



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

Given n functions of n variables in a user-defined model file it is sometimes possible to estimate zeros as long as good starting estimates are input, and a reasonable tolerance factor is provided.

The model file must define a system of n equations f_i in n variables x_i and the SIMFIT program **usermod** will attempt to locate x_1, x_2, \dots, x_n such that

$$f_i(x_1, x_2, \dots, x_n) = 0, \text{ for } i = 1, 2, \dots, n.$$

Users must supply good starting estimates by editing the default starting estimates y_1, y_2, \dots, y_n , or installing a new y vector from a file, and the accuracy can be controlled by varying $xtol$, since the program attempts to ensure that

$$\|x - \hat{x}\| \leq xtol \times \|\hat{x}\|,$$

where \hat{x} is the true solution, as described for NAG routine C05NBF. Failure to converge will lead to nonzero *IFAIL* values, requiring a re-run with new starting estimates.

From the main SIMFIT menu choose [A/Z] then open program **usermod** and input test file `usermodn_e.tf4` which defines 9 equations in 9 variables for the following tridiagonal system.

$$\begin{aligned} (3 - 2x_1)x_1 - 2x_2 + 1 &= 0 \\ -x_{i-1} + (3 - 2x_i)x_i - 2x_{i+1} + 1 &= 0, \quad i = 2, 3, \dots, 8 \\ -x_8 + (3 - 2x_9)x_9 + 1 &= 0. \end{aligned}$$

After setting the starting estimates $y(i) = 0$ for $i = 1, 2, \dots, 9$ proceed to locate zeros of n equations in n variables when the following table will result.

IFAIL = 0, *FNORM* = 7.448E-10, *xtol* = 1.000E-03

Variable	Value	Function	Value
$x(1)$	-5.7065289E-01	<i>fvec</i> (1)	2.5267933E-06
$x(2)$	-6.8162532E-01	<i>fvec</i> (2)	1.5688139E-05
$x(3)$	-7.0173246E-01	<i>fvec</i> (3)	2.8357029E-07
$x(4)$	-7.0421463E-01	<i>fvec</i> (4)	-1.3083878E-05
$x(5)$	-7.0136741E-01	<i>fvec</i> (5)	9.8768418E-06
$x(6)$	-6.9186497E-01	<i>fvec</i> (6)	6.5557114E-06
$x(7)$	-6.6579418E-01	<i>fvec</i> (7)	-1.3053615E-05
$x(8)$	-5.9603414E-01	<i>fvec</i> (8)	1.1777047E-06
$x(9)$	-4.1641142E-01	<i>fvec</i> (9)	2.9510981E-06

The values displayed at the solution point are as follows.

<i>IFAIL</i>	<i>IFAIL</i> = 0, otherwise re-run.
<i>FNORM</i>	final 2-norm of the residuals.
<i>xtol</i>	Tolerance factor.
$x(i)$	Estimates for x_i .
<i>fvec</i> (i)	$f_i(x)$ values.

As values less than about 10^{-7} are effectively zero compared to 1, this represents a satisfactory outcome since $f_i(x) \approx 0$ for $i = 1, 2, \dots, n$ at the solution point.

For reference, the model is as follows.

```

%
Example: 9 functions of 9 variables as in NAG C05NBF
        set y(1) to y(9) = -1 or 0 for good starting estimates
f(1)=(3-2x(1))x(1)-2x(2)+1, &, f9=-x(8)+(3-2x(9))x(9)+1
%
9 equations
9 variables
0 parameters
%
begin{expression}
f(1) = (3 - 2y(1))y(1) + 1 - 2y(2)
f(2) = (3 - 2y(2))y(2) + 1 - y(1) - 2y(3)
f(3) = (3 - 2y(3))y(3) + 1 - y(2) - 2y(4)
f(4) = (3 - 2y(4))y(4) + 1 - y(3) - 2y(5)
f(5) = (3 - 2y(5))y(5) + 1 - y(4) - 2y(6)
f(6) = (3 - 2y(6))y(6) + 1 - y(5) - 2y(7)
f(7) = (3 - 2y(7))y(7) + 1 - y(6) - 2y(8)
f(8) = (3 - 2y(8))y(8) + 1 - y(7) - 2y(9)
f(9) = (3 - 2y(9))y(9) + 1 - y(8)
end{expression}

```