes a run-time error if \(|x| > 1\)

---

**arcsin**

function arcsin(x:extended):extended;

arcsin returns the arcus sine (the inverse sine) of x. Causes a run-time error if \(|x| > 1\)

---

**arctan**

function arctan(x:extended):extended;

arctan returns the arcus tangent of x

---

**arcosh**

function arcosh(x:extended):extended;

arcosh returns the inverse of the hyperbolic cosine of x. Causes a run-time error if \(|x| < 1\). arcosh is defined by

\[
\text{arcosh}(x) = \ln(x + \sqrt{x^2 - 1}).
\]

---

**arsinh**

function arsinh(x:extended):extended;

arsinh returns the inverse of the hyperbolic sine of x. arsinh is defined by

\[
\text{arsinh}(x) = \ln(x + \sqrt{x^2 + 1}).
\]

---

**artanh**

function artanh(x:extended):extended;

artanh returns the inverse of the hyperbolic tangent function of x. Causes a run-time error if \(|x| > 1\). artanh is defined by

\[
\text{artanh}(x) = \ln\left( \frac{x + 1}{\sqrt{x^2 + 1}} \right).
\]
function Ask\(s:\text{Str255}\):Boolean;

Presents a dialog box displaying the string \(s\). The box has a Yes and a No button. If the user clicks Yes, ask returns true, if he clicks No, ask returns false.

Example: Calling \(\text{Ask('Continue transformation ?')}\) displays the following window:

![Continue transformation ? dialog box]

In external modules, this routine is called \(\text{AskBox}\).

function AskBox(var retval:integer; \(s:\text{Str255}\)):Boolean;

External Module name. See \(\text{Ask}\). The return values depend on the button that was clicked:

\begin{itemize}
  \item Yes button: \(\text{retval}\) is 1 and \(\text{AskBox}\) returns false.
  \item No button: \(\text{retval}\) is 0 and \(\text{AskBox}\) returns false.
  \item Stop button: \(\text{retval}\) is undefined and \(\text{AskBox}\) returns true.
\end{itemize}

If \(\text{AskBox}\) returns true, you should stop executing your function or program.

procedure Beep;

produces an alert sound.

procedure BringWindowToFront\(\text{windowID}:\text{longint}\);

\textit{Obsolete.} Use \textit{SelectWindow} instead.

Moves the specified window in front of all other windows. \(\text{windowID}\) is a window id, such as it is e.g. returned by \textit{GetWindowID} or \textit{GetCurrentWindow}.

function Button:Boolean

Returns true if the mouse button is pressed.

function CalcStat\(\text{column}:\text{longint};\)

\begin{itemize}
  \item \(\text{selRowsOnly, withBasics, withSkewAndKurt, withMedian:Boolean}\):Boolean;
\end{itemize}

\textit{Obsolete.} Use \textit{Statistics} instead.

Runs a statistical analysis on the numbers in the current data window. The results of the calculations can be accessed using the routines \textit{GetBasics}, \textit{GetMedian}, and \textit{GetSkew}.

\(\text{CalcStat}\) returns false if an error occurred, true if the calculation completed correctly. Set \(\text{column}\) to 0 to include all columns, set it to -1 to use the current selection. Set \(\text{selRowsOnly}\) to true if you only want to analyze the currently selected rows.
If you consequently want to use the results of GetBasics, set withBasics to true. If you want to use the results of GetMedian, set withMedian to true. If you want to use the results of GetSkew, set withSkewAndKurt to true.

---

**CallFunction**

function CallFunction(name:Str255;x:extended):extended;

Calls a function from the Func menu. name is the name of the function as it appears in the menu. This parameter is case sensitive. Pass an empty string to call the currently selected function. x is the x-value passed to the function.

CallFunction causes a run-time error if the specified function does not exist.

Example:

```#
    k:=CallFunction('Polynom', 1.23)
    m:=CallFunction('',0);
```

k is set to the value of the built-in function Polynom at x=1.23, using the parameters as given in Polynom's parameters window. m is set to the value returned by the currently selected functions at x=0.

If you want to set a parameter of the function before calling it, use SetFunctionParam.

In external modules, after you call CallFunction you should call TestStop to check if the called function has interrupted execution.

---

**CallProgram**

procedure CallProgram(name:Str255);

Calls a program, module or AppleScript. name is its name as it appears in the Misc menu. causes a run-time error if the specified program or script does not exist. Note that name is case-sensitive.

In external modules, after calling CallProgram, you should call TestStop to check if the called program has interrupted execution.

---

**CancelEvent**

function CancelEvent(var theEvent: EventRecord):Boolean;

External modules only. For advanced programming. Returns true if the given event is a key down event for the escape-key or for command and '.'

---

**Capture**

procedure Capture(optional parameter list);

Controls redirection of results window to a text file. Parameters:

- **file** (String) The file to capture the window into. Use a simple name or a file path. If you pass this parameter, a new capture file is opened and capturing starts. Omit this parameter when passing the parameter ‘option’.

- **option** (Integer) captureOn (= start capturing into the file), captureOff (= stop capturing but leave capture file open), captureClose (= stop capturing and close capture file). Omit this parameter when passing the parameter ‘file’.

Example:

```#
    Capture(file 'myFile');  # now, output is redirced to the given file
    Capture(option captureOff);  # now, output to the file is temporarily suspended
    Capture(option captureOn);  # now, output to the file is again turned on
```
Capture(option captureClose);

*now, output to the file is turned off and the file is closed*

**CellSelected**
function CellSelected(row, column: longint) Boolean;
Returns true if the given cell in the current data window is selected

**ChiSquared**
function ChiSquared: extended;
Returns the value of the mean deviation function $\chi^2_R$ obtained in the last fit. $\chi^2_R$ is the mean square deviation $\chi^2$ if the last fit was performed using Gaussian distributed errors. Otherwise it is the value obtained by applying whatever deviation function must be applied for the given error specifications. See chapter 8, “Fitting”, for more details. Causes a run-time error if the last fit was not successful. You can check if the last fit was good using the function `numFitParams`.

**Chr**
function Chr(i: integer): char;
Converts the given (extended) ASCII code i to a character.

**Clear**
procedure Clear;
Equivalent to selecting “Clear” from the “Edit” menu.

**ClearData**
procedure ClearData(row, col: longint);
Removes any numerical value in the given cell (row/column) of the current data window and leaves an empty cell. Causes a run-time error if no data window is open or if the given cell lies outside the bounds of the list.

**ClearLabels**
procedure ClearLabels(whichAxis: integer);
Kills all labels in the current axis. `whichAxis` is either `xAxis` or `yAxis`.

**ClearTicks**
procedure ClearTicks(whichAxis: integer);
Kills all ticks in the current axis. Call before using `AddTick`, `whichAxis` is either `xAxis` or `yAxis`.

**CloseCurve**
procedure CloseCurve;
Stops data collection for the current curve.

**CloseDataSet**
procedure CloseDataSet;
Stops data collection for the current data set.

**ClosePoly**
procedure ClosePoly;
Stops data collection for the current polygon, opened by calling `OpenPoly`
CloseTextFile

procedure CloseTextFile(fileRefNumber: longint);
Closes the given text file. fileRefNumber is the reference number returned by CreateTextFile.

CloseWindow

procedure CloseWindow(optional parameter list);
Closes a window. Parameters:
  window     (Longint or String) The name or window ID of the window. Default: Front window
  saveOption (Integer) saveToFile (= always save into its file), dontSave (= never save), askUser (= if window has been changed, ask user if it should be saved). Default is askUser.
There is also an obsolete version of CloseWindow, which is supported for compatibility with older versions. Do not use it in new programs:

procedure CloseWindow(windowID:longint; saveIt:Boolean);
Set saveIt to false if you do not want to save the window, even if it was changed. windowID specifies the window.
This procedure cannot be called while a function is running.

ColEmpty

function ColEmpty(columnNumber:longint)Boolean;
Returns true if the given column of the current data window doesn’t contain any data.

Compile

procedure Compile(windowID:longint);
Compiles the given text window. Equivalent to choosing “Add to Menu” from the Misc menu. Generates a run time error if windowID does not belong to a function window, or if a syntax error occurs. windowID is a window id, such as it is returned by GetWindowID or FrontWindow.

Compl

function Compl(r1,r2: extended)complex;
Returns the complex number with r1 for real part and r2 for imaginary part.

ConfidenceInterval

procedure ConfidenceInterval(i:integer;var min,max:extended);
Returns (in min,max) the confidence interval for parameter i as it was calculated in the last fit. Note that this routine does not return meaningful results if the confidence interval for a given value was not determined, e.g. because the given parameter was not active during a fit or because the chosen fitting algorithm did not calculate confidence intervals.
See also: ParamSD

Conj

function Conj(z: complex)complex;
Returns the complex conjugate of z.

Copy

procedure Copy;
Equivalent to selecting “Copy” from the “Edit” menu.
Function cos(x: extended): extended;
Returns the cosine of x.

Function cosh(x: extended): extended;
Returns the hyperbolic cosine of x. cosh is defined by
\[ \cosh(x) = \frac{e^x + e^{-x}}{2}. \]

Function CovarMatrix(i, j: integer): extended;
Returns the values of the covariance matrix obtained in the last fit. i and j are the indices corresponding
to the parameter numbers.
CovarMatrix returns an invalid number (NAN: Not A Number) if i or j corresponds to a parameter that
was not active during the last fit. You can test the validity of the return value using the function
Invalid.
Causes a run-time error if the last fit was not successful or if i, j are out of range. You can check if the
last fit was successful by using the function NumFitParams.

Procedure CreateNewGraph(xmin, xmax, ymin, ymax: extended;
xScaling, yScaling: integer);
Creates a new graph in the current drawing window. xmin, xmax, ymin, ymax are the ranges of the graph
axes. xScaling, yScaling must be set to either 0, 1, 2, or 3 for linear scaling, logarithmic scaling, 1/x
scaling and probability scaling, respectively.
Causes a run-time error if there is no drawing window or if the ranges or axes styles are inconsistent.

Function CreateTextFile(fileName: Str255): longint;
Creates a text file with the given name and returns a reference number used to identify this file. Call
WriteToTextFile to redirect the output from calls to Write/Writeln/WriteNumber into this file and
use CloseTextFile to close the file when you are through.

Procedure Cut;
Equivalent to selecting “Cut” from the “Edit” menu.

Array data[row, col: longint] of extended
This array holds the data of the current data window. Assigning a value to data[row, col] sets the
value of a cell in this window. Reading the cell data[row, col] returns the value of a cell. Causes run-
time errors if the data cell is not within window, if the cell is empty, if the cell is part of a text column, or
if no data window is open. Always call DataOK(row, col) before using the value of data[row, col].
The array data does not exist for external modules. External modules must use the routines SetData
and GetData for numeric cells and GetCell and SetCell for text cells. In addition to this, the routines
GetData, GetColHandle and SetColHandle provide some fast low-level access.

Function DataExportOptions(optional parameter list);
Sets the options for exporting data windows as text files.
Parameters:

**mode**
Specifies the basic format. Pass withTitles (for standard format with column titles), withoutTitles (for standard format without column titles), or customFormat (for a customized format as specified in the following parameters).

**withTitles**
(Boolean) Add the text from the info field to the beginning of the file.

**copyInfo**
(Boolean) Write the text from the info field.

**optimize**
(Boolean) Remove leading spaces and trailing zeros in all numbers.

**delimiter**
(String) Column delimiter, at least 1 character. Typical values are:
- '\t' which defines a tabulator (decimal 8),
- '' which is a simple space,
- ',' which is a simple comma,
- Any combination of characters and '\t'.

Usually, '\n' (line feed) or '\r' (carriage return) should not be used.

**terminator**
(String) Line terminator appended after each row, at least 1 character. Typical values are:
- '\r' which defines a carriage return (decimal 13),
- '\n' which defines a line feed (decimal 10),
- Any combination of characters and '\r', '\n'.

Note that the line terminator must not be equal to the column delimiter.

**firstLine**
(String) A string to be added to the first line of the file.

To export data into a text file, first call DataExportOptions for setting the desired file format. Then call SaveWindow and pass textFieldType for the parameter.

See also: DataImportOptions

---

**DataImportOptions**

function DataImportOptions(optional parameter list);

Sets the options for importing text files. Parameters:

**mode**
(Integer) Specifies the basic format. Pass asFunction (for loading text files into a text window), withTitles (for loading text files as data in standard format with column titles), withoutTitles (for loading text files as data in standard format without column titles), or customFormat (for loading text files as data in a customized format as given by the following parameters).

**headerLines**
(Integer) The number of lines to be skipped at the beginning of the file.

**copyInfo**
(Boolean) Copy the header lines (specified with parameter headerLines) into the info field of the data window.

**withTitles**
(Boolean) Read the column titles.

**delimiter**
(String) Column delimiter, at least 1 character. Typical values are:
- '\t' which defines a tabulator (decimal 8)
- '' which is a simple space,
- ',' which is a simple comma,
- '\s' stands for “1 or more spaces”,
- '\w' stands for “1 or more spaces and/or tabulators in any sequence”,
- Any combination of characters and '\t'.

---

A-20  Appendix A: Predefined functions, procedures and arrays
**terminator** (String) Line terminator after each row, with at least 1 character. Typical values are:
- `'\r'` which defines a carriage return (decimal 13),
- `'\n'` which defines a line feed (decimal 13),
- Any combination of characters and `'\r'`, `'\n'`.  
Note that the line terminator must not be equal to the column delimiter.

To import data from a text file, first call `DataImportOptions` for setting the desired file format. Then call `OpenFile` and pass `textType` (for loading the file into a function window) or `dataType` (for loading the file into a data window) for the parameter “type”.

---

**DataTransform**

procedure DataTransform( optional parameter list )

Performs various data transformations on a data window. Corresponds to the command “Data Transform...” of the “Calc” menu.

Parameters:

- **window** (String or Longint) The name or window ID of the data window.
- **selectionOnly** (Boolean) True if operating on current selection, false if operating on x and y column.
- **selRowsOnly** (Boolean) True if operating on the selected rows only.
- **xColumn** (Longint) The x-column (omit if you pass true for selectionOnly)
- **yColumn** (Longint) The y-column (omit if you pass true for selectionOnly)
- **function** (String) The function to be used if operation is `functionOp`.
- **formula** (String) The formula if operation is set to `formula`.
- **argumentColumn** (Longint) The column to be used as argument if the operation works on a column argument.
- **argumentValue** (Real) The value to be used if the operation works on a value argument.

To use this command, you best choose “Start Recording” from the Misc menu, then choose “Data Transform...” from the Calc menu and set the desired options. Hit ok. The correct call is then recorded in your function window.

---

**DataOK**

function DataOK(row,col:longint):Boolean;

Returns `true` if the given cell of the current data window contains a numeric value, returns `false` if the cell is empty, if it is part of a text column, or if it lies outside the data window. Use this function before reading a data cell.

Example:

```plaintext
if DataOK(i,j) then myVariable := data[i,j];
```

`DataOK` causes a run-time error if no data window is open.  
The external module name for this function is `TestData`.
function DateString(format: integer):String;
Returns a string with today's date. format defines the formatting of the string and can take the following values: shortDate ('1/31/92'), abbrevDate ('Fri, Jan 31, 1992'), longDate ('Friday, January 31, 1992').
See also: TimeString

procedure DeactivateProFitWindows;
External modules only. For advanced programmers only. Deactivates all of pro Fit's windows and disables all menus. Call this routine before showing a window or creating a dialog. Each call to DeactivateProFitWindows must be matched with a call to ActivateProFitWindows.

procedure Delete(s: String; first, length: integer);
Deletes length characters in s, starting from character first. To delete all characters until the end of the string, pass 255 for length.
Example:
   s := 'hi there';
   Delete(s, 4, 2);
   WriteLn(s);     {writes 'hi ere'}

procedure DeleteAxis(whichAxis:integer;axisID:integer);
Deletes the given axis. axisID corresponds to the number used in the axis popup menu in the dialog box that appears when double clicking an axis, e.g. axisID=2 for axis X2. whichAxis is either xAxis or yAxis.

procedure DeleteFunction(func:String)
Removes the given function from the “Func” menu. func is the name of the function.
See also: DeleteProgram

procedure DeleteParameterSet(optional parameter list);
Deletes a parameter set previously saved with SaveParameterSet. Does nothing if the parameter set is not found. Parameters:
   name (String) The name of the set. Omit to delete all the sets belonging to the given function.
   ofFunction (String) The function the parameter set belongs to. Omit if the parameter set was available to all functions.
   file (String) The file from which the parameter set must be deleted. Omit to delete from permanent set.
   fromMenu (Boolean) True if the param set must be deleted from the parameter set menu. Default: true)
   fromFile (Boolean) True if the param set must be deleted from the file. Default: true.
See also: AddParameterSet, UseParameterSet, SaveParameterSet, LoadParameterSet
procedure DeleteProgram(prog:String)
Removes the given program, module or script in the “Misc” menu. prog is its name.
See also: DeleteFunction

function Derivative(name:Str255; x, scale:extended):extended;
Returns the derivative of a function. name is the name of the function as it appears in the Func menu.
This parameter is case sensitive. Use an empty string ("") for the function that is currently selected in the
Func menu. x is the x-coordinate where the derivative must be calculated. scale is the length of a typical
interval of x-values over which the function’s value changes.
For the parameter scale, a rough estimation is good enough. scale is typically something like the
length of the x-axis when you plot your function. It must not be too small. As an example, if your
function describes a 20 ns laser pulse and uses time in seconds as its input, set scale e.g. to \(10^{-8}\) (10
ns).
Causes a run time error if the function does not exist.

procedure DisableDrawingUpdates;
By default, proFit draws a shape immediately after a program created it. If you don’t want shapes to be
drawn immediately, call this routine before you start drawing. This can accelerate the execution of your
program.
There isn’t any “EnableDrawingUpdates” routine. DisableDrawingUpdates inhibits drawing until
your program has finished.

procedure DoCloseWindow(windowID:longint; saveIt:Boolean);
External module name, see CloseWindow

procedure DoMenu(theMenuItem:Str255);
Executes a command appearing in proFit’s menus. theMenuItem defines the command to be executed.
To execute a command from a normal (not hierarchical) menu, theMenuItem has the format:

\['menu name:item name'\]

To execute a command from a hierarchical menu, theMenuItem has the format:

\['menu name:submenu name:item name'\]

Instead of specifying an item name, you can also specify the number of the item in the menu preceded by
'#'.
This procedure cannot be called while a function is running.
Examples:

DoMenu('Edit:Copy');
DoMenu('Calc:Nonlinear Fit...');
DoMenu('Calc:Fourier Transform:FFT...$OK');
DoMenu('Draw:Rotate:#1');

If the command that you select in this way brings up a dialog box and if you want to automatically click
the OK button of this dialog box, add \'$OK' to the end of the string. Adding \'$OK' to the end of the
string has the same effect as immediately clicking OK when the dialog box comes up, but the dialog box
will not appear.
procedure DoScript(window: integer);

Runs the script in the given window. window is its window ID. Equivalent to selecting “Run” or “Run Selection” from the menu “Misc”.

procedure DoNewWindow(windowType: OSType);

External modules name. See NewWindow.

procedure DrawArc(left, top, right, bottom, start, length: extended);

Creates an arc inside the specified bounds in the current drawing window. It is a part of an ellipse. The arc extends from the angle start to the angle start+length.

procedure DrawDataPoint(x, y: extended);

Creates a data point at the coordinates x,y in the current drawing window. It uses the point style set by SetDataPointStyle, SetBGDataPointStyle.

If OpenDataSet has been called before calling DrawDataPoint, then DrawDataPoint creates a new data point in the current graph instead of drawing in the drawing window. In this case DrawDataPoint adds a point with zero error bars, a call to DrawDataPoint(x,y) is then equivalent to a call to AddDataPoint(x,y,0,0,0,0);

procedure DrawEllipse(left, top, right, bottom: extended);

Creates an ellipse inside the specified bounds in the current drawing window.

procedure DrawLine(start_h, start_v, end_h, end_v: extended);

Creates a line in the current drawing window extending between the given start and end points start_h, start_v, end_h, end_v.

procedure DrawNumber(theNum: extended; decs: integer; theAngle: extended; docenter: Boolean);

Converts theNum to a string and draws it in the current drawing window. decs defines the number of digits after the decimal point that must be displayed.

The text appears at the current pen position, set with MoveTo. If docenter is true, the number is centered on the current pen position and the current pen position remains unchanged. If docenter is false, the text starts at the current pen position and the current pen position is offset to the end of the text.

theAngle defines the rotation of the text and can take the values 0, 90, 180 and 270.

If docenter is false, the current pen position is offset to the end of the string.

procedure DrawPICT(left, top, right, bottom: extended; thePict: PicHandle);

External modules only. Creates a new picture in the current drawing window using the Mac OS PicHandle thePict. left and top give left top corner of the picture. right and bottom are used to define the size of the picture if they are larger than left and top, respectively. Otherwise the size is derived from the information given in thePict.
procedure DrawRect(left, top, right, bottom: extended);

Creates a new rectangle with the given borders in the current drawing window.

procedure DrawText(theString: Str255; theAngle: extended; docenter: Boolean);

Draws a text in the current drawing window. The text appears at the current pen position, set with MoveTo. If doCenter is true, the text is centered on the current pen position and the current pen position remains unchanged. If doCenter is false, the text starts at the current pen position and the current pen position is offset to the end of the text. theAngle defines the rotation of the text and can take the values 0, 90, 180 and 270. If doCenter is false, the current pen position is offset to the end of the string.

procedure DrawTextLine(theString: Str255; theAngle: extended; docenter: Boolean);

External module name. See DrawText.

function Erf(x: extended): extended;

The error function, defined by

\[ \text{erf}(x) = \frac{2}{\sqrt{\pi}} \int_{0}^{x} e^{-t^2} dt \]

function Erfc(x: extended): extended;

The complementary error function, \( \text{erfc}(x) = 1 - \text{erf}(x) \)

(Erf and Erfc are also available as P Erf and P Erfc for external Pascal modules to avoid ambiguities when using the unit fp.p, which defines erf and erfc.)

procedure Exit;

Exits a local function or procedure. If called in main body of a program or function, exits the program or function. See also: Halt.

procedure Extrema(optional parameter list);

Finds the minima/maxima of a function by varying its x-value within a given interval. Parameters:

- function (String) The function to be used. Omit for current function.
- xMin (Real) The start of the x-interval to be searched for extrema.
- xMax (Real) The end of the x-interval to be searched for extrema.
- subintervals (Integer) The number of sub-intervals to be searched in the x-interval. When the function’s derivative changes its sign over a sub-interval, the sub-interval is searched for a minimum or maximum.
- printResults (Boolean) Set to true for printing the results to the Results window. Omit “printResults” or set it to false for suppressing this.

To retrieve the results of a call to procedure Extrema, call the function GetResult(selector...). Use one of the following selectors:
extremaCount: the number of extrema found (≤ 100)

extremaXValue: x-value of each extremal point*

extremaYValue: y-value of each extremal point*

extremaSign: specifies if given point is minimum (extremaSign has value –1) or maximum (value 1) *

* pass an index (1..extremaCount) as second parameter to GetResult

The following example finds the maxima of the current function between –1 and 1, then prints them:

```pascal
program MaximaFinder;
var i, nrPoints:Longint;
begin
  Extrema(xMin -1, xMax 1, subIntervals 50);
  nrPoints:= GetResult(extremaCount);
  for i := 1 to nrPoints do
    if GetResult(extremaSign,i) > 0 then {if max.}
      Writeln(GetResult(extremaXValue, i));
end;
```

**Exp**

function Exp(x:extended):extended;
The exponential function.

\[ \exp(x) = e^x \]

**false**

const false = 0
This constant stands for the logical value of false.

**Fit**

procedure Fit(optional parameter list);
Runs a fit. Parameters:

- **function** (String) Function to be fitted. Omit for current function.
- **algorithm** (Integer) Algorithm to be used: levenberg, montecarlo, robust, linear, polynomial.
- **window** (String or Longint) The data window’s name or window ID. Omit for fitting the front window.
- **xColumn, yColumn** (Longint) The columns containing the x- and y-data. Pass -99 for using the row index as x-column.
- **xErrKind** (Integer) Errors of the x-data: individualError (if the x-errors are found in a column, passed in parameter “xErrColumn”), constantError (if the x-errors are constant, passed in parameter “xError”), percentError (if the x-errors are in percent, passed in parameter “xError”), zeroError (if the x-errors are assumed to be zero).
  Omit if x-errors are unknown.
- **xErrColumn** (Longint) The column containing the x-errors if “xErrKind” is individualError.
xError (Real) The x-error if “xErrKind” is constantError or percentError.

yErrKind (Integer) Errors of the y-data: individualError (if the y-errors are found in a column, passed in parameter “yErrColumn”), constantError (if the y-errors are constant, passed in parameter “yError”), percentError (if the y-errors are in percent, passed in parameter “yError”), unknownError (if the y-errors are unknown)
Omit if the y-errors are unknown.

yErrColumn (Longint) The column containing the y-errors if “yErrKind” is individualError.

yError (Real) The y-error if “yErrKind” is constantError or percentError.

fullDescription (Boolean) True if a complete protocol of the fit is to be printed in the results window, false if a shortened protocol is to be printed.

onlyActiveParameters (Boolean) True if all parameters are to be printed in the results window, false if only the fitted parameters are to be printed.

stopCounter (Longint) Defines the number of iterations if algorithm is montecarlo. Set to 0 if you want the fit to continue until it is interrupted manually. Omit for all other fitting algorithms.

doErrorAnalysis (Boolean) True for running a statistical error analysis after the fit (slow), false if errors are to be derived from the covariance matrix (Levenberg-Marquardt algorithm only). Default: false

confidence (Real) The desired confidence interval for statistical error analysis. Omit if doErrorAnalysis is false.

printResults (Boolean) Set to true for printing the results to the Results window. Omit “printResults” or set it to false for suppressing this.

To retrieve the results of the fit, use the function GetResult(selector...). Use one of the following selectors:

chiSquared chi squared
nrFittedParameters number of fitted parameters
fittedParameter fitted parameters*
covariance elements of the covariance matrix **
confidenceMin, confidenceMax lower and upper limits of the fitted parameters *
standardDeviation standard deviation of fitted parameters
nrIterations number of used iterations
goodnessOfFit goodness of fit
nrDataPoints number of fitted data points
sumOfDeviations sum of deviations (only after robust fit)
correlation linear correlation between x- and y-values (only after linear fit)
probCorrelation significance of linear correlation (only after linear fit)
* Pass parameter index (1 based) as second argument to GetResult
** Pass matrix indices (1 based) as second and third arguments to GetResult

Note: The old definition

```pascal
procedure Fit(funcName:String; xCol, yCol,
errCol:longint; errVal: extended;
selectionOnly:Boolean
```

is still supported but obsolete – do not use it in new programs.

---

**FittedParams**

```pascal
function FittedParams(i:integer):extended;
```

*Obsolete. Use GetResult(fittedParameters, i) instead.*

Returns the parameter values obtained in the last fit. \( i \) is the parameter index.
Causes a run-time error if \( i \) is out of range or if the last fit was not a successful fit.

---

**FFT**

```pascal
procedure FFT(optional parameter list)
```

Performs a Fourier transform on a data window. Input is a column of real values in the time domain, output are two columns of real/imaginary or amplitude/phase in the frequency domain. Parameters:

- `window` (String or Longint) Data window, specified by name or window ID.
- `inputCol` (Longint) Input column
- `outputCol1` (Longint) Output column for real part or amplitude in the frequency domain.
- `outputCol2` (Longint) Output column for imaginary part or phase in the frequency domain.
- `outFrequencyCol` (Longint) Output column to hold the frequency values (Hertz) of the data in `outputCol1` and `outputCol2`. Calculated from parameter “timeInterval”. Omit if no frequency column is to be calculated.
- `timeInterval` (Real) The time interval (Seconds) between consecutive data points in the input column. Used for calculating the frequency column. Omit if no frequency column is to be calculated.
- `realImaginary` (Boolean) True if the output columns are to hold the real and imaginary values in the time domain, false if they are to hold their amplitude and phase.
- `printResults` (Boolean) True if statistical information on the processed data is to be printed in the Results window.

See also: InverseFFT.

---

**FrontmostWindow**

```pascal
function FrontmostWindow(windowType:OSType):longint;
```

Returns the ID of the front most window of the given type, returns 0 if no window of the given type exists. `windowType` can either be `dataType`, `textType` or `drawingType` for specifying data windows, function windows and drawing windows, respectively.

---

**FrontWindow**

```pascal
function FrontWindow:longint;
```

Returns the window ID of the front window. The ID will be valid as long as the window exists. For more information about window IDs, see the section “Windows and Documents” above.
function Gamma(x: real/complex):real/complex;
Gamma function. x must be larger than 0 for real valued results. Real value accuracy > 12 digits.

function GammaI(a, x: real/complex):real/complex;
Incomplete gamma function. x and a must be larger than 0 if they are both real-valued. Real value accuracy approximately 8 digits. Complex value accuracy up to 12 digits.

function GammaLn(x: real/complex):real/complex;
Natural logarithm of the gamma function. Real value accuracy > 12 digits.

function GammaP(a,x: real/complex):real/complex;
Incomplete gamma function “P”.
\[
\Gamma_P(a,x) = 1 - \frac{\Gamma(a,x)}{\Gamma(a)}.
\]
x and a must be larger than 0 when they are both real-valued. Real value accuracy approximately 8 digits. Complex value accuracy up to 12 digits.

function GetAndSetStatus(newStatus:integer; var s:Str255):integer;
External modules only. For advanced programming. Returns the present execution status, then sets it to newStatus. The status can be 0(if normal operation), 1 (if the user interrupted operation), 2 (if a warning has been posted), 3 (if a run-time error has been posted). Set newStatus to -1 if you don't want to change the current status. If you set a status 2 or 3, pass a suitable error or warning message in s, it will be shown once your module is finished. On return, s holds the current message (if status was 2 or 3). Note: Calling StopExecution is equivalent to setting error status to 1 and TestStop returns true if error status is 1 or 3.

procedure GetBasics(var count:longint var sum,mean,variance,stdDev,meanAbsDev:extended);
Obsolete. Use Statistics and GetResult instead.
Returns some of the results obtained in the last statistics evaluation performed with the routine CalcStat. CalcStat must have been called with the withBasics parameter set to true if GetBasics is to be used.

procedure GetCell(var s:String;row,column:longint);
Returns the string in the given cell of the current data window. If the cell is in a number column, it converts the number to a string and returns the string.

procedure GetClickedCoord(var x,y:extended);
Returns the window-coordinates where the last mouse click took place in the current drawing window.
procedure GetColHandle(col:longint; var colH:Handle; 
  var length:longint; var colType:longint; 
  forWriting:Boolean);

External modules only. For advanced programming.
This routine returns a Mac OS handle to the data of the given column. You can read and/or modify the data in the handle. This is much faster than accessing a column's data through GetData/SetData and GetCell/SetCell.

colH can be nil if the corresponding column is empty. length is the number of rows held by this column, presently always equal to nrRows. forWriting must be set to true if you intend to change the contents of the column, set to false otherwise. If you change the data in the returned handle, you must subsequently call SetColHandle. colType is the type of the column (textColumn, floatColumn, doubleColumn)

Do not call DisposeHandle(colH) — colH is allocated and deallocated by pro Fit.
The organization of the data in colH depends on the data type of the column as returned by colType:
if colType = floatColumn, colH is a handle of type FloatColumnHandle (handle to an array of 4-byte floating point values), if colType = doubleColumn, colH is of type DoubleColumnHandle (handle to an array of 8-byte floating point values), if colType = textColumn, colH is of type TextColumnHandle (handle to a record of type StringData).

Note: For columns of type floatColumn and doubleColumn, the first entry of the array is reserved. The value of the first cell is found in the array element having index 1.

Warning 1: This routine should by used by experienced programmers only.
Warning 2: Accessing text columns in this way is not recommended. The definition of the data structure may change in the future.

While you are working on the data in colH, you should not call any other routines accessing the data window except GetColumnHandle and SetColumnHandle. When you modify the data in colH, you should avoid calling any pro Fit routines until you have called SetColHandle — if you want to call other pro Fit routines, first make a copy of the data by using HandToHand; once you have made all modifications to the data, call SetColHandle.

procedure GetColName(var name:Str255; col:longint);
Returns the title of the column col.

function GetColType(columnNumber:longint)longint;
Returns the type of the data of the given column (in the current data window).
Return values are textColumn (for text columns), floatColumn (for numeric columns having a range of -1e30 ... 1e30, i.e. 4-byte floating point values) or doubleColumn (for numeric columns having a range of -1e300 ... 1e300, i.e. 8-byte floating point values).

function GetCurrentAxis(whichAxis:integer)integer;
returns the ID number of the current x- or y-axis. whichAxis is either xAxis or yAxis.

function GetCurrentGraph:longint;
Returns a unique number identifying the current graph as long as it exists. Returns 0 if no current graph exists.
GetCurrentWindow

function GetCurrentWindow(windowType:longint):longint;

Returns the ID of the current window with type windowType.
windowType can be dataType, drawingType or textType specifying data windows, drawing windows and function windows.

GetData

function GetData(row,column:longint)extended;

External modules only. Returns the numerical value of the given cell in the current drawing window.
GetData replaces the predefined matrix data[i,j] used from functions within proFit.

GetDefaultData

procedure GetDefaultData(xColH,yColH, xErrColH, yErrColH:ExtendedArrayHandlePtr;
indecesH:LongArrayHandlePtr; var arraySize:longint;
selectedRowsOnly:Boolean; info:DataInfoPtr);

DataInfo = record
xMin,xMax,xPosMin,xNegMax: extended;
yMin,yMax,yPosMin,yNegMax: extended;
ordered: Boolean;
zeroYErrors,invalidYErrors,
zeroXErrors,invalidXErrors: Boolean;
end;
DataInfoPtr = ^DataInfo;

This routine provides a copy of the default x-y data in the current data window. It allocates memory for the x,y arrays, for the x,y-Error arrays, and for the array that gives the corresponding row numbers in the data window. Then it fills them with the data. It copies only the data where both the x and the y cell contain valid numbers. The arrays are returned in xColH^, yColH^, xErrColH^, yErrColH^.
Pass nil for one of these arrays if you are not interested in it.
The record info holds some more information about the returned data.
The arrays returned by GetDefaultData contain valid data starting from the element with index 1. The value of the element with index 0 is undefined. The last element has index arraySize.
arraySize is set to zero in case of out-of-memory situations or other problems.
Warning: This routine should only be used by advanced programmers.

GetFileDirectory

function GetFileDirectory(ID:longint; s:string):boolean;

Returns the directory where the document displayed in the given window is stored.
ID is the windowID. The path-name of the directory is returned in the string s. This function returns false if the path-name had to be truncated.

GetFrontWindow

function GetFrontWindow:longint;

External module name. See FrontWindow.

GetFunctionName

function GetFunctionName:Str255;

Returns the name of the current function.
GetFunctionParam

function GetFunctionParam(name:Str255; i:integer):extended;

Returns the default value of a parameter. name is the name of the function. This parameter is case-sensitive. Use an empty string ("") to specify the function currently selected in the Func menu. i is the parameter index.

Example:
GetFunctionParam('Polynom', 1) returns the degree of the built-in function “Polynom”.

GetFunctionParamMode

function GetFunctionParamMode(name:Str255; i:integer):integer;

Returns the fitting mode (active, inactive, constant) of a parameter. name is the name of the function. This parameter is case-sensitive. Use an empty string ("") to specify the function currently selected in the Func menu. i is the parameter index.

GetFunctionParamName

function GetFunctionParamName(name:Str255; i:integer):integer;

Returns the name of a parameter. name is the name of the function the parameter belongs to. This parameter is case-sensitive. Use an empty string ("") to specify the function currently selected in the Func menu. i is the parameter index.

GetGlobalData

function GetGlobalData(index:integer):real;

Returns the value stored under the given index in a global data array. This data array is shared between all functions and programs. It can be used for communication between programs, functions, scripts and modules.

The index must between 0 and 99.

See also: GetGlobalData

GetGraphCoordinates

procedure GetGraphCoordinates(var xmin,xmax,ymin,ymax:extended);

Returns the minimum and maximum values of the main x- and y-coordinate axes of the current graph in xmin, xmax, ymin, ymax.

If the current graph looks like the one to the right, GetGraphCoordinates returns xmin=0, xmax=6, ymin=-1, ymax=1.

GetGraphFrame

procedure GetGraphFrame(var left,top,right,bottom:extended);

Returns the enclosing rectangle of the current graph.

GetMarkedCoord

procedure GetMarkedCoord(i:integer;var x,y:extended);

Returns the coordinates of the preview window marker with index i in x, y. Pass i=0 for the reference marker.
procedure GetMedian(var count:longint; var mean,median,minimum,maximum:extended);

Obsolete. Use Statistics and GetResult instead.
Returns some results of the last call to CalcStat. CalcStat must have been called with the withMedian parameter set to true before this function can be used.

function GetModuleFile:FSSpecPtr;
External modules only. Returns a pointer to the FSSpec record of the file where the currently running external module was found. Returns nil if no such file exists.

function GetNextGraph(graphID:longint)longint;
Returns the graph following the one with the given ID, returns the first graph if graphID=0. Returns 0 if graphID points to the last graph. Returns 0 if no graph exists with the given ID.
Called repeatedly, GetNextGraph cycles through all graphs and returns their ID. Start with GetNextGraph(0) to make sure that all graphs are scanned.

function GetNumFunctionParams(name:Str255):integer;
Returns the number of parameters used by a function. name is the name of the function. This parameter is case sensitive. Use an empty string ("") to specify the function currently selected in the Func menu.

function GetResult(selector, [index1,[index2]]);
This function returns the results of various commands. The desired result is selected by the resultSelector. If the result is an array or matrix, you have to add one or two indices index1, index2. If the result is a simple number, omit the indices.
These are the commands that GetResult returns results for: Fit, Optimize, Statistics, Root, Extrema, Integral
See the definitions of the respective commands for the selectors to be passed to GetResult.

function GetSelection:Rect;
External modules only. Returns the coordinates of the contiguous selection in the current drawing window. The rectangle's coordinates correspond to SelectLeft, SelectTop, SelectRight, SelectBottom.

function GetSelectionBounds(var left, right, top, bottom: extended);
Returns the boundaries of the current selection in the current drawing window.

procedure GetSkew(var count:longint; var mean,variance,skewness,kurtosis:extended);

Obsolete. Use Statistics and GetResult instead.
Returns some results of the last call to CalcStat. CalcStat must have been called with the withSkewAndCurt parameter set to true before this function can be used.
function GetWindowID(windowName:Str255)longint;
Returns the window ID of the window having the given title. Returns 0 if there is no window with this title.

procedure GetWindowTitle(windowID:longint; var name:Str255);
Returns the title of the given window. windowID is the window ID of the window, such as it is e.g. returned by GetWindowID or FrontWindow.

function GetWindowType(windowID:longint)longint;
Returns the type (dataType for data windows, textType for function windows, drawingType for drawing windows) of the given window. Returns 0 if the given window is of any other type.

windowID is the window ID of the window, such as it is returned by GetWindowID or FrontWindow.

globalData: array[0..100] of extended
Obsolete. Not supported in version 5.1 or later. Use GetGlobalData and SetGlobalData instead.

procedure GrLine(x,y:extended);
External modules name. See Line.

procedure GrLineTo(x,y:extended);
External modules name. See LineTo.

procedure GrMove(x,y:extended);
External modules name. See Move.

procedure GrMoveTo(x,y:extended);
External modules name. See MoveTo.

procedure GroupBegin;
Starts the definition of a group. All drawing taking place after this call will be part of a group. Call GroupEnd when you have finished drawing the parts of the group.

procedure GroupEnd;
Ends the definition of a group. See GroupBegin.

procedure Halt;
Exits the running a program or function. See also: Exit.
procedure HandleEvent(var theEvent: EventRecord);
External Modules only. For advanced programming. Passes theEvent to pro Fit for handling it. Use this call to handle update events when creating your own window. theEvent is a pointer to the Mac OS event record.

\[
\text{const } ii = \text{compl}(0,1);
\]
The imaginary unit.

\[
\text{function } \text{Im}(z: \text{complex}) \text{extended};
\]
Returns the imaginary part of the complex number \( z \). To get the real part, call function \( \text{Re} \).

\[
\text{const } \text{inf} = 1/0;
\]
An infinitely large number. Use \(-\text{inf}\) for an infinitely large negative number.

procedure Input(s1:Str255; var v1; s2:Str255; var v2; ...);
Brings up a dialog box where you can enter new values for v1, v2... Input can set up to 6 variables of type Real or String. Each variable can be preceded by a string defining a title to be shown for the variable. If you omit this string, the variable’s name is used. The title of the dialog box can be set using the \text{SetBoxTitle}. Example:

\begin{verbatim}
program test;
 var
 a:extended;
 i:integer;
begin
 a := 0.5;  i := 10;
 SetBoxTitle('starting parameters');
 Input('value of a',a,'value of i',i);
end;
\end{verbatim}

This program first assigns default values to the variables \( a \) and \( i \). Then it asks the user to change these variables if she wants to. The program displays the following dialog box:

The title was set using the routine \text{SetBoxTitle}. The user can enter new values for the variables. If she clicks ‘OK’, the program continues, if she clicks ‘Stop’, the program is interrupted immediately.
**Input** checks if the title for a parameter starts with ' $ ' followed by one or more special characters. Use this option if the corresponding variable is to be entered by means of a pop-up menu or a check box. If the title starts with:

'- $W...':

a pop-up menu with a list of all data windows is used. Initialize the variable for the window to 0 or the reference ID of a data window before passing it to Input. On return, it contains the reference ID of the selected window.

'- $C...':

a pop-up menu with a list of a columns in a data window is used. If there is a popup menu with data windows in the same dialog box, then the columns of the selected data window are shown, otherwise the columns of the current data window are shown.

'- $Pxxxx$...':

a pop-up menu with user defined items is used. The items are defined by string xxxx (terminated by ' $ '). xxxx recognizes the metachars defined for the Mac OS routine `AppendMenu`, e.g. use semicolons to separate the items in xxxx.

'- $X...':

a check box is used. It is unchecked if the variable is 0, checked otherwise. The returned value will be 0 (unchecked) or 1 (checked).

**Example:**

```plaintext
Input('$Wwindow', w, '$Cdata column', col, '$Pyes;no;-;maybe$do it?', fuzzy);
```

brings up the following dialog box:

![Dialog Box Example]

**Limitations:**

You can only specify one data window pop-up.

If you have a data window pop-up as well as one or more column pop-up menus, the data window pop-up must appear before the column pop-up.

---

**InputBox**

```plaintext
function InputBox(nrArgs:integer;var r:InputRec):Boolean;
```

External Modules Only. Replaces the routine *Input*. The parameter `nrArgs` gives the number of elements of the record `r`. The record `r` has the type `inputRec`.

---

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type
ExtendedPtr = ^extended;

InputRec =
  packed array[1..maxNrInputValues] of record
    x: ExtendedPtr;
    s: ^str255;
  end;

Strings and values are set according to the explanations given for the routine Input. In addition to the
'..' meta-commands recognized by Input, InputBox also understands the meta command 'SS..' which
specifies that the parameter is a string pointer.
The following is an abbreviated example showing how to call InputBox in Pascal:

var
d1: extended;
s1, s2: Str255;
r: InputRec;
Str255: s;
begin
d1 := 1.1;  { default values }
s := 'default text';
s1 := 'data1';  { and names }
s2 := '$Sdata2';
r[1].x := @d1;  { set entries of r }
r[2].x := ExtendedPtr(@s);
r[1].s := @s1;
r[2].s := @s2;
if InputBox(2, r) then ...
(If you are programming in C: @ is Pascal’s address operator (corresponding to & in C). For C, the
indices of the InputRec range from 0 to 5.)

function Integral(name:Str255; min,max:extended;
  iterations:integer):extended;
  Obsolete. Use Integrate instead.
  Returns the integral of a function. name is the name of the function as it appears in the Func menu. This
  parameter is case-sensitive. Use an empty string ("") to specify the function currently selected in the Func
  menu. min and max are the lower and upper limits of the integral. iterations is the number of
  iterations for calculating the integral (must be in the range 5..15). A small number of iterations makes
  execution faster but decreases accuracy — a large value slows down execution but yields a more accurate
  result.

procedure Integrate(optional parameter list)
  Calculates the integral of a function over a given x-range. Parameters:
    function          (String) The function to be used. Omit for current function.
    xMin             (Real) The start of the x-range.
    xMax             (Real) The end of the x-range.
iterations (Integer) The number of iterations (5 .. 15). The more iterations you use, the more accurate the result becomes.

printResults (Boolean) Set to true for printing the results to the Results window. Omit “printResults” or set it to false for suppressing this.

To retrieve the results, use the function GetResult(selector) with one of the following selectors:

- integralValue: the integral
- integralAccuracy: the correction in the last iteration

The following piece of code calculates the integral of the current function between -1 and 1, then prints it:

```
Integrate(xMin -1, xMax 1, iterations 10);
Writeln(GetResult(integralValue));
```

See also: TabulateIntegral

---

Invalid

function Invalid(val:extended):Boolean;

Returns true if val is an invalid number (a NaN: Not A Number). Use this function to test the results of Root, Maximum and Minimum, or of other functions that can return a NaN in some cases.

---

InverseFFT

procedure InverseFFT(optional parameter list)

Performs an inverse Fourier transform on a data window. Input are two columns of of real/imaginary or amplitude/phase in the frequency domain. Output is a column of real values in the time domain. Parameters:

- window (String or Longint) Data window, specified by name or window ID.
- inputCol1 (Longint) Input column for real part or amplitude in the frequency domain.
- inputCol2 (Longint) Input column for imaginary part or phase in the frequency domain.
- outputCol (Longint) Output column
- outTimeCol (Longint) Output column to hold the time values (Seconds) of the data in outputCol. Calculated from parameter “frequencyInterval”. Omit if no time column is to be calculated.
- frequencyInterval (Real) The frequency interval (in Hertz) between consecutive data points in the input columns. Used for calculating the time column. Omit if no time column is to be calculated.
- realImaginary (Boolean) True if the input columns hold the real and imaginary values in the time domain, false if they hold their amplitude and phase.
- printResults (Boolean) True if statistical information on the processed data is to be printed in the Results window.

See also: FFT.

---

invalidNum

const invalidNum = "not a number";

An invalid number, a NaN.
function KeyPressed(key:integer):Boolean;
Returns true if the given key of the keyboard is currently held down. key can be optionKey, commandKey, shiftKey, controlKey.

function Ord(s: String)integer;
Returns the length of the given string s.

procedure Line(dx,dy:extended);
Draws a line from the current pen position x, y to the position x+dx, y+dy. Offsets the current pen position by dx, dy.

procedure LineTo(x,y:extended);
LineTo draws a line from the current pen position to x,y. Sets the current pen position to x,y.

function Ln(x:extended):extended;
Returns the natural logarithm (base e) of x. Causes a run-time error for x < 0. Returns -INF for x=0.

procedure LoadParameterSet(optional parameter list);
Loads a given parameter set previously saved with SaveParameterSet. The loaded parameters appear in the Parameter window. Parameters:

- name (String) The name of the set.
- ofFunction (String) The function the parameter set belongs to. Omit if the parameter set was available to all functions.
- file (String) The file from where the parameter set must be loaded. Omit to load from permanent sets.

See also: AddParameterSet, UseParameterSet, SaveParameterSet, DeleteParameterSet

function Log(x:extended):extended;
Returns the base 10 logarithm of x. Causes a run-time error for x < 0. Returns -INF for x=0.

procedure LowerString(var s: String);
Converts all characters of s to lower case. See also UpperString

procedure MakeNewAxis(whichAxis:integer; min,max:extended;
    scaling:integer; position: extended);
Creates a new x (whichAxis = xAxis) or y (whichAxis = yAxis) axis in the current graph. The newly created axis becomes the current axis. Use GetCurrentAxis to find the ID of the newly created axis.

position gives the coordinate of the new axis in the coordinate system of the main axes X1, Y1.
scaling can take the values 0 (linear scaling), 1 (logarithmic scaling), 2 (1/x-scaling), 3 (probability scaling).
procedure MakeTicks(whichAxis: integer; firstMaj, distance: extended; nrMinTicks: integer);

Creates a new set of ticks for the given axis.
whichAxis is xAxis or yAxis. firstMaj and distance give the position of the first major tick and the distance between major ticks. nrMinTicks defines the number of minor ticks between consecutive major ticks.

function MarkedX(i: integer): extended;

function MarkedY(i: integer): extended;

Return the x-coordinate and y-coordinate of the preview window marker with index i. Pass i=0 for the reference marker. Returns a NaN if no marker with index i exists.

function Maximize(theFunction: Str255; precision: extended; varyX: Boolean; var x, y: extended): Boolean;

Obsolete. Use Optimize instead.
Finds the parameter set that gives a maximum value for the given function.
theFunction is the name of the function as it appears in the Func menu. This parameter is case-sensitive. Use an empty string ("") to specify the currently selected function. precision defines the accuracy of the calculation – Maximize will run repeated iterations until the function value changes by less than precision in consecutive iterations. If varyX is true, Maximize varies the active parameters as well as the x-value of the function, if false, only the active parameters are varied and the x-value is not changed.
The variables x and y return the x- and y-values where the maximum is found.
The algorithm used is the Simplex method.

function Maximum(name: Str255; min, max: extended): extended;

Obsolete. Use Extrema instead.
Returns the maximum of a function, i.e. the x-value where the function's value is largest. name is the name of the function as it appears in the Func menu. This parameter is case-sensitive. Use an empty string ("") to specify the currently selected function. min and max are the boundaries of the interval where the maximum must be found.
Maximum starts looking for a maximum only if the slope of the function is positive at x=min and negative at x=max.
If no maximum is found, the function returns NaN (Not A Number). Use the function Invalid to test if the result is an NaN.

function Minimize(theFunction: Str255; precision: extended; varyX: Boolean; var x, y: extended): Boolean;

Obsolete. Use Optimize instead.
Finds the parameter set that gives a minimum value for the given function.
theFunction is the name of the function as it appears in the Func menu. This parameter is case-sensitive. Use an empty string ("") to specify the currently selected function in the Func menu. precision defines accuracy of the calculation – Minimize will run repeated iterations until the function's value changes by less than precision in consecutive iterations. If varyX is true, Minimize varies the active
parameters as well as the x-value of the function, if false, only the active parameters are varied and the x-
value is not changed.
The variables $x$ and $y$ return the x- and y-values where the maximum is found.
The algorithm used is the Simplex method.

---

**Function: Minimum**

```plaintext
function Minimum(name:Str255; min,max:extended):extended;
```

*Obsolete.* Use Extrema instead.
Returns the minimum of a function, that is the x-value where the function value is the smallest. `name` is the name of the function as it appears in the Func menu. This parameter is case-sensitive. Use an empty string ("") to specify the currently selected function. `i` is the parameter index. `min` and `max` are the boundaries of the interval where the minimum must be found.
This function starts looking for a minimum only if the slope of the function is negative at $x=\text{min}$ and positive at $x=\text{max}$.
If no minimum is found the function returns `NAN` (Not A Number). Use the function `invalid` to test if the result is an `NAN`.

---

**Procedure: Move**

```plaintext
procedure Move(dx,dy:extended);
```

Offsets the current pen position from its current position by $dx$, $dy$.

---

**Procedure: MoveTo**

```plaintext
procedure MoveTo(x,y:extended);
```

Moves the current pen position to $x,y$ without drawing anything.

---

**Procedure: NewDataWindow**

```plaintext
procedure NewDataWindow(optional parameter list);
```

Opens a new data window. Parameters:
- `nrRows` (Longint) The number of rows. Omit for default (200)
- `nrCols` (Longint) The number of columns. Omit for default (10)
- `name` (String) The name of the new window. Omit for using a default name.
- `boundsLeft, boundsTop, boundsBottom, boundsRight` (Integer) The bounds of the window in global screen coordinates, omit for default position and size.
- `info` (String) The info text attributed to the window. Omit for leaving it empty.
- `fontName` (String) The font to be used for the new window.
- `fontSize` (Integer) The font size to be used for the new window.

---

**Procedure: NewDrawingWindow**

```plaintext
procedure NewDrawingWindow(optional parameter list);
```

Opens a new drawing window. Parameters:
- `name` (String) The name of the new window. Omit for using a default name.
- `boundsLeft, boundsTop, boundsBottom, boundsRight` (Integer) The bounds of the window in global screen coordinates, omit for default position and size.
<table>
<thead>
<tr>
<th>info</th>
<th>(String) The info text attributed to the window. Omit for leaving it empty.</th>
</tr>
</thead>
<tbody>
<tr>
<td>fontName</td>
<td>(String) The font to be used for the new window.</td>
</tr>
<tr>
<td>fontSize</td>
<td>(Integer) The font size to be used for the new window.</td>
</tr>
<tr>
<td>fontStyle</td>
<td>(Integer) The font style to be used for the new window (bold, italic, ...)</td>
</tr>
</tbody>
</table>

**NewFunctionWindow**

procedure NewFunctionWindow(optional parameter list);

Opens a new text window. Parameters:

- **name** | (String) The name of the new window. Omit for using a default name.
- **boundsLeft, boundsTop, boundsBottom, boundsRight** | (Integer) The bounds of the window in global screen coordinates, omit for default position and size.
- **info** | (String) The info text attributed to the window. Omit for leaving it empty.
- **fontName** | (String) The font to be used for the new window.
- **fontStyle** | (Integer) The font style to be used for the new window (bold, italic, ...)
- **fontSize** | (Integer) The font size to be used for the new window.

**NewWindow**

procedure NewWindow(windowType: longint);

*Obsolete*. Use NewDataWindow, NewDrawingWindow or NewFunctionWindow instead.

Creates a new window of the given type. windowType is drawingType (for drawing windows), dataType (for data window) or textType (for function windows). The new window becomes the “current window” of its type.

This procedure cannot be called while a function is running.

**NextWindow**

function NextWindow(windowID: longint) longint;

Returns the window (i.e. the window ID) of the window behind the window having the given windowID. If windowID is 0, it returns the frontmost window. Returns 0 if no window behind the given window.

The following example tiles all data, text and drawing windows. It first cycles through the windows to count them. Then it moves them.
program TileWindows;
const hTile = 5;        {horizontal tiling offset}
    vTile = 18;       {vertical tiling offset}
var windID: longint;
    nrWindows: integer;
    left, top: integer;
begin
    nrWindows := 0;
    windID := FrontWindow;
    while windID <> 0 do        {count the windows}
    begin
        if windID > 0 then       {if a data, drawing}
        begin
            nrWindows := nrWindows+1;         {or text}
            windID := NextWindow(windID);
        end;
        left := nrWindows*hTile;
        top := nrWindows*vTile;
        windID := FrontWindow;
    end;
    windID := FrontWindow;
    while windID <> 0do        {place the windows}
    begin
        if windID > 0 then {if a data, drawing}
        begin                              {or text}
            PlaceWindow(windID, 3+left, 30+top, 0, 0);
            top := top-vTile; left := left-hTile;
        end;
        windID := NextWindow(windID);
    end;
end;

function NrCols:longint;
Returns the number of columns (numeric and text columns) of the current data window. Causes a run-time error if no data window is open.

function NrRows:longint;
Returns the number of rows of the current data window. Causes a run-time error if no data window is open.

function NumberInvalid(val:extended):Boolean;
External modules name. See Invalid.

procedure NumberToStr255(x:extended; var s:Str255;
    format,digits:integer);
External modules only. Converts the number x into a string. format/digits control the conversion process:
    format = 0: normal conversion

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if digits > 0: the number of digits after the '.', if digits < 0: the total number of digits (approx.)

format = 1: optimized conversion, removes unnecessary trailing zeros after the decimal point, unnecessary '+' signs, decimals points, etc.
digits: the number of digits

NumberToString

procedure NumberToString(x: real; var s: String; minimize: Boolean; digits: integer);
Converts x to a string and returns it in s. If digits is positive or 0, it specifies the number of digits after the decimal point, otherwise the total number of digits of the resulting string. If minimize is true, trailing zeroes and any trailing decimal point are/is removed.

NumFitParams

function NumFitParams:integer
Returns the number of parameters of the last fitted function. This is the total number of parameters, including constant and inactive parameters.
Returns 0 if the last fit was not successful. Use this function to check the validity of the last fit before using such functions as CovarMatrix or ParamSD.

OpenCurve

procedure OpenCurve(curveName:Str255);
Opens a new curve in the current graph. After having called OpenCurve, calls to MoveTo, LineTo, Move, Line will add segments to the curve. curveName is the name of the curve in the legend. Call CloseCurve when you have completed the curve.
DrawDataPoint is not affected by this procedure. It will continue drawing point shapes. Don't use AddDataPoint between OpenCurve and CloseCurve.
Note that the parameters to be passed to MoveTo, LineTo, Move, Line are in the coordinates of the current x- and y-axes. (Use SetCurrentAxis to set these axes before calling OpenCurve.)
OpenCurve causes a run-time error if no current graph is available.

OpenData

procedure OpenData(fileName:Str255);
Opens the given file as a data file. The file must either be a proFit data file or a text file with valid data. The new window becomes the “current data window”.
If fileName contains a simple file name, the file is loaded from pro Fit's folder. If fileName contains a file path, the file is loaded from the folder defined in the file path. Set fileName to '? ' to bring up a dialog box prompting the user for the name. A run-time error occurs if the file cannot be opened.
This procedure cannot be called while a function is running.
If you want to open a text file with custom format, use SetTextFileFormat to set the format.

OpenDataSet

procedure OpenDataSet(errors:integer; connected:Boolean; name:Str255);
Opens a new data set in the current graph. Once you have called OpenDataSet, call AddDataPoint or DrawDataPoint to add data points. Once you have added all data points, call CloseDataSet.
Parameters:
This parameter is 0 (if the data points should not have error bars) or a sum of the constants \(eBarX\) (symmetric error bars in X), \(eBarY\) (symmetric error bars in y), \(asymEBarX\) (asymmetric error bars in X), \(asymEBarY\) (asymmetric error bars in Y).

**name**

The name associated with the curve. It appears in the legend of the graph.

By passing the appropriate value in errors, you tell proFit if it should allocate space for holding error values or not. If you want to use error bars, you have to call the routine AddDataPoint to add data points and their error bar lengths in the currently open data set. If you are not interested in error bars, simply call DrawDataPoint. AddDataPoint ignores its xErr parameter if errors is noErrorBars or errorBarsY. It ignores the yErr parameter if errors is noErrorBars or errorBarsX. OpenDataSet causes a run-time error if no current graph is available.

**Example:** The following program draws a graph with all types of data points.

```plaintext
program test;
var i,j;
begin
CreateNewGraph(0,18,0,3,0,0);
for i := 1 to 17 do
begin
SetDataPointStyle(i,9,0.5);
OpenDataSet(0,false,'name');
DrawDataPoint(i,1);
DrawDataPoint(i,2);
CloseDataSet;
end;
end;
```

---

**OpenFile**

Opens a file. Parameters:

- **file** (String) The file to open. Use a simple name or a file path.
- **type** (Integer) The type of the window to be opened (textType, dataType). Omit for default type.

Use FrontWindow if you need the window ID of the new window.

To import data from text files, call DataImportOptions before calling OpenFile.

See also GetFileDirectory, SetDefaultDirectory, SaveWindow.

There is also an obsolete definition of OpenFile, supported for compatibility with earlier versions of proFit:

```plaintext
procedure OpenFile(fileName:Str255);
```

Opens a data, drawing or function file in a new window. The new opened window becomes the “current window”. If the given file is a text file, the user will be asked if the file should be loaded into a data or a function window. To automatically load a text file into a data window, use OpenData, to automatically open a text file into a function window, use OpenText.
If `fileName` contains a simple file name, the file is loaded from the proFit folder. If `fileName` contains a file path, the file is loaded from the folder defined in the file path. If you pass ‘?’ for `fileName`, the user will be asked to locate the file.

If the specified file is a proFit module or a compiled AppleScript, it is added to the Misc or Func menu.

Causes a run-time error if the file could not be opened

This procedure cannot be called while a function is running.

---

**OpenPoly**

```
procedure OpenPoly(smoothing:integer; closed:Boolean);
```

Starts the creation of a polygon. After having called `OpenPoly`, use multiple calls to `Line` or `LineTo` to draw it, then call `ClosePoly` when you are through. Set `closed` to true if the polygon should be closed at the end.

- `smoothing` = 0 for no smoothing,
- `smoothing` = 1 for normal smoothing,
- `smoothing` = 2 for Bézier smoothing with the curve going through the polygon definition points.

---

**OpenText**

```
procedure OpenText(fileName:Str255);
```

Opens the given file as a function file. The file must either be a proFit function file or a text file. The new window becomes the “current text window”.

If `fileName` contains a simple file name, the file is loaded from the proFit folder. If `fileName` contains a file path, the file is loaded from the folder defined in the file path. If you pass ‘?’ for `fileName`, the user will be asked to locate the file.

This procedure cannot be called while a function is running.

---

**Optimize**

```
procedure Optimize(optional parameter list)
```

Finds a maximum or minimum of a function by varying its x-value and/or its parameters. Parameters:

- `function` (String) The function to be used. Omit for current function.
- `getMinimum` (Boolean) true if you want to find the function’s minimum, false for its maximum.
- `varyParams` (Boolean) true if you want to vary the function’s parameters to find the minimum/maximum. Only the active parameters of the function are varied.
- `varyX` (Boolean) true if you want to vary the function’s x-value to find the minimum/maximum.
- `xValue` (Real) If “varyX” is false, this parameter gives the value of the function’s x-value. If “varyX” is true, it gives the starting value for x.
- `fullDescription` (Boolean) true if a complete protocol is to be printed in the results window, false if only the resulting parameters, x- and y-values are to be printed.
- `printResults` (Boolean) Set to true for printing the results to the Results window. Default: false.

To retrieve the results of a call to procedure `Optimize`, call the function `GetResult(selector...)`.

Use one of the following selectors:

- `optimizedX` the optimized x-value
- `optimizedY` the optimized x-value
- `fittedParameter` the optimized parameters. Pass parameter index (1 based) as second argument to `GetResult`
The following example finds the minimum of the current function by varying its x-value and its active parameters, then prints the optimized value of the second parameter:

```plaintext
Optimize(xValue 0, precision 0, getMinimum true, varyParams true, varyX true);
Writeln(GetResult(fittedParameter, 2));
```

**Ord**

function Ord(ch: char):integer;
Returns the (extended) ASCII code of character ch.

**PageSetup**

procedure PageSetup(optional parameter list);
Shows the Page Setup dialog box for a given window. Parameters:

- `window` (Longint or String) The name or window ID of the window.
  - Default: Front window

See also: Print

**ParamSD**

function ParamSD(i:integer):extended
Returns the standard deviation calculated for parameter i in the last Levenberg-Marquardt fit. Returns an invalid number (NAN) if the index i corresponds to a parameter that was not active during the last fit. You can test if the return value is a NAN using the function Invalid. Causes a run-time error if the last fit was not successful or if i is out or range. Use NumFitParams to check if the last fit was successful.

**Paste**

procedure Paste;
Equivalent to selecting “Paste” from the “Edit” menu.

**Phase**

function Phase(z: complex):extended;
Returns the argument of the complex number z, i.e. the angle between the vector pointing to the complex point and the positive real axis. The function Abs gives the amplitude of the number.

```plaintext
abs(c)*exp(ii*phase(c)) = c
```

**pi, π**

```plaintext
const pi = 3.1415926535897932;
π = 3.1415926535897932;
```

Approximation of the ratio between the circumference and the diameter of a circle:

\[ \pi \approx 3.1415926535897932384626433832795028841971 \]

First approximations for this peculiar number were already known by 2000 B.C. The Babylonians found \( \pi = 3 + 1/8 \), the Egyptians \( \pi = 4(8/9)^2 \). In the 5th century A.D. in China, Tsu Chung-Chih and Tsu Kengh-Chih established \( 3.1415926 < \pi < 3.1415927 \).

**PlaceWindow**

procedure PlaceWindow(windowID:longint;
  left,top,right,bottom:integer);
Moves the given window to a new place on screen. left, top, right and bottom give the position of the margins of the new window in “global coordinates” (which have their origin at the top left of the main screen). PlaceWindow does nothing if the new window position would be off screen. If right <=
left, the width of the window remains unchanged, if bottom <= top, the height of the window remains unchanged.

windowID is the window ID of the window, such as it is returned by GetWindowID or FrontWindow. Use windowID = 0 for the front window.

---

**PlaceWindow**

```pascal
procedure PlaceWindow(windowID: longint; windowRect: Rect);
```

External modules only. Same as the internal function but accepts a Rect data structure as a parameter.

**PlotData**

```pascal
procedure PlotData(optional parameter list);
```

Plots a data set into a graph. Parameters:

- `xColumn, yColumn` (Longint) The x- and y-columns.
- `window` (Longint or String) The window to take the data from. You can either pass a window ID or the window’s name.
- `autoX, autoY` (Boolean) True if the limits of the x-axis (y-axis) of the graph are to be selected automatically to contain all data points, false if explicit limits are given in parameters xFirst, xLast (yFirst, yLast). Default is false.
- `xFirst, xLast` (real) The start and end of the x-axis. Specify these values if you set autoX to false.
- `yFirst, yLast` (real) The start and end of the y-axis. Specify these values if you set autoY to false.
- `xScaling, yScaling` (Integer) The scaling of the x- and y-axes. Values can be linScaling, logScaling, recSclaing (for 1/x-scaling), probScaling (probability scaling). Omit this parameter(s) to use the current default scaling.
- `xAxis, yAxis` (Integer) The axis to be used as x- and y-axis. Omit these parameters to use the default axes.
- `newWindow` (Boolean) True if graph is to appear in a new window, false if it is to appear in the current drawing window.
- `newGraph` (Boolean) True if plot is to appear in a new graph, false if it is to appear in the current graph.
- `selRowsOnly` (Boolean) True if only the currently selected rows are to be plotted, false if all rows are to be plotted.
- `drawErrors` (Boolean) True if error bars are to be plotted, false otherwise.
- `pointType` (Integer) Index of point type in the point style menu.
- `pointSize` (Real) Size of point, between 2 and 128.
- `pointThickness` (Real) Thickness of lines for drawing points: 0 (auto), 0.25, 0.5, 1.0.
- `bgPointType` (Integer) The same as pointType but for the background part of the point.
- `bgPointSize` (Real) The same as pointType but for the background part of the point.
- `connected` (Boolean) True if the data points are to be connected by lines, false otherwise. Default: false.
- `curveThickness` (Real) Thickness of the lines connecting the data points. Omit for using default thickness.
- `curveDash` (Integer) Line dash number (corresponding to the dash menu) if points are connected. Pass the position of the dash pattern in the dash popup menu. The values between 1 and 8 always correspond to:
1 2 3 4
5 6 7 8

curveRed,
curveGreen,
curveBlue

(Integer) The colour of the lines connecting data points. Pass values between 0 (dark) and 65535 (bright). Omit to use the default color.

procedure PlotFunction(optional parameter list);
Plots a function into a graph. Parameters:

**function**
(String) The name of the function to plot. Default: current function.

**xFirst, xLast**
(real) The start and end of the x-axis.

**yFirst, yLast**
(real) The start and end of the y-axis. Specify these values if you set autoY to false.

**autoY**
(Boolean) True if the limits of the y-axis of the graph are to be selected automatically to contain the whole plot, false if explicit limits are given in parameters yFirst, yLast. Default is false.

**from, to**
(Real) The x-coordinates where the plot begins/ends. Default: equal to xFirst, xLast.

**xScaling, yScaling**
(Integer) The scaling of the x- and y-axes. Values can be linScaling, logScaling, recSclaing (for 1/x-scaling), probScaling (probability scaling). Omit this parameter(s) to use the current default scaling.

**xAxis, yAxis**
(Integer) The axis to be used as x- and y-axis. Omit these parameters to use the default axes.

**newWindow**
(Boolean) True if graph is to appear in a new window, false if it is to appear in the current drawing window.

**newGraph**
(Boolean) True if plot is to appear in a new graph, false if it is to appear in the current graph.

**xStep**
(Real) Step width for plotting. Set to 0 for using automatic step width selection.

**fittedParams**
(Boolean) True if last fitted parameters are to be used for the function, false if the parameters in the Parameter window are to be used.

**curveThickness**
(Real) Thickness of the curve. Omit for using default thickness.

**curveDash**
(Integer) Line dash number (corresponding to the dash menu) of the curve. Pass the position of the dash pattern in the dash popup menu. The values between 1 and 8 always correspond to:

1 2 3 4
5 6 7 8

curveRed,
curveGreen,
curveBlue

(Integer) The colour of the curve. Pass values between 0 (dark) and 65535 (bright). Omit to use the default color.
function Pos(pattern, s: String):integer;
Returns the position of the given pattern in string s. Returns 0 if the pattern is not found in string s.
Example:
Pos('hi', 'hi there') returns 1
Pos('there', 'hi there') returns 4
Pos('glue', 'hi there') returns 0

function PRandom:extended;
External modules name. See Random.

procedure Print(optional parameter list);
Shows the Print dialog box for a given window. Parameters:
window (Longint or String) The name or window ID of the window. Default: Front window
See also: PageSetup

function Random:extended;
Returns a random number evenly distributed between 0 and 1.

function Re(z: complex):extended;
Returns the real part of the complex number z. To get the imaginary part, call function Im.

procedure ReduceData(optional parameter list)
Reduces and/or smoothes the data in data window Parameters:
window (String or Longint) The window, specified by name or window ID. Omit for front window.
action (Integer) keepSome (= keep every n-th row), removeSome (= remove every n-th row), average (= replace n consecutive rows by one single row holding their average), smooth (= replace each row by the average of the row and its n-1 neighbouring rows), keepSelRows (= remove all rows except the ones that are selected), removeSelRows (= remove all rows that are presently selected). n is given by the parameter “points”
points (Integer) additional parameter if action is keepSome, removeSome, average or smooth.
selectionOnly (Boolean) True if only the currently selected cells are to be affected, false if all cells in the data window are to be affected. (Ignored if parameter “action” is removeSelRows or keepSelRows)
procedure Root(optional parameter list);

Finds the root(s) of a function or finds the x-value of a function where its y-value is equal to a given value. A given x-interval is searched. Parameters:

**function**  (String) The function to be used. Omit for current function.

**xMin**  (Real) The start of the x-interval.

**xMax**  (Real) The end of the x-interval.

**subintervals**  (Integer) The number of sub-intervals to be searched in the x-interval. When the function’s sign changes over a sub-interval, the sub-interval is searched for a root.

**yValue**  (Real) The desired y-value. Omit or set to 0 if finding the x-value where the function becomes zero (roots).

**printResults**  (Boolean) Set to true for printing the results to the Results window. Omit “printResults” or set it to false for suppressing this.

To retrieve the results of a call to procedure `Root`, call the function `GetResult`. Use one of the following selectors:

- `rootsCount`  the number of roots found  \( \leq 100 \)
- `rootsXValue`  x-value of each root*
- `rootsYValue`  y-value of each root*

*pass an index (1..rootsCount) as second parameter to `GetResult`.

The following example finds the roots of the current function between -1 and 1, then prints them:

```pascal
program RootFinder;
var i, nrRoots:Integer;
begin
  Roots(xMin -1, xMax 1, subIntervals 50);
  nrRoots := GetResult(rootsCount);
  Writeln(nrRoots);
  for i := 1 to nrRoots do
    Writeln('     ', GetResult(rootsXValue, i));
end;
```

Note: There's also an obsolete version of `Roots`:

```pascal
function Root(name:Str255; min,max: extended):extended
```

which is supported for compatibility with older versions of pro Fit. Don't use it for new developments.

---

**Round**

**function Round(x:extended):extended;**

Rounds x to the closest integer and returns its value.

---

**RowSelected**

**function RowSelected(rowNumber:longint):Boolean;**

Returns true if anything in the given row of the current data window is selected.

---

**SaveDataAsText**

**procedure SaveDataAsText(windowID:longint; fileName:Str255);**

Saves a data window as a text file. `windowID` is the window ID of the window, such as it is e.g. returned by `GetWindowID` or `FrontWindow`. 

---
fileName is the name of the file. If fileName contains a simple file name, the file is placed in pro Fit's folder. If fileName contains a file path (e.g. 'HD:MyFolder:file'), the file is placed in the folder defined in the file path. Pass '?' for fileName to bring up a dialog box asking the user where to save the file. Use SetTextFileFormat if you want to specify how the text file must be formatted.

**SaveDrawingAs**

```pascal
procedure SaveDrawingAs(windowID:longint; fileName:Str255;
                          format:longint);
```

Saves a drawing window as a pro Fit file (if format = defaultFormat), a PICT file (if format = pictFormat) or a EPS file (if format = epsFormat).

- **windowID** is the window ID of the window, such as it is returned by GetWindowID or FrontWindow.
- **fileName** is the name of the file. If fileName contains a simple file name, the file is placed in pro Fit's folder. If fileName contains a file path (e.g. 'HD:MyFolder:file'), the file is placed in the folder defined in the file path. Pass '?' for fileName to bring up a dialog box asking the user where to save the file.

SaveDrawingAs(L,'bla',default) is equivalent to SaveWindowAs(L,'bla').

**SaveParameterSet**

```pascal
procedure SaveParameterSet(optional parameter list);
```

Saves the the parameters that currently appear in the Parameter window. Parameters:

- **set** (String) The name of the set. Omit to save all sets belonging to the given function.
- **forAll** (Boolean) True if the parameter set is to be available for all functions, false if the parameter set is only to be available for the current function. Default: false
- **file** (String) The file where the parameter set must be saved. Omit to save as permanent sets.

See also: AddParameterSet, UseParameterSet, LoadParameterSet, DeleteParameterSet

**Save**

```pascal
procedure Save(windowID:longint);
```

Equivalent to choosing Save from the File menu. Causes a run time error the window has never been saved.

**SaveWindow**

```pascal
procedure SaveWindow(optional parameter list);
```

Saves a window. Parameters:

- **window** (Longint or String) The name or window ID of the window. Default: Front window
- **file** (String) The file to save the window into. Use a simple name or a file path. Default: the file currently attributed to the window.
- **type** (Integer) The type of the file if non-default type (textFileType, PICTType, EPSFType). Omit for default type. To control the format for exporting data to a text file, call DataExportOptions before calling SaveWindow.

See also GetFileDirectory, SetDefaultDirectory, OpenFile.
There is also an obsolete version of `SaveWindow` supported for compatibility with earlier versions. Do not use it in new programs:

```pascal
procedure SaveWindowAs(windowID: longint; fileName: Str255);

Saves the contents of the given window into a file with the specified file name.
`windowID` is the window ID of the window, such as it is e.g. returned by `GetWindowID` or `FrontWindow`.
`fileName` is the name of the file. If `fileName` contains a simple file name, the file is placed in pro Fit's folder. If `fileName` contains a file path (e.g. 'HD:MyFolder:file'), the file is placed in the folder defined in the file path. Pass '?' for `fileName` to bring up a dialog box asking the user where to save the file.
```

```pascal
procedure SelectAll;

Equivalent to selecting “SelectAll” from the “Edit” menu.
```

```pascal
function SelectBottom: longint;

Returns the row number of the bottom-most selected cells of the current data window or 0 if no cells are selected. Causes a run-time error if no data window is open.
External modules must use `GetSelection`.
```

```pascal
procedure SelectCell(optional parameter list)

Selects one or more cells in the current data window. Parameters:
- `row` (Longint) A row index if you want to select data in a single row. Omit if you use `fromRow`, `toRow`.
- `fromRow, toRow` (Longint) The range of rows if you want to select data in several rows. Omit if you use the parameter “row”.
- `col` (Longint) A column index if you want to select data in a single column. Omit if you use `fromCol`, `toCol`.
- `fromCol, toCol` (Longint) The range of columns if you want to select data in several columns. Omit if you use the parameter “col”.
- `options` (Integer) Controls what happens with the previous selection. Pass `addContinuously` (= add to present selection), `forgetOld` (= forget present selection, default)
```

```pascal
procedure SelectCells(left, top, right, bottom: longint);

Obsolete. Use `SelectCell` instead.
Removes the current selection from the current data window and selects all cells within the given rectangle. Call with all arguments = 0 to deselect all cells.
```

```pascal
procedure SelectColumn(optional parameter list)

Selects a column or a range of columns in the current data window. Parameters:
- `col` (Longint) The column to select. Omit if you use `fromCol`, `toCol`.
- `fromCol, toCol` (Longint) The range of columns to select if you want to select several columns. Omit if you use the parameter “col”.
```
**options** (Integer) Controls what happens with the previous selection. Pass 
*addContinuously* (= add to previous selection) or *forgetOld* (= forget previous selection, default)

---

**SelectFunction**

```pascal
procedure SelectFunction('myFunc');
```

Selects the given function in the “Func” menu and makes it the current function. `func` is the name of the function. A call to `SelectFunction('myFunc')` is equivalent to `SetOptions(currentFunction 'myFunc')`.

---

**SelectLeft**

```pascal
function SelectLeft:longint;
```

Returns the column number of the leftmost selected cells of the current data window or 0 if no cells are selected. Causes a run-time error if no data window is open.

External modules must use `GetSelection`.

---

**SelectRight**

```pascal
function SelectRight:longint;
```

Returns the column number of the rightmost selected cells of the current data window or 0 if no cells are selected. Causes a run-time error if no data window is open.

External modules must use `GetSelection`.

---

**SelectRow**

```pascal
procedure SelectRow(optional parameter list)
```

Selects a row or a range of rows in the current data window. Parameters:

- **row** (Longint) The row to select. Omit if you use fromRow, toRow.
- **fromRow, toRow** (Longint) The range of rows to select if you want to select several columns. Omit if you use the parameter “row”.
- **options** (Integer) Controls what happens with the previous selection. Pass *forgetOld* (= forget present selection, default), *addContinuously* (= add to present selection, extending it continuously), *addDiscontinuously* (= add to present selection, extending it discontinuously), *deselectIt* (= deselect the specified rows)

---

**SelectRows**

```pascal
procedure SelectRows(top, bottom:longint; select:Boolean);
```

*Obsolete.* Use `SelectRow` instead.

Selects all rows between top and bottom if select = true, deselects them if select = false.

If there are selected rows outside top/bottom, they remain selected.

---

**SelectTop**

```pascal
function SelectTop:longint;
```

Returns the row number of the topmost selected cells of the current data window or 0 if no cells are selected. Causes a run-time error if no data window is open.

External modules must use `GetSelection`.

---

**SelectWindow**

```pascal
procedure SelectWindow(wind:String or Longint)
```

Moves the specified window in front of all other windows. `wind` is the windowID or the name of the window.
SetArrowStyle

procedure SetArrowStyle(location: integer; style: integer; size: extended);

Specifies the default arrow style for lines and polygons.
location defines if you want to change the style of the arrow at the beginning of the line (location = 1), end (2) or both beginning and end (3).
Set style to 0 if there should be no arrow at the specified location. Set style to 1...12 to select the arrow style corresponding to the entry in the arrow style popup menu. style values from 1 to 6 correspond to the 6 predefined styles:

```
1
2
3

4
5
6
```

style values from 7 to 12 correspond to the 6 custom styles which appear in the arrow style menu. Set style to -1 for leaving it unchanged.
size: The size in points (1/72 inches). Set it to 0 for leaving it unchanged.
The following program draws a bent arrow as shown on the right.
```
program OneArrow;
begin
  SetLineStyle(5, 1);  {line thickness}
  SetArrowStyle(1, 2, 20); {start arrow style}
  SetArrowStyle(2, 1, 20); {end arrow style}
  OpenPoly(1, false);  {draw a smooth polygon}
  MoveTo(100,100); LineTo(150,100); LineTo(150,50);
  ClosePoly;
end;
```

SetAxisAttributes

procedure SetAxisAttributes(whichAxis: integer; flags: longint);

Sets various drawing options of an axis in the current graph.
whichAxis is equal to xAxis or yAxis and defines if you want to change the current x- or y-axis. (To set the current axis, call SetCurrentAxis.)
flags is 0 or a sum of the following constants: equalToMain, drawAxisLine, drawTicks, drawMajorTickLabels, drawMinorTickLabels, plusSideTicks, minusSideTicks, plusSideLabels, labelsOutsideFrame.
Example:
```
SetAxisAttributes(xAxis,sameAsMain+drawAxisLine+ticksPlusSide+drawTicks);
```

SetAxisPosition

procedure SetAxisPosition(whichAxis: integer; position: extended);

Changes the position an axis in the current graph.
whichAxis is equal to xAxis or yAxis and defines if you want to change the current x- or y-axis. (To set the current axis, call SetCurrentAxis.)
position is the position in the coordinates of the main axis perpendicular to the specified axis. If position is outside the range of this main axis, it is set to its minimum/maximum.

SetBGDataPointStyle

procedure SetBGDataPointStyle(style: integer; size: extended);

Sets the default background style of data points.
style, size have the same meaning as for the routine SetDataPointStyle. If style designates a “composite point”, only the background of this composite point is used. Always call SetDataPointStyle before calling SetBGDataPointStyle. For more information see SetDataPointStyle.

SetBoxTitle

procedure SetBoxTitle(title:Str255);
Sets the title of the dialog box invoked with the next call to the predefined function Input (or InputBox for external modules).

SetCell

procedure SetCell(row,column:longint; s:Str255);
Sets the string in the given cell of the current data window to s. If the given cell is in a numeric column, SetCell attempts to convert s into a number. If this conversion fails, the given cell is cleared.

SetColHandle

procedure SetColHandle(col:longint; colH:Handle);
External modules only. For advanced programming. Sets a given column to the data in colH. The organization of the data in colH depends on the data type of the column. See also the entry for GetColHandle.
If the column is of type floatColumn, colH is a handle of type FloatColumnHandle (handle to an array of 4-byte floating point values), if it is doubleColumn, colH is of type DoubleColumnHandle (handle to an array of 8-byte floating point values), if it is textColumn, colH is of type TextColumnHandle (handle to a record of type StringData). (To get a column's type, call GetColType. You can find more information in the files proFit_interface.p / proFit_interface.h)
Once you call SetColHandle, the handle becomes property of pro Fit — do not dispose it. colH can either be:
• a handle that you allocated yourself. In this case, the Handle's size must be:
  4*(nrRows+1) for columns of type floatColumn
  8*(nrRows+1) for columns of type doubleColumn
  14 + size of all strings for columns of type textColumn
• a handle that you obtained from GetColHandle
• nil if you want to clear the given column
This routine should be used by experienced programmers only. Warning: Accessing text columns in this way is not recommended. The definition of the data structures may change in the future.

SetColName

procedure SetColName(col:longint; name:Str255);
Obsolete. Use SetColumnProperties instead.
Changes the name of a column in the current data window. col is the number of the column, name its new name.
SetColName causes a run-time error if there is no data window open or if col is outside the bounds of the data window.

SetColType

procedure SetColType(columnNumber:longint; theType:longint);
Obsolete. Use SetColumnProperties instead.
Changes the type of the column specified by columnNumber to theType. theType can have the values textColumn (for text columns), floatColumn (for numeric columns having a range of -1e30 ... 1e30,
i.e. 4-byte floating point values) or doubleColumn (for numeric columns having a range of -1e300 ... 1e300, i.e. 8-byte floating point values)

procedure SetColumnProperties(optional parameter list)
Sets the properties of one or more columns in the current data window. Parameters:

- col (Longint) The index of the column to change. Omit if passing values for a column range in parameters “firstCol”, “lastCol”.
- firstCol, lastCol (Longint) The range of columns to change. Omit if passing a single column in parameter “col”.
- name (String) The title of the column(s). Omit for leaving it unchanged.
- nrDecimals (Integer) The number of decimals for numeric columns. Omit for leaving it unchanged.
- format (Integer) The format for numeric columns: scientificFormat or floatingFormat. Omit for leaving it unchanged.
- width (Integer) The width of the column(s) in pixels. Omit for leaving it unchanged.
- type (Integer) The type of the column(s) floatColumn (4 byte floating point having a range of -1e30 ... 1e30), doubleColumn (8 byte floating point having a range of -1e300 ... 1e300), textColumn. Omit for leaving it unchanged.

procedure SetColWidth(columnNumber:longint; width:integer);
Obsoleted. Use SetColumnProperties instead.
Sets the width of the column specified in columnNumber to the value (in pixels) passed in width. width must be an even number between 14 and 510.

procedure SetCurrentAxis(whichAxis:integer; axisID:integer);
Sets the current (x- or y-) axis. The current axis is used for plotting as well as in various other calls, such as SetAxisAttributes.
whichAxis is either xAxis or yAxis. axisID designates the number of the axis.
Example: SetCurrentAxis(xAxis,2) makes X2 the current x-axis.

procedure SetCurrentGraph(graphID:longint);
Sets the current graph to the graph identified by graphID. To make no graph the current graph, set graphID to 0.

procedure SetCurrentWindow(windowID:longint);
This routine makes a window the current window of its kind.
There is a “current data window”, a “current drawing window”, and a “current text window”. These are the windows used by the output routines such as LineTo and SetData.
When a new window is opened, it automatically becomes the current window of its kind.
windowID is the window ID of the window, such as it is returned by GetWindowID or FrontWindow.
procedure SetCurveFill(whichAxis:integer; axisID:integer);

Sets the fill style of the next plotted curve. To fill the area between the curve and an x-axis or an y-axis, set whichAxis to xAxis or yAxis, respectively. axisID specifies the index of the axis. To disable curve filling, set axisID to 0.

A call to SetCurveFill affects all subsequent calls to OpenCurve and OpenDataSet calls.

procedure SetData(row,column:longint;ex:extended);

External modules only. Sets the value of the specified cell of the current data window to ex.

procedure SetDataPointStyle(style:integer; size:extended; thickness:extended);

Sets the default data point style. This style is used for all subsequent plotting of data points. style defines the “shape” of the data point:

- 0: pixel (the smallest point),
- 1-17: 0 1 2 3 4 5 6 7 8
- 9 10 11 12 13 14 15 16 17
- -1..-8: the eight custom points in the last row of the point style menu. size is the size in points size is the size of the point in pixels.

thickness is 0, 0.25, or 0.5, or 1.0. Use 0 if you want to automatically use smaller lines for smaller points.

Points can be simple or composite. A simple point consists of a single symbol, such as the styles 0 – 13 above. Composite points consist of two symbols (a foreground and a background one) plotted on top of each other, such as the styles 14 – 17 above.

SetDataPointStyle sets the foreground symbol or, if a composite point is used, both foreground and background symbols. To set the background symbol separately, call SetBGDataPointStyle.

procedure SetDataSize(numberOfRows, numberOfColumns:longint);

Obsolete. Use SetDatawindowProperties instead.

Sets the number of columns and rows of the current data window. The number of rows and columns must be between 1 and 30000.

Set numberOfRows to 0 if you only want to change the number of columns. Set numberOfColumns to 0 if you only want to change the number of rows.

To get the current size of a data window, use the functions NrRows and NrCols.

procedure SetDataWindowProperties(optional parameter list)

Sets the properties of a data window. Parameters:

- window name (String or Longint) The name or windowID of the window to be affected.
- boundsLeft, boundsRight, boundsTop, (String) The title of the window. Omit for leaving it unchanged.
boundsBottom (Integer) The bounds of the window in global screen coordinates. Omit for leaving them unchanged.

info (String) The info text attributed to the window. Omit for leaving it unchanged.

fontName (String) The font to be used in the window. Omit for leaving it unchanged.

fontStyle (Integer) The font style to be used in the window (plain, bold, italic, underline, outline, extended, condensed or any sum of these values). Omit for leaving it unchanged.

fontSize (Integer) The font size to be used in the window. Omit for leaving it unchanged.

nrRows, nrCols (Integer) The number of rows/columns. Omit for leaving this unchanged.

---

**SetDefaultCols**

procedure SetDefaultCols(xCol,yCol,xErrCol, yErrCol:longint);

Sets the “default columns” of the current data window. The default x- and y-columns are those columns that are shown in the preview window. Default columns are marked with “x”, “y”, “Δx”, “Δy” in their column header.

You can set xErrCol, yErrCol to zero to “undefine” the column.

Set any of the xCol, yCol, xErrCol, yErrCol to -1 if you don’t want to change it.

---

**SetDefaultDirectory**

procedure SetDefaultDirectory(path: string);

Sets the default directory for saving files to the one specified by the given path-name. Pass the empty string as a paramter to re-set the default directory to its original setting, i.e. the directory where the pro Fit application is found.

---

**SetEBarStyle**

procedure SetEBarStyle(capLength, capThick, lineThick:extended);

Sets the style of the error bars that will be generated by OpenDataSet/AddDataPoint/CloseDataSet. Error bars are generated by AddDataPoint when the error parameter of OpenDataSet says so.

capLength: The length of the cap in pixels, -1 to make the caps as wide as the data points, -2 to get a box (works only if x- and y-errors are given).

capThick, lineThick: The thickness of the caps and of the bar lines in pixels (0.001 – 50)

---

**SetErrorAnalysis**

procedure SetErrorAnalysis(confidence:extended; iterations:longint);

Sets the options for the error analysis to be used in the next call to Fit. confidence is the confidence interval probability in percent. iterations is the number of simulated data sets to be analyzed.

---

**SetFillColor**

procedure SetFillColor(red,green,blue: longint);

Sets the default RGB color used for filling shapes. Used for drawing or filling curves. red, green, blue are integers between 0 and 65535.
procedure SetFillPattern(pattern: integer);

Sets the default fill pattern used for filling drawing objects. Set pattern to 0 for making the shapes transparent. The following figure shows a list of all patterns and their pattern number:

<table>
<thead>
<tr>
<th>Pattern Number</th>
<th>Pattern</th>
</tr>
</thead>
<tbody>
<tr>
<td>0</td>
<td>transparent</td>
</tr>
<tr>
<td>1</td>
<td></td>
</tr>
<tr>
<td>2</td>
<td></td>
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<td>15</td>
<td></td>
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procedure SetFitDefaults(algorithm: integer;
yErrDistribution, xErrDistribution: integer;
xErrColumn: longint; xErrValue: extended;
stopTime: extended);

Sets advanced fitting options. It sets the x-error column and type, the algorithm and the stopping criteria to be used in all subsequent calls to `Fit`.

- **algorithm**: the algorithm to be used (1: Levenberg-Marquardt, 2: Montecarlo, 3: Robust, 4: linear regression, 5: polynomial)
- **yErrDistribution, xErrDistribution**: the distribution of the x- and y- errors. They can be `gaussDistr`, `doubleExpDistr`, `lorentzDistr`, `andrewDistr`, or `tukeyDistr`
- **xErrColumn** tells if x-errors should be used: set it to 0 if x-errors are unknown, to -1 if they are constant (pass the value in `xErrValue`), to -2 if they are given in percent (pass the percentage in `xErrValue`), or to the number of an x-error column.
- **stopTime** tells when to stop Monte Carlo fitting: pass a value > 0 to give the maximum number of iterations, a value < 0 to give a negative maximum time in seconds, 0 for continuing fitting until manual interruption.

procedure SetFitParamRange(paramNr: integer; rangeMin: extended;
rangeMax: extended; asPercent: Boolean);

Sets the fitting range for parameter `paramNr` as it is used for Monte-Carlo fits. If `asPercent` is true the range values can be given as a percentage offset from the parameter value. The fitting ranges set by this command stay valid until the next fit command has been executed.

procedure SetFunctionParam(name: Str255; i: integer; value: extended);

Sets the default value of a function parameter as it appears in the parameters window. `name` is the name of the function as it appears in the Func menu. Use an empty string (""') to specify the function currently selected in the Func menu. This parameter is case sensitive. `i` is the parameter index, `value` its new value.

Example:

```
setFunctionParam('Polynom', 1, 6)
```

sets the degree (=a[i]) of the built-in function "Polynom" to 6.
**SetFunctionProperties**

*SetFunctionProperties*(optional parameter list)

Sets the properties of a function in the Func menu. Parameters:

- **function** (String) The function (omit for currently selected function)
- **shown** (Boolean) True if the function is shown in the Preview window, false if not. Omit to leave unchanged.
- **nrParams** (Integer) The number of parameters. Omit to leave unchanged. Do not change the number of parameters while a function is being used, e.g. for fitting.

**SetGlobalData**

*SetGlobalData*(value: real; index: integer);

Sets the value under the given index in a global data array. This data array is shared between all functions and programs. It can be used for communication between programs, functions, scripts and modules.

The index must between 0 and 99.

See also: GetGlobalData

**SetGraphAttributes**

*SetGraphAttributes*(flags:longint);

Sets various attributes of the current graph.

- **flags** is 0 or a sum of the following constants:
  - `drawFrame`: draw the frame
  - `drawMajorGridX`: grid lines at major x-ticks
  - `drawMinorGridX`: grid lines at minor x-ticks
  - `drawMajorGridY`: grid lines at major y-ticks
  - `drawMinorGridY`: grid lines at minor y-ticks
  - `plotBehindAxes`: first draw curves, then axes
  - `gridInFront`: first draw the rest, then the grid
  - `gridInMiddle`: draw grid between axes and curves

The last two constants cannot be used at the same time

**SetGraphFrame**

*SetGraphFrame*(left, top, right, bottom:extended);

Changes the position and size of the current graph to match the new values. (Use *SetNewGraphRect* for setting the default size of future graphs.)

**SetLabel**

*SetLabel*(whichAxis:integer; tickNum:integer; labelNumber:extended);

Sets the label of tick mark having number *tickNum* to correspond to the given value. Accesses the current x- or y-axis (use *whichAxis=xAxis* or *whichAxis=yAxis*).

**SetLabelsFormat**

*SetLabelsFormat*(whichAxis:integer; format:integer; decimals:integer);

Sets the number format of the labels of the current x- or y-axis. *whichAxis* is either *xAxis* or *yAxis*.

- `format`: -1,0,1 for auto, decimal, and exponential, respectively.
- A format parameter equal to any other number sets the labels format to fixed exponential and uses format as the number in the exponent.
SetLegendProperties

procedure SetLegendProperties(optional parameter list);
Sets the visibility, position and size of the legend of the current function.
Parameters are:

visible (Boolean) Show or hide the legend.
offsetx, offsety (Real) Offset between topleft of legend and topright of graph.
width, height (Real) Size of an entry in the legend (left part).

SetLabelText

procedure SetLabelText(whichAxis:integer; tickNum:integer; labelText:Str255);
Sets the label of the given tick mark to the to given string. Accesses the current x- or y-axis (use whichAxis=xAxis or whichAxis=yAxis).
This routine is usually used after calls to AddTick.

SetLineColor

procedure SetLineColor(red,green,blue: longint);
Sets the line default color to be used for any future drawing in the current drawing window. red, green, blue are integers between 0 and 65535.

SetLineStyle

procedure SetLineStyle(thick:extended; dash: integer);
Sets the default line style to be used for any future drawing in the current drawing window.
thick is the line thickness in points (1/72 inches). Set it to 0 for leaving it unchanged.
dash is the dash pattern, and its numerical value corresponds to the position of the dash pattern in the dash popup menu. The values between 1 and 8 always correspond to:

```
1 2 3 4
5 6 7 8
```
Values between 9 and 12 correspond to the four last customizable entries in the dash styles menu. A value of 0 leaves the dash style unchanged.

SetNewGraphRect

procedure SetNewGraphRect(left,top,right, bottom:extended);
Sets the size and position of the next graph generated with CreateNewGraph, PlotData and PlotFunction. Subsequent calls to CreateNewGraph, PlotData and PlotFunction will use the normal default position and size, i.e. the effect of SetNewGraphRect only extends to the one graph created next. (Use SetGraphFrame for setting the size of the current graph.)

SetOptions

procedure SetOptions(optional parameter list);
Sets some options of pro Fit. Parameters:

currentFunction (String) The current function. (Alternative call to SetOptions( currentFunction 'myFunc') is SelectFunction('myFunc') ).
Omit for leaving the current function unchanged.
decimals (Integer) The number of decimals to be used for writing numbers in the results window. Pass a negative value for setting the total number of digits, a positive value for setting the number of digits after the decimal point. Omit for leaving the setting unchanged.
errorAlerts (Boolean) true if error alerts are to be shown when running into errors during the execution of programs or scripts. Omit for leaving this option unchanged.

scriptDebugging (Boolean) Set to true if debug info is to be printed while running AppleScripts. Omit for leaving this option unchanged.

### SetParamDefaults

```plaintext
procedure SetParamDefaults(i:integer; value:extended; mode:integer; name:Str255; min,max:extended);
```

*Obsolete.* Use `SetParameterProperties` instead.

Sets the value, fitting mode, name and limits of a parameter of the currently running function. `i` is the parameter index, `value` its new value, `mode` its new fitting mode (can be `constant`, `inactive`, or `active`), `name` its new name, and `min`, `max` the lower and upper boundaries of the parameter.

### SetParamDefaultValue

```plaintext
procedure SetParamDefaultValue(i:integer; value:extended);
```

*Obsolete.* Use `SetParameterProperties` instead.

Sets the default value of a parameter of the currently running function. The default value is the value that appears in the parameters window. `i` is the parameter index, `value` the new value. This function is generally used within the predefined function “Initialize”.

### SetParameterProperties

```plaintext
procedure SetParameterProperties(optional parameter list);
```

Sets some properties of a parameter of the current function. Parameters:

- `param` (Integer) The index (1 based) of the parameter to be changed.
- `name` (String) The name of the parameter as it appears in the Parameter window. Omit for leaving it unchanged.
- `value` (Real) The value of the parameter as it appears in the Parameter window. Pass `equalX` for setting it “=x”. Omit for leaving it unchanged.
- `min`, `max` (Real) The lower and upper limits of the parameter. Omit for leaving the corresponding limit unchanged.
- `mode` (Integer) The mode of the parameter. Use `paramInactive`, `paramActive`, `paramConstant` for making the parameter inactive, active or constant. Omit for leaving the mode unchanged.

### SetParamLimits

```plaintext
procedure SetParamLimits(i:integer; min,max:extended);
```

*Obsolete.* Use `SetParameterProperties` instead.

Sets the limits of a parameter of the currently running function. Parameter limits define the range of values that are admissible for a given parameter (for example during a fit). `i` is the parameter index, and `min`, `max` its lower and upper boundaries.

### SetParamName

```plaintext
procedure SetParamName(i:integer; name:Str255);
```

*Obsolete.* Use `SetParameterProperties` instead.

Sets the name of a parameter of the currently running function. `i` is the parameter index, `name` its new name.
procedure SetRange(whichAxis: integer; min, max: extended; scaling: integer);

Sets the range and scaling of the current x-axis (if whichAxis=xAxis) or y-axis (if whichAxis=yAxis).
min, max is the new range of the axis. scaling is its new scaling and can take the values 0 (linear scaling), 1 (logarithmic scaling), 2 (1/x-scaling), 3 (probability scaling), -1 (keep scaling unchanged).

procedure SetTextStyle(fontName: Str255; size: extended; style: integer);

Sets the default font, font size, and style for subsequent text drawing. Text color can set using the SetLineColor routine.

procedure SetWaitText(s1, s2, s3, s4, s5, s6: Str255);

Writes the strings s1 ... s6 into pro Fit’s progress window, which is displayed during lengthy operations. The strings are arranged in a two columns by three rows arrangement:

\[
\begin{array}{cc}
  s1 & s2 \\
  s3 & s4 \\
  s5 & s6 \\
\end{array}
\]

Use an empty string if you don’t want to change it. See also SetWaitTitle.

procedure SetWaitTitle(s: Str255);

Writes the string s as a title into pro Fit’s progress window, which is displayed during lengthy operations. See also SetWaitText.

procedure SetWindowInfo(windowID: longint; info: Str255);

Obsolete. Use SetWindowProperties instead.
Sets the info field of a window to the given string. (The info field of a window can be viewed by choosing the Get Info... command from the File menu. For data windows, it is the text that appears when you drag down the info hook.) windowID is the window ID of the window, such as it is returned by GetWindowID or FrontWindow.
SetWindowInfo

procedure SetWindowInfo(windowID:longint; length:longint; info:Ptr);

External Modules only. Sets the info field of a window to the given text.
info is a pointer to the new info text and length is its length in bytes. Call
SetWindow(windowID,0,nil) to clear the info text.
windowID is the window ID of the window, such as it is returned by GetWindowID or FrontWindow.

SetWindowProperties

procedure SetWindowProperties(optional parameter list)

Sets the properties of a window. Parameters:
window (String or Longint) The name or windowID of the window to be affected.
name (String) The title of the window. Omit for leaving it unchanged.
boundsLeft, boundsRight, boundsTop, boundsBottom (Integer) The bounds of the window in global screen coordinates. Omit for leaving them unchanged.
info (String) The info text attributed to the window. Omit for leaving it unchanged.
fontName (String) The font to be used in the window. Omit for leaving it unchanged.
fontStyle (Integer) The font style to be used in the window (plain, bold, italic, underline, outline, extended, condensed or any sum of these values). Omit for leaving it unchanged.
fontSize (Integer) The font size to be used in the window. Omit for leaving it unchanged.

SetWindowTitle

procedure SetWindowTitle(windowID:longint; name:Str255);

Obsolete. Use SetWindowProperties instead.
Sets the title of the given window to the string name.
windowID is the window ID of the window, such as it is e.g. returned by GetWindowID or FrontWindow.

Sin

function Sin(x:extended):extended;

Returns the sine of x.

Sinh

function Sinh(x:extended):extended;

Returns the hyperbolic sine of x. sinh is defined by
\[ \sinh(x) = \frac{e^x - e^{-x}}{2} \]

Sort

procedure Sort(optional parameter list)

Sorts rows in a data window. Parameters:
window (String or Longint) The window, specified by name or window ID. Omit for front window.

referenceCol (Longint) The column to be used for sorting.

order (Integer) sortAscending or sortDescending, the sort order

selectionOnly (Boolean) True if only the rows of the currently selected columns are to be sorted, false (or omitted) if the rows of all columns are to be sorted

---

**SpeakString**

procedure SpeakString(s:Str255);

Lets your hardware read the text contained in the string s. If text-to-speech extensions are not installed on your computer, this routine does nothing.

---

**Sqr**

function Sqr(x:extended):extended;

Returns the square of x. \( s(x) = x^2 \)

---

**Sqrt**

function Sqrt(x:extended):extended;

Returns the square root of x. Causes a run-time error for a negative argument

---

**Statistics**

Statistics(optional parameter list);

Performs statistical analysis on a data window. Parameters:

- **window** (String or Longint) The window’s name or window ID of your data. Omit for using the frontmost datawindow.
- **column** (Longint) The column to work on or 0 for all columns. Omit if “selectionOnly” is true.
- **selRowsOnly** (Boolean) True if only the currently selected rows are to be analyzed. Only used when parameter “selectionOnly” is false.
- **selectionOnly** (Boolean) True if the currently selected cells are to be analyzed. False if the columns specified in parameter “column” are to be analyzed.
- **withBasic** (Boolean) False for suppressing calculation of the sum, mean, variance, standard deviation and absolute deviation. Default: true.
- **withSkew** (Boolean) False for suppressing calculation of skewness and kurtosis. Default: true.
- **withMedian** (Boolean) False for suppressing calculation of mean median, maximum and minimum. Default: true.
- **printResults** (Boolean) True for printing the results to the Results window. Omit “printResults” or set it to false for suppressing this.

To retrieve the results of this command, call GetResult with one of the following selectors:

- **statCount**: number of evaluated values
- **statSum**: sum
- **statMean**: mean
- **statMedian**: median
- **statStdDeviation**: standard deviation
- **statMeanAbsDeviation**: mean absolute deviation
- **statMinumum**: minimum value
statMaxumum: maximum value
statVariance: variance
statKurtosis: kurtosis

StopExecution

procedure StopExecution;
External modules only. Tells proFit to interrupt execution of the current module as soon as possible.

Str255ToNumber

function Str255ToNumber(s: Str255; var x: extended): integer;
External modules only. Converts the string s to a number x. s can be a numeric string or an expression.
Return values are 0 (conversion successful), 1 (x is infinite), 2 (s is empty), 3 (x is an NAN (invalid number), 4 (user aborted), or 5 (run time error).

StringToNumber

function StringToNumber(s: String; var x: real): integer;
Converts the string s to a number x and returns a result code as follows:
0: conversion successful
1: x is infinite
2: s is empty
3: x is an NAN (not a number)
4: user aborted calculation
5: run time error

Tabulate

procedure Tabulate(optional parameter list)
Tabulates a function to a data window. Parameters:

function (String) The function to be tabulated, omit for current function.
from, to (Real) The first and last value to be tabulated.
stepValue (Real) The step between tabulated points. Omit if you pass autoStep or pointsStep for parameter "step"
step (Integer) numericStep (= tabulate for equally spaced points as defined in stepValue), autoStep (= choose step width automatically, use a larger number of points where the function varies quickly), pointsStep (tabulate for all values of the x column in the current data window).
Default if omitted: numericStep
parameter (Integer) Omit or set to 0 if tabulating the function by varying its x-value. Set to the number of a parameter for tabulating the function by varying this parameter.
xValue (Real) defines the function’s x-value if you pass a non-zero value for “parameter”. Omit otherwise.
fittedParams (Real) true for tabulating the function with the parameters obtained in the last fit, false (default) if tabulating the function with the parameters given in the Parameter window.
TabulateExtrema

procedure TabulateExtrema(optional parameter list)
Finds the minima/maxima of a function by varying its x-value in a given interval. Calculates a table of
the extrema for different values of a parameter of the function. Parameters:

- **function** (String) The function to be used. Omit for current function.
- **xMin, xMax** (Real) The start and end of the x-interval.
- **parameter** (Integer) The parameter to be varied for tabulating. Pass -2 for varying
  “xMin”, -1 for varying “xMax” (however, these two options do not make much sense!)
- **from, to** (Real) The start and end value of the parameter to be varied.
- **stepValue** (Integer) The step for increasing the parameter.
- **subintervals** (Integer) The number of sub-intervals to be searched in the x-interval.

When the function’s derivative changes its sign over a sub-interval, the
sub-interval is searched for a minimum or maximum.

See also: Extrema, Optimize

TabulateIntegral

procedure TabulateIntegral(optional parameter list)
Calculates the integral of a function over a given x-range. Creates a table of the integral for different
values of a parameter of the function or for different values of a limit of the x-range. Parameters:

- **function** (String) The function to be used. Omit for current function.
- **xMin, xMax** (Real) The start and end of the x-range to be integrated.
- **parameter** (Integer) The parameter to be varied. Pass -2 for varying “xMin”, -1 for varying
  “xMax”
- **from, to** (Real) The start and end value of the parameter (or xMin, xMax) to be
  varied.
- **stepValue** (Integer) The step for increasing the parameter (or xMin, xMax).
- **iterations** (Integer) The number of iterations (5 .. 15). The more iterations you use,
  the more accurate the result becomes.

See also: Integrate

TabulateRoots

procedure TabulateRoots(optional parameter list)
Finds the root(s) of a function (or finds the x-value of a function where its y-value is equal to a given
value) within a given x-range. Varies a parameter and tabulates the roots for different values of this
parameter in a data window. Parameters:

- **function** (String) The function to be used. Omit for current function.
- **xMin, xMax** (Real) The start and end of the x-range.
- **parameter** (Integer) The parameter to be varied. Pass -2 for varying “xMin”, -1 for varying
  “xMax” (however, these two options hardly ever will make sense)
- **from** (Real) The start value of the parameter to be varied.
- **to** (Real) The end value of the parameter to be varied.
- **stepValue** (Integer) The step for increasing the parameter.
- **subintervals** (Integer) The number of sub-intervals to be searched in the x-interval.

When the function’s sign changes over a sub-interval, the sub-interval is
searched for a root.
yValue  (Real) The desired y-value. Omit or set to 0 if finding the x-value where the function becomes zero.

See also: Root

function Tan(x:extended):extended;
Returns the tangent of x. \( \tan(x) = \frac{\sin(x)}{\cos(x)} \).

function Tanh(x:extended):extended;
Returns the hyperbolic tangent of x. \( \tanh(x) = \frac{e^x - e^{-x}}{e^x + e^{-x}} = \frac{\sinh(x)}{\cosh(x)} \).

function TenTo(x:extended):extended;
Returns 10 to the power of x. \( \text{ten}to(x) = 10^x \).

function TestData(row,column:longint)Boolean;
External modules name. See DataOK.

function TestStop:Boolean;
External modules only. Returns true if the current operation should be interrupted (because of user wish or proFitwish).

function TickCount:extended;
Returns the number of 1/60 seconds since your computer was started. It can be useful for timing your programs or functions or for writing intermediate results or status information at regular time-intervals to the Results window.

function TimeString(secs: Boolean):String
Returns a string with the current time. Set secs to true for appending seconds. See also: DateString

procedure Transpose(optional parameter list)
Transposes a data window, i.e. exchanges its rows and columns. Parameters:
window  (String or Longint) The window’s name or window ID. Omit for transposing the front window.

const true = 1;
This constant stands for the logical value of true.
procedure Undo;
Equivalent to selecting “Undo” from the “Edit” menu.

procedure UpperString(var s: String);
Converts all characters of s to upper case. See also LowerString

procedure UseParameterSet(optional parameter list);
Moves a parameter set appearing in the parameter set menu to the parameter window. Parameters:
  set (String) The name of the set.
  forAll (Boolean) True if the parameter set is one available for all functions.
  Default: false
  ofFunction (String) The function the parameter set belongs to. Omit for the current function.
See also: AddParameterSet, SaveParameterSet, LoadParameterSet, DeleteParameterSet

procedure Write(string or expressions);
This procedure can have any reasonable number of strings or expressions as parameters. They will be written into the Results window.
Example:
  Write('x value is: ', x);
Note: The format fields of standard Pascal (:x:y after numerical values or :x after all other values) are not supported. The number of digits after the decimal point for the write and writeln procedures can be specified by choosing “Preferences” from the File menu. Use SetOptions(decimals ...) for setting it from a program or function.
You can redirect the output of Write to a text file using the routines CreateTextFile and WriteToTextFile.

procedure Writeln(string or expressions);
This procedure writes strings and numbers into the Results window. Then it moves the insertion mark to a new line. It uses the same parameters as the procedure write.
Example:
The following writes the value of the top left data cell of the current data window into the results window:
  Writeln('data cell (1,1) = ',data[1,1]);
You can redirect the output of Writeln to a text file using the routines CreateTextFile and WriteToTextFile.

procedure WritelnString(s:Str255);
External modules only. Writes the string s to the results window and starts a new line.

procedure WriteNumber(r:extended);
External modules only. Writes the number r to the results window.
procedure WriteInt(n:longint);
External modules only. Writes the integer number \( n \) to the results window.

procedure WriteString(s:Str255);
External modules only. Writes the string \( s \) to the results window

procedure WriteToTextFile(fileRefNum:longint);
Re-directs the output of Write, Writeln, WriteNumber etc. to a file.
fileRefNum is the number returned by CreateTextFile or 0 if you want to direct output to the results window.
Call CloseTextFile to close the file when you are through

function XColumn:longint;
Returns the column number of the x-column in the current data window. It returns zero if no x-column was set and produces a run-time error if no data window is available.

function XErrColumn:longint;
Returns the column number of the \( \Delta x \)-column in the current data window. It returns zero if no \( \Delta x \)-column was set and produces a run-time error if no data window is available.

function YColumn:longint;
Returns the column number of the y-column in the current data window. It returns zero if no y-column was set and produces a run-time error if no data window is available.

function YErrColumn:longint;
Returns the column number of the \( \Delta y \)-column in the current data window. It returns zero if no \( \Delta y \)-column was set and produces a run-time error if no data window is available.
Appendix B: About numbers

proFit uses three different formats for representing floating point numbers (or float):

- **Real** (or float): This format has smallest accuracy but requires minimum size. It is used in data windows if you set the range of a column to “−1E30 ... 1E30”.
- **Double**: This format has better accuracy but requires more size. It is used in data windows if you set the range of a column to “−1E300 ... 1E300”.
- **Extended** (or native double): This is the format used for internal calculations. It has the same or better accuracy as the double format.

The following list summarizes the features of each data type for the Power Macintosh and the 68k version of pro Fit:

<table>
<thead>
<tr>
<th></th>
<th>real</th>
<th>double</th>
<th>extended (native double)</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td>Power Mac</td>
<td>68k</td>
<td></td>
</tr>
<tr>
<td>minimum negative number</td>
<td>−3.4E38</td>
<td>−1.8E308</td>
<td>−1.8E308</td>
</tr>
<tr>
<td>maximum negative number</td>
<td>−1.2E-38</td>
<td>−2.2E-308</td>
<td>−2.2E-308</td>
</tr>
<tr>
<td>minimum positive number</td>
<td>1.2E-38</td>
<td>2.2E308</td>
<td>2.2E308</td>
</tr>
<tr>
<td>maximum positive number</td>
<td>3.4E38</td>
<td>1.8E308</td>
<td>1.8E308</td>
</tr>
<tr>
<td>decimal digits</td>
<td>7–8</td>
<td>15–16</td>
<td>15–16</td>
</tr>
<tr>
<td>size (bytes)</td>
<td>4</td>
<td>8</td>
<td>8</td>
</tr>
</tbody>
</table>

† The FPU version uses 12 bytes, the non-FPU version 10.

Apart from the values in the list above, pro Fit knows four other numbers: 0, +INF (infinity), -INF (−infinity), NAN. The first three of them will do what you expect them to do. E.g. 1/0 = +INF, INF/3 = INF etc. NAN (Not A Number) is the result of any computation that cannot be carried out, such as sqrt(-1). The occurrence of NAN values in computations is reported as a run-time error.
Appendix C: File formats

This appendix describes the file formats used by proFit for transferring data or drawings to and from other applications.

Data

The default text format

To exchange data between proFit and other applications, text files are used. Usually, such files hold one or more lines of text. Each line contains all values of a row separated by “tabs” (→). The lines are separated by “carriage returns” (¶). It is possible to use other characters instead of tabs and carriage returns (see below).

There are two standard formats of data text files produced by proFit:

The standard format with titles is defined as follows:

1st line: name1 → name2 → name3 ¶
2nd line: 0.123 → 1.732 → 1.122 ¶
3rd line: 2.233 → 2.125 → 2.126 ¶
.....

The standard format without titles is very similar, but without the column titles line.

There is an interesting exception for data text files to be loaded into proFit. If the first line is a single star (*) proFit reads the second line as the column titles even if the file is loaded as being standard format without titles.

Lines are separated by carriage returns ((char) (13) or \r’ for C programmers, chr(13) for Pascal programmers).

The first line with the column titles is optional. These names are separated by tabs (character code 9, here denoted as → – (char) (9) or \t’ for C programmers, chr(9) for Pascal programmers). If proFit reads a file without column titles, it sets the columns names to “Column 1”, “Column 2” etc.

A typical Pascal program for writing such a file would be:

```
var out:text;
...
rewrite(text,'filename');
writeln(text,'x',chr(9),'y');
writeln(text,'1.234',chr(9),'2.341');
writeln(text,'-1.244',chr(9),'3.412');
...
close(text);
```

Some applications produce data text files using other formats, or read data text files only when they are in special formats. proFit provides options to read and write text files in other formats as well. The details are given in the next section.
Loading text files

For reading text files, choose Open... from the File menu, choose “Text Files” from the View pop-up and select the file to be read. You will be prompted for the following information:

If you select **Function or program file**, the file is opened as a non-data text file and loaded into a new function window.

If you select **Data file**, the file is opened as a data file and loaded into a data window. In this case you can select either one of the standard formats or the custom format.

- If “Custom” format is not selected, proFit uses an intelligent translation algorithm, which recognizes most data file formats automatically. By selecting the “With Titles” format pro Fit interprets the first line in the text file as the column titles.
- If “Custom” format is selected, you can specify the file format yourself.

You can import any file where the data is stored as lines of text, each line containing the values of a row. You can specify one or more characters (**Column delimiter**) that separate individual values in a line.
and the characters (Line terminator) that separate the individual lines. For both, column delimiter and
line terminator, pro Fit gives you a selection of the most common combinations.

Furthermore, you can check
- Contains header lines for skipping the first line(s) of the file, or to copy them into the info field
  of the data window, and
- Contains column titles if the file contains column titles in the first line following the optional
  header lines.

Sometimes you do not exactly know how the text file is formatted. Therefore, you may want to have a
look at the starting lines of that file by clicking Show contents. Pro Fit will show you the following
dialog box:

![TEXT File to be Loaded dialog box]

Note that special characters such as a tabulator, line feed or carriage return are written in a double
caracter form with a backslash (\) as the first character.

It is possible to display the text with different Line breaks. If Wrap long lines is checked, the lines
will not be cut at the right border but wrapped to the next line.

Saving text files

You can also save data into text files in a custom format. To do this, choose Save as... from the File
menu for your data window and choose “Text File” from the Format pop-up. In the dialog box that
appears, select Custom format:
This dialog box is very similar to the one for loading text files. Again, you can select the **Column delimiter** and the **Line terminator**.

If **Write header lines** is checked, you have the option to either write a single first line with the text specified in the edit field to the right, or to copy the whole text contained in the info field of the data window as the header of the file.

If **Write column titles** is checked, the next line contains the column names separated by the column delimiter.

Check **Optimize size** to write the numbers with as few characters as possible, without losing precision.

**The native data format**

If you want to exchange binary data with pro Fit, you can use pro Fit’s native file format. A description of this format is given in the technical note “pro Fit binary data file format” that comes with the pro Fit package.

**Drawings**

pro Fit drawings can be saved as PICT files (file type ‘PICT’) or EPS files (file type ‘EPSF’). These formats are used for export to other applications only and cannot be read by pro Fit.

To save a drawing as a PICT file, bring the drawing window to the front and choose Save as... from the File menu. In the dialog box that comes up, check the option “PICT”.

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C-6 Appendix C: File formats
PICT files contain standard Macintosh PICT information and can be read by most drawing applications. The exact format of the PICT files created by proFit depends on the current PICT settings. See Chapter 13, "Preferences", for more information on the different PICT settings.

Note that PICT files cannot contain QuickDraw GX shapes. Do not use the option “QuickDraw GX shape” when saving PICT files.

EPS files are Encapsulated PostScript Files. They are essentially text files containing a standard PostScript representation of the drawing. This representation is used by other applications that understand and work with PostScript. In addition to the PostScript text, a PICT representation of the drawing is included. The file type of EPS files is ‘EPSF’. Hold down the option key while saving the file to produce a file type of ‘TEXT’.

To save a drawing as a EPS file, bring the drawing window to the front and choose Save as... from the File menu. In the dialog box that comes up, check the option “EPS File”.