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

When a theoretical model has been fitted to a data set it is sometimes required to employ the model evaluated using the m best-fit parameters θ_i for calculations. The SIMFIT program **qnfit** provides the following options for doing this using the best-fit model

$$\hat{f}(x) = f(x, \hat{\Theta}), \text{ where } \hat{\Theta} = (\hat{\theta}_1, \hat{\theta}_2, \ldots, \hat{\theta}_m)$$

after displaying the goodness of fit.

1. Plotting the best fit curve together with the data.
2. Plotting residuals in several ways.
3. Extrapolating the best-fit curve beyond the data range.
4. Displaying the contribution of individual components to the overall fit with those models that are sums of sub-models. This type of graphical deconvolution requires the use of those models in the SIMFIT library that are defined in this way. Actually the user-friendly curve-fitting programs also provide this feature where it is appropriate, e.g. **exfit** for sums of exponentials.
5. Evaluating the best-fit model at specific values of the independent variable.
6. Calculating the area under the best-fit curve between defined end points, i.e. the AUC.
7. Plotting the derivative of the best-fit curve over a data range in order to estimate the maximum and minimum slopes.
8. Evaluating the derivative at selected points.
9. Using the best-fit curve for inverse prediction, i.e. calibration.

Some explanation is required for those options in this list that require numerical techniques.

- **Calculating the AUC**

  This can only be done within **qnfit** using Simpson's rule. However the option is provided to vary the number of divisions so that this number can be increased if required until a stable result is obtained.

  Perhaps the most common reason for using this technique is to calculate the area under a curve where the range can be specified, e.g. in pharmacokinetics to estimate bioavailability such as drug plasma levels.

- **Calculating derivatives**

  Here the derivative is estimated at a specific point x using the parameter h in the approximation

$$\frac{dy}{dx} \approx \frac{\hat{f}(x+h) - \hat{f}(x)}{h}$$

  and the option is provided to alter h until a stable result is obtained.

  A very common use for this technique is to estimate the points where the maximum and minimum gradients occur in growth curve studies.

- **Calibration**

  For this procedure to reverse-predict x given it is necessary to solve the nonlinear equation

  $$y - \hat{f}(x) = 0$$

  for a specified y and the unknown x using an iterative technique. If the default starting values do not lead to a satisfactory solution the option is provided to choose new starting estimates A and B where

  $$(y - \hat{f}(A))(y - \hat{f}(B)) < 0.$$

  This functionality means that **qnfit** can be used as a general purpose calibration curve program in those instances where a non-typical calibration curve has to be constructed using a specific model rather than using the SIMFIT polynomial, GLM, or spline smoothing calibration curve programs.

As a very simple example to illustrative these calculations take the data file `qnfit_data.tf1` together with the model file `qnfit_model.tf1` and first fit the model to the data to obtain a best-fit curve. Then continue through the display of goodness of fit until the main **qnfit** menu is reached. The calculation options will then be seen.

This data-model pair is very convenient because the data are very accurate and the model is linear in parameters and very simple, being the quadratic

$$f(x) = \theta_1 x + \theta_2 x^2 + \theta_3,$$

using the usual SIMFIT scheme that constants in theoretical models come last. So, for this extreme case, we can perform the calculations analytically both for the best-fit parameters (2.12035, -0.115647, 0.103471) and the exact parameters (2, -0.1, 0.1) before random error was added using **adderr**, leading to the following results.

Procedure	QNFIT using $\hat{\Theta}$	Calculated using $\hat{\Theta}$	Exact using Θ
Area from 0 to 10	68.5031	68.5032	67.6667
Derivative for $x = 1$	1.88905	1.88906	1.8
Derivative for $x = 2$	1.65776	1.65776	1.6
Derivative for $x = 3$	1.42647	1.42647	1.4
x given $y = 1$	0.43305	0.43305	0.46068
x given $y = 2$	0.94294	0.94294	1.0
x given $y = 3$	1.48658	1.48660	1.57385
Function value for x = 1	2.10817	2.10817	2.0
Function value for x = 1	3.88158	3.88158	3.7
Function value for x = 1	5.42369	5.42370	5.2

Of course this is a ridiculously simple example which is just given to demonstrate how these numerical techniques could be used in more typical situations.