



Tutorials and worked examples for simulation, curve fitting, statistical analysis, and plotting.

<https://simfit.org.uk>

<https://simfit.silverfrost.com>

It is often required to fit two or more possible models in sequence to a data set in order to decide which model is best justified for the data supplied. SIMFIT has several programs designed to do this automatically, e.g., **exfit** for sums of exponentials, **mmfit** for sums of Michaelis-Menten equations, **rffit** for positive rational functions, etc. At each stage of model fitting these programs output goodness of fit measures, and perform an *F* tests for excess variance. The SIMFIT program **qnfit**, like these other programs, also allows users to store *F* test details for retrospective testing which can also be done interactively, as now described.

Open the SIMFIT main menu, choose [Statistics], then [Standard tests], and select the *F* test option. This requires you to input the following values.

1. The objective function Q_1 and number of parameters m_1 in the simpler model.
2. The objective function Q_2 and number of parameters m_2 in the richer model.
3. The number of experimental data points n .

Obviously this test requires $Q_1 > Q_2$, $m_2 > m_1$, and $n > m_2$.

For instance, using the default parameters gives these results.

<i>F</i> test results	
Q_1 ((<i>W</i>).SSQ for model 1)	12.00
Q_2 ((<i>W</i>).SSQ for model 2)	10.00
m_1 (number of parameters in model 1)	2
m_2 (number of parameters in model 2)	3
n (number of experimental points)	12
Numerator degrees of freedom	1
Denominator degrees of freedom	9
<i>F</i> test statistic <i>TS</i>	1.800
$P(F \geq TS)$	0.2126
$P(F \leq TS)$	0.7874
5% upper tail critical point	5.117
1% upper tail critical point	10.56
Conclusion:	
Model 2 is not justified ... Tentatively accept model 1	

From such values SIMFIT calculates the test statistic *TS* given by

$$TS = \frac{(Q_1 - Q_2)/(m_2 - m_1)}{Q_2/(n - m_2)}$$

which may be distributed, or more usually only approximately distributed, according to the *F* distribution with $m_2 - m_1$ and $n - m_2$ degrees of freedom. The table indicates that, as *TS* was less than the upper 5% critical point, there are no grounds for accepting the richer model in this particular case.

It must be emphasized that, while simulations suggest that this test is fairly robust in simple cases like distinguishing one exponential from two, the test is only really justified for fitting linear nested model families like polynomials, or multilinear regression, as now outlined.

Justification for the F test can be illustrated by successive fitting of polynomials to the same data

$$\begin{aligned} H_0 : f(x) &= \alpha_0 \\ H_1 : f(x) &= \alpha_0 + \alpha_1 x \\ H_2 : f(x) &= \alpha_0 + \alpha_1 x + \alpha_2 x^2 \\ &\dots \\ H_k : f(x) &= \alpha_0 + \alpha_1 x + \alpha_2 x^2 + \dots + \alpha_k x^k \end{aligned}$$

in a situation where experimental error is normal with zero mean and constant variance, and the true model is a polynomial, a situation that will never be encountered in real life.

The important distributional results, can be illustrated for the case of two models i and j , with $j > i \geq 0$, so that the number of points and parameters satisfy $n > m_j > m_i$ while the sums of squares are $Q_i > Q_j$, then

1. $(Q_i - Q_j)/\sigma^2$ is $\chi^2(m_j - m_i)$ under model i
2. Q_j/σ^2 is $\chi^2(n - m_j)$ under model j
3. Q_j and $Q_i - Q_j$ are independent under model j .

So the likelihood ratio test statistic

$$F = \frac{(Q_i - Q_j)/(m_j - m_i)}{Q_j/(n - m_j)}$$

is distributed as $F(m_j - m_i, n - m_j)$ if the true model is model i , which is a special case of model j in the nested hierarchy of the polynomial class of linear models.

In most experiments the models $f(x, \theta)$ fitted to n observations y_i are nonlinear in the parameters θ , and the variance of the experimental error usually increases as the measured responses increase. In an attempt to allow for this, weighting factors w_i are introduced so that the objective function at the minimum would be the sum of weighted squared residuals $WSSQ$ given by

$$WSSQ = \sum_{i=1}^n w_i \{y_i - f(x_i, \hat{\theta})\}^2.$$

However, the choice of weighting factors is highly controversial. For instance, if the variances of the experimental errors were known to be σ_i^2 , then an obvious choice for the weighting factors would be

$$w_i = \frac{1}{\sigma_i^2}$$

effectively reducing the problem to the special case of constant variance, much beloved by theoreticians.

To study individual cases, these options are available using SIMFIT, especially with program **qfit**.

- Set all $w_i = 1$.
Fitting will tend to be unduly dominated by large responses y_i .
- Set all $w_i = 1/s_i^2$, where s_i are standard errors determined from replicates.
Standard error estimates will be unreliable unless large number of replicates are available.
- Set all $w_i = 1/g(y_i)$, for some specified function $g(y)$.
Fitting may be dominated by small responses y_i if $g(y) = (\alpha y)^2$ for some α .
- Set all $w_i = 1/h(f)$, for some specified function $h(f(x, \theta))$.
Weights will change for each cycle of optimization as the parameters change.

All these can lead to bias and using s , $g(y)$ or $h(f)$ should be justified by further investigation.