



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

Given a function of one variable it is possible to estimate zeros as long as two values of the independent variable are provided where the function has opposite signs.

The steps involved are as now detailed.

1. Select a model $f(\Theta, x)$, i.e. a function of one variable, and possibly some parameters Θ .
2. Adjust the parameters Θ if required.
3. Input a constant term C to define the function $g(x) = f(\Theta, x) - C$.
4. Just set $C = 0$ if a root of $g(x) = f(\Theta, x) = 0$ is required.
5. Plot the function $f(\Theta, x)$ to locate two values A, B such that $g(A)g(B) < 0$.
6. Input the proposed limits A, B then solve $g(x) = 0$.
7. If this fails, adjust the limits A, B or tolerance factor *epsrel* and try again.

As an example, the procedure required to input a user-defined model will be described.

From the main SIMFIT menu select [A/Z], open program **usermod** then read in the SIMFIT model-defining test file `usermods_e.tf1` which has the following form.

```
%  
phi(x) = normal cdf  
%  
1 equation  
1 variable  
0 parameters  
%  
begin{expression}  
f(1) = phi(x)  
end{expression}  
%
```

This is a model file for special functions for which the normal cdf function $\Phi(x)$ has been selected, that is

$$\Phi(x) = \frac{1}{\sqrt{2\pi}} \int_{-\infty}^x \exp\left(-\frac{t^2}{2}\right) dt$$

and it will now be available to program **usermod** for calculations such as root finding or plotting.

The steps necessary to find a root of the equation $g(x) = 0$ where $g(x)$ is defined as

$$g(x) = \Phi(x) - C$$

for some constant C will now be described.

Users must supply a relative error accuracy factor *epsrel*, two values A and B , and a constant C such that, for $g(x) = \Phi(x) - C$, then $g(A)g(B) < 0$.

If the values supplied are such that $g(A)g(B) > 0$, the program will attempt to enlarge the interval in order to bracket a zero, but it will not change the sign of A or B .

Users must do this if necessary by editing the starting estimates A and B .

The program returns the root as X if successful, where X and Y have been located such that

$$|X - Y| \leq 2.0 \times \text{epsrel} \times |Z|$$

and $|g(Z)|$ is the smallest known function value, as described for NAG routine C05AZF.

For instance, input $C = 0.975$ so the routine is required to estimate x such that

$$0.975 = \frac{1}{\sqrt{2\pi}} \int_{-\infty}^x \exp\left(-\frac{t^2}{2}\right) dt$$

and, after setting some reasonable starting estimates, e.g., the defaults $(-1,1)$, the following message will be printed

```
Success : Root = 1.96 (EPSREL = 0.001)
```

giving the root estimated by the SIMFIT implementation of C05AZF.

In other words, this calculation has located the upper 2.5% point of the standard normal distribution as illustrated by the following plot.

