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

Often experimental data have been obtained for several responses as a function of the same independent variable and it is wished to fit a model consisting of several deterministic equations to the combined data set. For example, in a chemical experiment several components of a complex reaction can sometimes be measured simultaneously. There are two distinct situations.

- **The equations do not involve the same parameters**

  In this situation there is nothing to be gained from performing a joint determination of all parameters and it is more sensible to analyze the components separately.

- **The equations have common parameters**.

  Separate analysis of the components can be used to get some idea of possible starting estimates but, as the equations are linked, it will necessary to fit the comprehensive model to obtain meaningful parameter estimates.

This type of multiple curve fitting using SimFIT program **qnfit** requires the following steps.

1. **Choosing the correct option**

   From the [A/Z] option on the main SimFIT menu open program **qnfit** then choose to fit a model defining *n* functions of 1 variable.

2. **Providing data**

   The *n* data sets can be input in sequence by file-selection or from your curve fitting project archive, but by far the best method is to input a library file. This has the additional advantage that a percent sign can be used to imply a missing data set.

3. **Providing starting estimates**

   These can be input interactively but it is infinitely preferable to supply starting estimates using the `begin{limits} ... end{limits}` technique appended to the first data set because the program can then be run in EXPERT mode.

4. **Providing a model**

   The model must be prepared as an ASCII text model file using SimFIT program **usermod**.

To illustrate this procedure an extremely simple data set and model with three linear equations unlinked by common parameters will be used.

Example 8: Case 1

From the [Demo] button on the file input control read in the library file `line3.tfl` which is as follows.

```
3 lines for line3.mod/qnfit
line1.data
line2.data
line3.data
```

The first line is the title of the library file and the next three lines are the names of the individual data files.

It is important to note that short names are used in this example because SimFIT recognizes that these three files are test files but, in your own examples, you must use the full path to your data files.

Now consider the first of these test data file, namely `line1.data` shown next.

```
data for line3.mod y = x + 1
5 3
1  1.1  1
2  2.0  1
3  2.9  1
4  4.2  1
5  4.8  1
begin{limits}
-10  0.5  10
-10  0.5  10
-10  1.0  10
-10  3.0  10
-10  2.0  10
-10  2.5  10
end{limits}
```

We see that, after the title, the file header dimension indicates that there 5 values in 3 columns, that is, $x = 1, 2, 3, 4, 5$ in column 1, $y = 1.1, 2.0, 2.9, 4.2, 4.8$ in column 2, and constant weights equal to 1 in column 3. These values are then followed by the limits and starting estimates.

The model

The model file is `line3.mod` which is now listed.

```
%
Three user supplied functions of 1 variable ... 3 straight lines
f(1) = p(1) + p(2)x: (line 1)
f(2) = p(3) + p(4)x: (line 2)
f(3) = p(5) + p(6)x: (line 3)
 %
 3 equations
 1 variable
 6 parameters
 %
 begin{expression}
 f(1) = p(1) + p(2)x
 f(2) = p(3) + p(4)x
 f(3) = p(5) + p(6)x
 end{expression}
 %
```

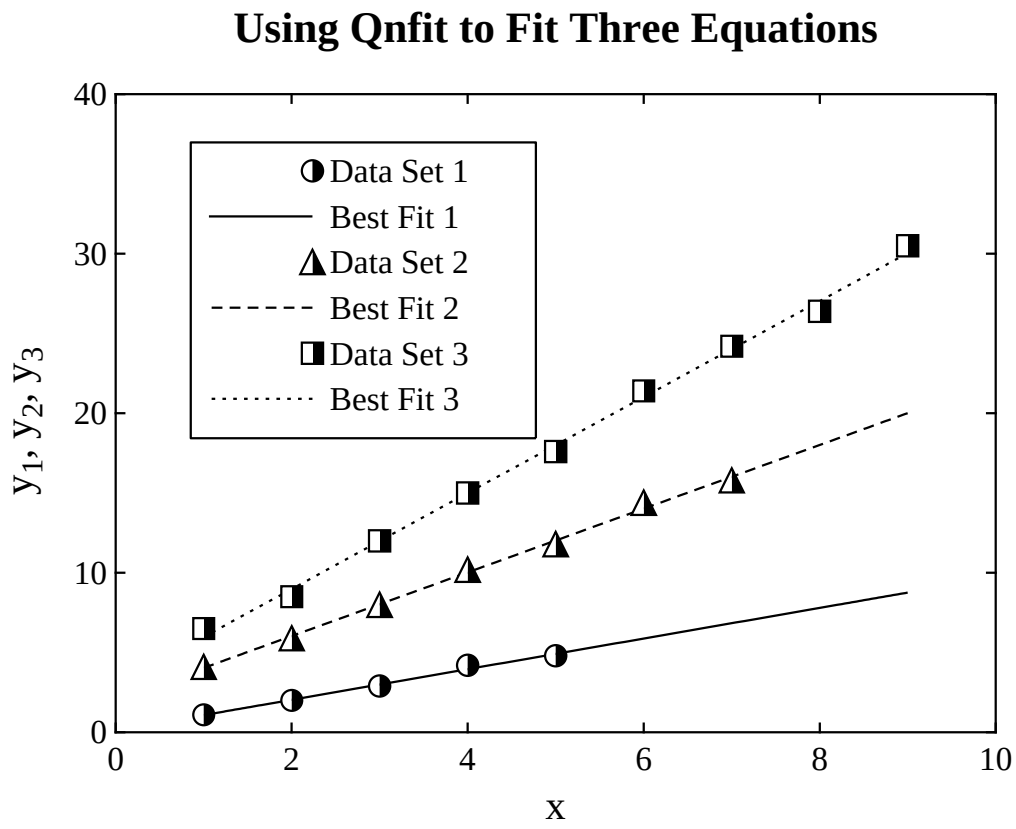
The parameter estimates

Upon proceeding to fit this model the following table of parameter estimates is obtained, indicating that, except for the intercept to line 1 all parameters were well–defined.

Number	Low-Limit	High-Limit	Value	Std.Error	Lower95%cl	Upper95%cl	*p*
1	-10.0	10.0	0.12001	0.367597	-0.66351	0.90352	0.7486 *
2	-10.0	10.0	0.96000	0.110835	0.72376	1.19623	0.0000
3	-10.0	10.0	2.04286	0.296218	1.41149	2.67423	0.0000
4	-10.0	10.0	1.99643	0.066236	1.85525	2.13761	0.0000
5	-10.0	10.0	2.96944	0.254625	2.42672	3.51216	0.0000
6	-10.0	10.0	3.00833	0.045248	2.91189	3.10478	0.0000

The best–fit curves

After fitting the best–fit curves can be displayed as below from the final menu by choosing the option to use the best fit model to plot/extrapolate/deconvolute.



Example 8: case 2

In cases linked by common parameters it is often necessary to fit a system of nonlinear differential equations using program **deqsol**, but the next example illustrates a case where an explicit solution can be obtained for the scheme

$$A \overset{k_1}{\rightarrow} B \overset{k_2}{\rightarrow} C$$

where $p_1 = k_1, p_2 = k_2, p_3 = A(0), p_4 = B(0), p(5) = C(0)$.

$$A(t) = p_3 \exp(-p_1 t)$$

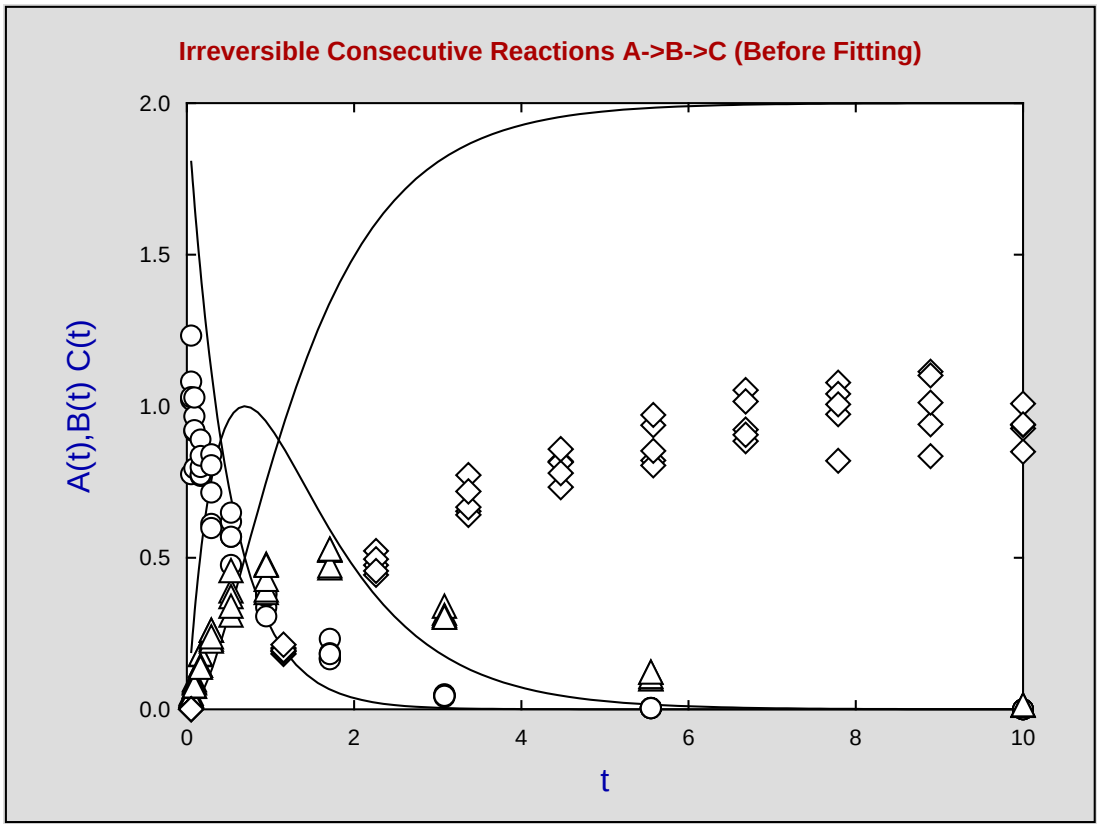
$$B(t) = \left\{\frac{p_1 p_3}{p_2 - p_1}\right\} \exp(-p_1 t) + \left\{p_4 - \frac{p_1 p_3}{p_2 - p_1}\right\} \exp(-p_2 t)$$

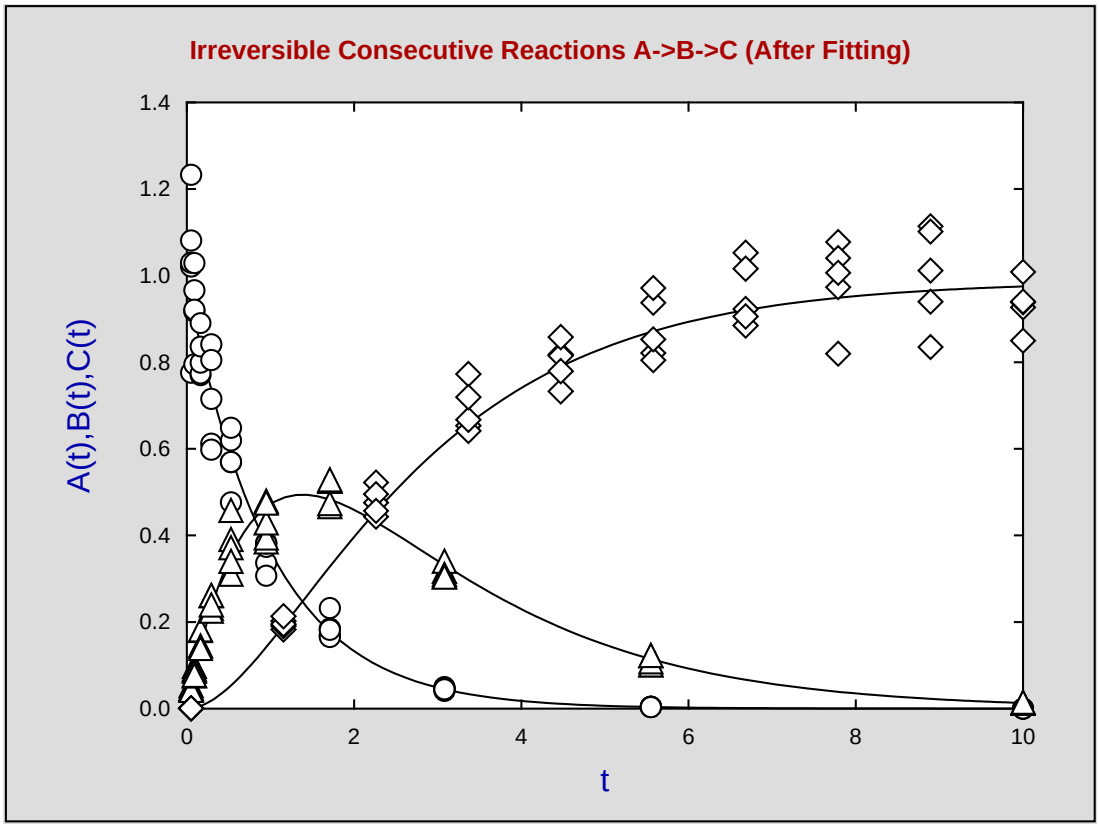
$$= (p_1 p_3 t + p_4) \exp(-p_1 t), \text{ if } k_1 = k_2$$

$$C(t) = p_3 + p_4 + p_5 - \left\{\frac{p_2 p_3}{p_2 - p_1}\right\} \exp(-p_1 t) - \left\{p_4 - \frac{p_1 p_3}{p_2 - p_1}\right\} \exp(-p_2 t)$$

$$= p_3 + p_4 + p_5 - A(t) - B(t), \text{ if } k_1 = k_2.$$

Using **qnfit** to analyze the data in library file `qnfit_data.tf8` with the model `qnfit_model.tf8`, which includes the alternative expression for the singular case $k_1 = k_2$, gives the results obtained before and after fitting shown next. Note that these two test files can be input using the [Demo] button from the **qnfit** file opening dialogue.


Irreversible Consecutive Reactions A->B->C (Before Fitting)
A(t),B(t) C(t)
2.0
1.5
1.0
0.5
0.0
0
2
4
6
8
10
t


Irreversible Consecutive Reactions A->B->C (After Fitting)
A(t),B(t),C(t)
1.4
1.2
1.0
0.8
0.6
0.4
0.2
0.0
0
2
4
6
8
10
t