

Tutorials and worked examples for simulation, curve fitting, statistical analysis, and plotting. http://www.simfit.org.uk

No plot is complete without labels to identify the data in a title, with specific information in the legends, and possibly additional text within the data plotting range to identify special features. However, the labels may not be simple character strings but may contain subscripts, superscripts, or mathematical symbols, which require an associated template to indicate such additional enhancements, as discussed next.

## Labels and corresponding templates

Consider the titles, legends, and additional text in the next figures from fitting a two site binding model displayed in standard space and Scatchard transformed space.



To appreciate how to edit labels and associate template keys to introduce subscripts, superscripts, maths, etc. consider the title, x legend and y legend in the standard plot are as follows

while the additional text and templates for the Scatchard plot are as shown next.

```
T = 21@C
00000030
[Ca++] = 1.3*10-7M
00022000000300220
```

Clearly a 0 indicates a normal character, a template value 1 indicates a subscript while a value 2 indicates a superscript, and these changes would be made by altering the template key interactively.

However the keys equal to 3 for maths or 6 for bold maths are done automatically by selecting the required character from a SIMFIT symbol or maths character substitution table.

## Labels in plots

Labels in  $SIMF_{I}T$  plots are text strings (with associated template strings) that do not have arbitrary positions, but are plotted at default coordinates to identify the data. Some examples would be as follows.

- Labels adjacent to segments in a pie chart.
- Labels on the X axis to indicate groups in bar charts.
- Labels on the X axis to identify clusters in dendrograms.
- Labels plotted alongside symbols in 2D plots, such as principal components.

Test files such as cluster.tfl illustrate the usual way to supply labels appended to data files in order to over-ride the defaults set from the configuration options, but sometimes it is convenient to supply labels interactively from a file, or from the clipboard, and not all procedures in  $SimF_IT$  use the labels supplied appended to data files. The next figures illustrate this.



Test file cluster.tfl was input into the procedure for exhaustive analysis of a matrix in simstat, and the option to plot columns as an advanced 2D plot was selected. This created the left hand figure, where default integer labels indicate row coordinates. Then the option to add labels from a file was chosen, and test file labels.txt was input. This is just lines of characters in alphabetical order to overwrite the default integers. Then the option to read in a template was selected, and test file templates.txt was input. This just contains a succession of lines containing 6, indicating that alphabetical characters are to be plotted as bold maths symbols, resulting in the right hand figure. The recommended procedure follows.

- 1. Write the column of case labels, or row of variable labels, from your data-base or spread-sheet program into an ASCII text file.
- 2. This file should just consist of one label per line and nothing else (like labels.txt)
- 3. Paste this file at the end of your SIMFIT data matrix file, editing the extra line counter (as in cluster.tfl) as required.
- 4. If there are *n* lines of data, the extra line counter (after the data but before the labels) must be at least *n* to use this label providing technique.
- 5. Alternatively use the more versatile begin {labels} ... end{labels} technique.
- 6. Archive the labels file if interactive use is anticipated as in the previous figure.
- 7. If Special symbols or accents are required, a corresponding templates file with character display codes can be prepared.

## Adjusting the position of labels

As an example, principal components for multivariate data can be explored by plotting scree diagrams and scattergrams after using the calculations options in program **simstat**. If labels are appended to the data file, as with cluster.tf2, they can be plotted, as in the next figures.



Labels similar to the ones that are usually plotted along the x axis are used to label the points, but displaced to one or other side of the plotting symbol for legibility. Colors are controlled from the [Colour] options as these are linked to the color of the symbol plotted, even if the symbol is suppressed. The font is the one that would be used to label the x axis if labels were plotted instead of numbers. Clearly arbitrary labels cannot be plotted at the same time on the x axis. Often it is required to move the labels because of clashes, as above. This is done by using the labels editing function, setting labels that clash equal to blanks, then using the normal mechanism for adding arbitrary text and arrows to label the coordinates in the principal components scattergram. To facilitate this process, the default text font is the same as the axes numbering font.

Alternatively, the plotting menus provide the option to displace any labels by defining parameters to shift individual labels horizontally or vertically. The movement is necessarily limited by a numerical scale or slider control, and some versions of  $S_{IM}F_{IT}$  allow label movement by dragging with the red arrow. Clearly, setting the additional *x* and *y* displacements to zero restores the label to the original position adjacent to the symbol being plotted.