Fitting convolution integrals is often required when an output function is the time–dependent response resulting from an input function interacting with a target function. Parameter estimates and goodness of fit criteria can then be used to justify the assumed functions

The convolution integral required in such situations is defined as $f_3(x) = f_1(t) * f_2(t)$ resulting from the functions $f_1(t)$ and $f_2(t)$ according to

$$\begin{aligned} f_3(x) &= \int_0^x f_1(t) f_2(x-t)\,dt \\ &= f_1 * f_2 \\ &= f_2 * f_1 \end{aligned}$$

where it is understood that functions f_1 and f_2 vanish for negative arguments. This presents no difficulty if the functions are known and the integral can be evaluated formally, but a variety of special situations are encountered experimentally. The case that SIMFIT program **qnfit** can analyze is where functions f_1 and f_2 are assumed deterministic functions but possibly with parameters that have to be estimated from observations on at least one of the functions f_1, f_2, or f_3, and where observations may have experimental error as well as arbitrary spacing and numbers of replicates. Because several situations can arise, for instance when $f_1(x)$ is known exactly, or where $f_2(x)$ cannot be determined independently, the method for supplying data must be sufficiently versatile to accommodate all possible cases and this will be explained first.

Example 9

In general there could be between 1 and 3 data sets and, for the example to be discussed, where the models are

$$\begin{aligned} f_1(t) &= \exp(-p_1 t) \\ f_2(t) &= p_2^2 t \exp(-p_2 t), \end{aligned}$$

the data will be accessed using the model test data set defined by the library file `qnfit_data.tf9`, and this file is as follows.

```
Convolution data
%
%
convolv3.data
```

Here the first line is the title of the library file and the next 3 lines identify the 3 individual data files for the three models f_1, f_2 and $f_3 = f_1 * f_2$. However, note that percentage signs at lines 2 and 3 indicate missing data so that only 1 data set is to be provided, i.e., for the output function. Users should note that when library files are created the files referenced must contain the fully qualified path and filename and not the short name. The reason a short name is used here is because SIMFIT recognizes that `convolv3.data` is a known test file that is to be found in the installation `dem` folder, e.g., `c:\program files\simfit\dem`.

The data set referenced by test file `qnfit_data.tf9` is as as shown next.

```
  p(1) = 1, p(2) = 2, 7.5% relative error
    50     3
  1.0000E-01,  1.9472E-02,  2.0200E-03
  1.0000E-01,  1.6683E-02,  2.0200E-03
  1.0000E-01,  1.8557E-02,  2.0200E-03
  1.0000E-01,  1.5427E-02,  2.0200E-03
  1.0000E-01,  2.0353E-02,  2.0200E-03
  1.5440E-01,  4.1841E-02,  2.3773E-03
  1.5440E-01,  4.0062E-02,  2.3773E-03
  1.5440E-01,  3.8858E-02,  2.3773E-03
  1.5440E-01,  3.6756E-02,  2.3773E-03
  1.5440E-01,  3.6039E-02,  2.3773E-03
  2.3850E-01,  7.6279E-02,  6.5248E-03
  2.3850E-01,  6.7460E-02,  6.5248E-03
  2.3850E-01,  8.4294E-02,  6.5248E-03
  2.3850E-01,  8.0786E-02,  6.5248E-03
  2.3850E-01,  7.3433E-02,  6.5248E-03
  3.6840E-01,  1.5220E-01,  1.0492E-02
  3.6840E-01,  1.4586E-01,  1.0492E-02
  3.6840E-01,  1.2986E-01,  1.0492E-02
  3.6840E-01,  1.5788E-01,  1.0492E-02
  3.6840E-01,  1.4757E-01,  1.0492E-02
  5.6900E-01,  2.5783E-01,  5.3012E-03
  5.6900E-01,  2.5305E-01,  5.3012E-03
  5.6900E-01,  2.5728E-01,  5.3012E-03
  5.6900E-01,  2.4757E-01,  5.3012E-03
  5.6900E-01,  2.4645E-01,  5.3012E-03
  8.7880E-01,  3.5996E-01,  4.3440E-02
  8.7880E-01,  3.4269E-01,  4.3440E-02
  8.7880E-01,  3.0933E-01,  4.3440E-02
  8.7880E-01,  3.2765E-01,  4.3440E-02
  8.7880E-01,  4.2261E-01,  4.3440E-02
  1.3570E+00,  4.2238E-01,  2.4938E-02
  1.3570E+00,  4.1043E-01,  2.4938E-02
  1.3570E+00,  4.3381E-01,  2.4938E-02
  1.3570E+00,  3.7102E-01,  2.4938E-02
  1.3570E+00,  3.9175E-01,  2.4938E-02
  2.0960E+00,  2.8337E-01,  1.5549E-02
  2.0960E+00,  2.9260E-01,  1.5549E-02
  2.0960E+00,  2.9741E-01,  1.5549E-02
  2.0960E+00,  3.1985E-01,  1.5549E-02
  2.0960E+00,  3.1586E-01,  1.5549E-02
  3.2370E+00,  1.2023E-01,  1.2802E-02
  3.2370E+00,  1.1852E-01,  1.2802E-02
  3.2370E+00,  1.4342E-01,  1.2802E-02
  3.2370E+00,  1.1157E-01,  1.2802E-02
  3.2370E+00,  1.1337E-01,  1.2802E-02
  5.0000E+00,  2.3755E-02,  1.9893E-03
  5.0000E+00,  2.9036E-02,  1.9893E-03
  5.0000E+00,  2.7638E-02,  1.9893E-03
  5.0000E+00,  2.7016E-02,  1.9893E-03
  5.0000E+00,  2.7876E-02,  1.9893E-03
begin{limits}
0.001  0.5  5.0
0.001  1.0  5.0
end{limits}
```

Parameter starting estimates and limits have been appended to the data, not the library file, so that program **qnfit** can be used in the EXPERT mode, and the model file is `qnfit_model.tf9` shown below.

```
%
convolution integral: from 0 to x of f1(u)*f2(x - u) du, where
f1(t) = exp(-p(1)*t), f2(t) = [p(2)^2]*t*exp(-p(2)*t)
f3(x) = f1*f2
%
3 equations
1 variable
2 parameters
%
begin{expression}
A = p(1)
B = p(2)
C = p(2)*p(2)
end{expression}
1
x
user1(x,m)
f(1)
2
x
user1(x,m)
f(2)
0.0001
epsabs
0.001
epsrel
0
blim(1)
x
tlim(1)
convolute(1,2)
f(3)
%
begin{model(1)}
%
Example: exponential decay, exp(-p(1)*x)
%
1 equation
1 variable
0 parameter
%
begin{expression}
f(1) = exp(-A*x)
end{expression}
%
end{model(1)}
begin{model(2)}
%
Example: gamma density of order 2
%
1 equation
1 variable
0 parameters
%
begin{expression}
f(1) = C*x*exp(-B*x)
end{expression}
%
end{model(2)}
```

As usual, the model starts with a title section followed by a main section using some commands that require explanation, as all models for fitting convolution integrals must have these features.

1. **Values returned**

   For each value of the independent variable x the model returns the following results.

   - $f_1(x)$
   - $f_2(x)$
   - $f_3(x)$

   The value of $f_1(x)$ can be used to fit model 1 independently, similarly the value of $f_2(x)$ corresponds to the response measured independently of f_1. but not at the same time as $f(3)$ where the argument for f_2 in the integrand is $x - t$. The intention to be used demonstrates how $f_3(x)$ could be fitted at the same time as $f_1(x)$ if data were supplied for both $f_1(x)$ and $f_3(x)$ but $f_2(x)$ could only be fitted at the same time if the data corresponded to the response as a simple function. More usually $f_1(x)$ and $f_2(x)$ are only made available for plotting, as per text–book examples.

2. **Communicating parameters to sub–models**

   ```
   begin{expression}
   A = p(1)
   B = p(2)
   C = p(2)*p(2)
   end{expression}
   ```

   This is a useful way to allow the parameters to be used by the sub–models without using the command `putpar` which is used for this purpose in the reverse Polish version `convolv3.mod`.

3. **Evaluating the sub–models**

   ```
   1
   x
   user1(x,m)
   f(1)
   2
   x
   user1(x,m)
   f(2)
   ```

   This code simply defines $f_1(x)$ and $f_2(x)$ at the current point x.

4. **Parameters controlling the integration**

   ```
   0.0001
   epsabs
   0.001
   epsrel
   0
   blim(1)
   x
   tlim(1)
   convolute(1,2)
   f(3)
   ```

This is how the relative and absolute tolerances are set then the convolution is performed.

5. **The sub–models**

   The sub–models are then defined as if they were standard models except that the number of parameters is set to zero in each model, since the parameters to be estimated have been declared globally using A, B, and C.

Example 9

The steps required to fit a convolution integral using data and models provided by SimFIT are now listed with additional comments.

1. **Opening the curve fitting program data**

   From the main SimFIT menu either choose [Fit] or [A/Z] and proceed to open program **qnfit**.

2. **Supplying data**

   Specify that you wish to fit n functions of 1 variable and then specify that n is to be 3. When asked to supply data press the [Demo] button on the file opening dialogue and select the library file `qnfit_data.tf9`.

3. **Supplying models**

   When asked for a model file use the [Demo] button on the file opening dialogue to choose the model file `qnfit_model.tf9`.

4. **Supplying starting estimates**

   The best way to supply parameter starting estimates and limits is to choose the EXPERT mode as that reads settings from the actual data set supplied which is `convolv3.data`, and not the library file `qnfit_data.tf9`.

5. **Performing a fit**

   At this stage you can preview the parameter starting estimates and limits, or view the fit of the model with starting estimates overlayed on the data before proceeding to fitting.

After fitting the following summary and a table of best-fit parameters will be displayed.

Results from curve-fit number 1	
Number of data points	50
Number of parameters	2 (0 currently fixed)
Degrees of freedom	48
WSSQ before entry	62318.7
IFAIL from LBFGSB	0
WSSQ from fitting	49.654
P($\chi^2 \geq$ WSSQ)	0.4072
Time taken to fit	0.194 (secs cpu time)

Best-fit parameters for curve-fit 1 using LBFGSB							
Number	Low-Limit	High-Limit	Value	Std.Error	Lower95%cl	Upper95%cl	p
1	0.001	5.0	0.99684	0.0089381	0.97887	1.01482	0.0000
2	0.001	5.0	2.00479	0.0115128	1.98164	2.02793	0.0000
For 50,90,95,99% parameter confidence limits using [parameter value +/- t(α/2)*std.err.]							
t(0.25) = 0.680, t(0.05) = 1.677, t(0.025) = 2.011, t(0.005) = 2.682							

Of course, now the model validity can be checked if the parameters are known independently by comparing the differences between the known and estimated parameters. Additional tests for goodness of fit can be displayed and eventually a plot showing the input function, response function (as a function of x and not shifted) and output convolution as illustrated next.