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1.1 How to use SimFIT test files

The SimFIT package provides a very large number of data analysis procedures as follows.

1. Creating and editing data files and mathematical models in SimFIT format
2. Simple curve fitting using defined models and automatically chosen starting estimates
3. Advanced curve fitting by constrained nonlinear regression using models from a built-in library or as user-defined equations
4. Simulating and fitting systems of nonlinear differential equations
5. Statistical analysis using standard and multivariate techniques
6. Data smoothing by polynomials or splines for constructing calibration curves
7. Plotting in two or three dimensions and as contours

So, in order to make SimFIT user-friendly, there are test files that can be used to experiment with any chosen procedure. For most of the SimFIT procedures a typical data set is automatically provided as a test file when a procedure is chosen. However, for all procedures there is a [Demo] option on the file-open widow that allows users to view or select possible data sets before trying with their own data sets, and there is also a [Paste] option to transform rectangular clipboard data tables into SimFIT format.

This document is just a list of the test files bundled with the SimFIT package, but the [View] option on the main menu also allows users to view any of the files listed.

1.2 Summary of SimFIT test files

Note that all SimFIT test files, data files, configuration files and graphics files (EPS and SVG) are ASCII text files that can be read and altered in any text editor, e.g., notepad. Data files can use integers, floating point, or scientific (i.e., exponential) notation and columns can be comma-separated or space-separated.

The test files consist of data sets that can be used to understand how SimFIT works. You can use a test file with a program, then view it to appreciate the format before running your own data. Library files are just collections of names of test files so you can enter many files at the same time. This is very useful with statistics (e.g., ANOVA, multiple comparisons with simstat) and plotting (e.g., supplying ASCII coordinate files to simplot).

Configuration and default files are used by SimFIT to store certain parameter values that are relevant to some particular functions. Some files are created automatically and upgraded whenever you make significant changes, and some are created only on demand. All such configuration and default files are ASCII text files that can be browsed in the SimFIT viewer. In general, the idea is that when a particular configuration proves satisfactory you could make a copy of the file to restore the current defaults after SimFIT has altered the settings. SimFIT generates many temporary files and if you exit from a program in an abnormal fashion (e.g., by Ctrl+Alt+Del) these are left in an unfinished state. Usually these would be automatically deleted, but expert users will sometimes want the facility to save temporary files on exit from SimFIT, so this possibility is provided but should be used sparingly.

You should not attempt to edit such files in a text editor but note that, if you suspect a fault may be due to a faulty configuration or default files, just delete them and SimFIT will create new versions.
1.3 List of test files by type

1.3.1 Test files (Data)

- **adderr.tf1**: Data for adding random numbers using `adderr`.
- **adderr.tf2**: Data for adding random numbers using `adderr`.
- **anova1.tf1**: Matrix for 1 way analysis of variance in `ftest` or `simstat`.
- **anova2.tf1**: Matrix for 2 way analysis of variance in `ftest` or `simstat`.
- **anova2.tf2**: Matrix for 2 way analysis of variance in `ftest` or `simstat`.
- **anova3.tf1**: Matrix for 3 way analysis of variance in `ftest` or `simstat`.
- **anova4.tf1**: Matrix for groups/subgroups analysis of variance in `ftest` or `simstat`.
- **anova5.tf1**: Matrix for factorial ANOVA (2 factors, 1 block).
- **anova5.tf2**: Matrix for factorial ANOVA (2 factors, 3 blocks).
- **anova5.tf3**: Matrix for factorial ANOVA (3 factors, 1 blocks).
- **anova5.tf4**: Matrix for factorial ANOVA (3 factors, 3 blocks).
- **anova6.tf1**: Matrix for repeated measures ANOVA (5 subjects, 4 treatments).
- **average.tf1**: Data for program `average`.
- **barchart.tf1**: Creates a barchart in `simplot`.
- **barchart.tf2**: Creates a barchart in `simplot`.
- **barchart.tf3**: Creates a barchart in `simplot`.
- **barchart.tf4**: Creates a barchart in `simplot`.
- **barchart.tf5**: Creates a barchart in `simplot`.
- **barchart.tf6**: Creates a barchart in `simplot`.
- **barchart.tf7**: Adds a curve to barchart created from `barchart.tf6`.
- **barchart3d.tf1**: Creates a 3 dimensional barchart in `simplot`.
- **barchart3d.tf2**: Creates a 3 dimensional barchart in `simplot`.
- **barchart3d.tf3**: Creates a 3 dimensional barchart in `simplot`.
- **binomial.tf1**: Fifty numbers from a binomial distribution with $N = 50$, $p = 0.5$.
- **binomial.tf2**: Analysis of proportions with no effector values, i.e. $X, N$.
- **binomial.tf3**: Analysis of proportions with effector values, i.e. $X, N, t$.
- **binomial.tf4**: Analysis of proportions with effector values, i.e. $X, N, t$.
- **binomial.tf5**: Analysis of proportions with effector values, i.e. $X, N, t$.
- **bivariate.tf1**: Data for fitting a scaled bivariate normal model.
- **calcurve.tf1**: Prepares a calibration curve in EXPERT mode using `calcurve`.
- **calcurve.tf2**: Calcurve.tf1 with no weights or EXPERT mode settings.
- **calcurve.tf3**: Predicts $y$ given $x$ with calcurve.tf1.
- **chisqd.tf1**: Fifty numbers from a chi-square distribution with $v = 10$.
- **chisqd.tf2**: Vector of observed values to be used with `chisqd.tf3`.
- **chisqd.tf3**: Vector of expected values to be used with `chisqd.tf2`.
- **chisqd.tf4**: Matrix for Fisher exact test in `chisqd` or `simstat`.
- **chisqd.tf5**: Contingency table for chi-square test in `chisqd` or `simstat`.
- **cluster.tf1**: Data for multivariate cluster analysis in `simstat`.
- **cluster.tf2**: Data for multivariate cluster analysis in `simstat`.
- **cochranq.tf1**: Matrix for Cochran Q test.
- **column1.tf1**: Vector for 1 way ANOVA in `ftest` or `simstat`.
- **column1.tf2**: Vector for 1 way ANOVA in `ftest` or `simstat`.
- **column1.tf3**: Vector for 1 way ANOVA in `ftest` or `simstat`.
- **column1.tf4**: Vector for 1 way ANOVA in `ftest` or `simstat`.
- **column1.tf5**: Vector for 1 way ANOVA in `ftest` or `simstat`.
- **column2.tf1**: Vector for nonparametric correlation in `rtest` or `simstat`.
- **column2.tf2**: Vector for nonparametric correlation in `rtest` or `simstat`.
- **column2.tf3**: Vector for nonparametric correlation in `rtest` or `simstat`.
- **compare.tf1**: Use with `compare` to compare with `compare.tf2`.
- **compare.tf2**: Use with `compare` to compare with `compare.tf1`.
consec4.tf1 Used by deqsol in consec4.TFL for A in 4 differential equations A=B=C=D
consec4.tf2 Used by deqsol in consec4.TFL for B in 4 differential equations A=B=C=D
consec4.tf3 Used by deqsol in consec4.TFL for C in 4 differential equations A=B=C=D
consec4.tf4 Used by deqsol in consec4.TFL for D in 4 differential equations A=B=C=D
consec5.tf1 Used by deqsol in consec4.TFL for A in 5 differential equations A=B=C=D=E
consec5.tf2 Used by deqsol in consec4.TFL for B in 5 differential equations A=B=C=D=E
consec5.tf3 Used by deqsol in consec4.TFL for C in 5 differential equations A=B=C=D=E
consec5.tf4 Used by deqsol in consec4.TFL for D in 5 differential equations A=B=C=D=E
consec5.tf5 Used by deqsol in consec4.TFL for E in 5 differential equations A=B=C=D=E
cox.tf1 Survival data for Cox proportional hazards model
cox.tf2 Survival data for Cox proportional hazards model
cox.tf3 Survival data for Cox proportional hazards model
cox.tf4 Survival data for Cox proportional hazards model
cox.tf5 Example of the preliminary flow cytometry format for c sadat
cox.tf6 Example of the preliminary flow cytometry format for c sadat
csa.fit.tf1 Geometric type data with 15% stretch for c safit
csa.fit.tf2 Arithmetic type data with 5% translation for c safit
csa.fit.tf3 Mixed type data for c safit
deqsol.tf1 Library data for fitting LV1.tf1 and LV2.tf1 by deqsol
deqsol.tf2 Library data for fitting LV1.tf1 by deqsol
deqsol.tf3 Library data for fitting LV2.tf1 by deqsol
deflt.tf1 Data for editing by deflt
deflt.tf2 Data for editing by deflt
deflt.tf3 Data for editing by deflt
deflt.tf4 Data for editing by deflt
defltm.tf1 Data for editing by defltm
defltm.tf2 Data for editing by defltm
defltm.tf3 Data for editing by defltm
errorbar.tf1 Normal error bars (4 columns)
errorbar.tf2 Advanced error bars (6 columns)
exfit.tf1 Exact data for 1 exponential for fitting by exfit
exfit.tf2 Random error added to exfit.tf1 by adderr
exfit.tf3 Exact data for 2 exponentials for fitting by exfit
exfit.tf4 Random error added to exfit.tf3 by adderr
exfit.tf5 Exact data for Model 5 in exfit
exfit.tf6 Exact data for Model 6 in exfit
exfit.tf7 Exact data for concave down exponentials in exfit
fdr_bh.tf1 Data for false discovery rate calculations in simstat
f test.tf1 Fifty numbers from the $\mathcal{U}_{11D439}$ distribution with $\mu_1 = 2$, $\sigma_1 = 5$
gauss3.tf1 3 Gaussians: starting estimates by begin{limits}...end{limits}
gauss3.tf2 3 Gaussians: starting estimates from start of trailer section
gcfit.tf1 Exact data for model 3 in gcfit
gcfit.tf2 Random error added to gcfit.tf1 by adderr
gcfit.tf3 Random error added to gcfit.tf1 by adderr
gcfit.tf4 Random error added to logistic equation by adderr
gcfit.tf5 Gompertz growth data
gcfit.tf6 Gompertz decay data by reversing gcfit.tf5
glm.tf1 Normal errors, reciprocal link
glm.tf2 Binomial errors, logistic link
glm.tf3 Poisson errors, log link
glm.tf4 Gamma errors, reciprocal link
gompertz.tf1 Data for gcfit in survival mode 2
hlfit.tf1 Exact data for 1 site for fitting by hlfit
hlfit.tf2 Random error added to hlfit.tf1 by adderr
hlfit.tf3  Exact data for 2 sites for fitting by hlfit
hlfit.tf4  Random error added to hlfit.tf3
hotcold.tf1  Data for mmfit/hlfit/qnfit in isotope displacement mode
hotel.tf1  Data for Hotelling 1-sample T-square test
houses.tf1  Data for constructing a biplot
incomplete.tf1  Incomplete matrix with missing values (comma-separated)
incomplete.tf2  Incomplete matrix with missing values (semicolon-separated)
incomplete.tf3  Incomplete matrix with missing values (tab-separated)
incomplete.mv1  Incomplete matrix with missing values (copy of incomplete.tf1)
incomplete.mv2  Incomplete matrix with missing values (copy of incomplete.tf2)
incomplete.mv3  Incomplete matrix with missing values (copy of incomplete.tf3)
inhibit.tf1  Data for fitting mixed inhibition as v = f(S,I)
inrate.tf1  Data for models 1 and 2 in inrate
inrate.tf2  Data for model 3 in inrate
inrate.tf3  Data for model 4 in inrate
inrate.tf4  Data for model 5 in inrate
latinsq.tf1  Latin square data for 3 way ANOVA in ftest or simstat
iris.tf1  Iris data for K-means clustering (see manova1.tf5)
iris.tf2  Starting K-means clusters for iris.tf2
kmeans.tf1  Data for K-means cluster analysis
kmeans.tf2  Starting clusters for kmeans.tf1
ld50.tf1  Dose-response data for LD50 by GLM as y,N,x
ld50.tf2  Dose-response data for LD50 by GLM as x,y,N,s
ld50.tf3  Dose-response data for LD50 by GLM as x,N-y,N,s
line.tf1  Straight line data
line.tf2  Straight line data
linfit.tf1  Multilinear regression data for linfit
linfit.tf2  Multilinear regression data for linfit
linfit.tf3  Weighted linear regression data for linfit
logistic.tf1  Data for binary logistic regression
logistic.tf2  Data to predict p after fitting logistic.tf1
logistic.tf3  Data for logistic regression
logistic.tf4  Data for logistic regression
logistic.tf5  Data for logistic regression
loglin.tf1  Data for log-linear contingency table analysis
lv1.tf1  Data for y(1) in the Lotka-Volterra differential equations
lv2.tf1  Data for y(2) in the Lotka-Volterra differential equations
maksim.tf1  Matrix for editing by maksim
maksim.tf2  Matrix for editing by maksim
manova1.tf1  MANOVA data: 3 groups, 2 variables
manova1.tf2  MANOVA data: 3 groups, 2 variables
manova1.tf3  MANOVA data: 2 groups, 5 variables
matrix_a.tf1  30 by 3 Directed correlation data
matrix_b.tf1  30 by 4 Directed correlation data
matrix_p.tf1  3 by 4 Matrix of probabilities
matrix.tf1  5 by 5 matrix for simstat in calculation mode
matrix.tf2  7 by 5 matrix for simstat in calculation mode
matrix.tf3  Positive-definite symmetric 4 by 4 matrix for simstat in calculation mode
matrix.tf4  Symmetric 4 by 4 matrix for simstat in calculation mode
matrix.tf5  25 by 4 matrix for simstat in correlation mode
mcnemar.tf1  Data for McNemar test
meta.tf1  Data for Cochran-Mantel-Haentzel Meta Analysis test
meta.tf2  Data for Cochran-Mantel-Haentzel Meta Analysis test
meta.tf3  Data for Cochran-Mantel-Haentzel Meta Analysis test
mmfit.tf1  Exact data for 1 Michaelis-Menten isoenzyme in mmfit
mmfit.tf2  Random error added to mmfit.tf1 by adderr
mmfit.tf3  Exact data for 2 Michaelis Menten isoenzymes in mmfit
mmfit.tf4  Random error added to mmfit.tf3 by adderr
normal.tf1  Fifty numbers from a normal distribution with $\mu = 0, \sigma = 1$
normal.tf2  Fifty numbers from a normal distribution with $\mu = 1, \sigma = 2$
normal.tf3  Fifty numbers from N(-1.5,1) plus fifty from N(1.5,1)
npcorr.tf1  Matrix for nonparametric correlation in rstest or simstat
pacorr.tf1  Correlation matrix for partial correlation in simstat
pabst-einstein.tf1  log10(Pabst-Einstein) equation
piechart.tf1  Creates a piechart in simplot
piechart.tf2  Creates a piechart in simplot
piechart.tf3  Creates a piechart in simplot
plot2.tf1  LHS axis data for double plot in simplot
plot2.tf2  LHS axis data for double plot in simplot
plot2.tf3  RHS axis data for double plot in simplot
plis_x.tf1  Partial least squares X matrix in simstat
plis_y.tf1  Partial least squares Y matrix in simstat
plis_z.tf1  Partial least squares Z matrix in simstat
poisson.tf1  Forty numbers from a Poisson distribution
poisson.tf2  Death from horse kicks in Prussian cavalry
polnom.tf1  Data for a quadratic in polnom
polnom.tf2  Predict x given y from polnom.tf1
polnom.tf3  Predict y given x from polnom.tf1
polnom.tf4  Fit after transforming to $x = \log(x), y = \log(y/(1 - y))$
primes.tf1  Single prime numbers up to 10000
primes.tf2  Twin prime numbers up to 10000
qnfit_data.tf1  Data for qnfit tutorials: Example 1 Quadratic
qnfit_data.tf2  Data for qnfit tutorials: Example 2 2D linear
qnfit_data.tf3  data for qnfit tutorials: Example 3 3D linear
qnfit_data.tf4  data for qnfit tutorials: Example 4 Sum of 2 MM curves
qnfit_data.tf5  data for qnfit tutorials: Example 5 B in A->B->C
qnfit_data.tf6  data for qnfit tutorials: Example 6 Sum of 2 normal pdfs
qnfit_data.tf7  data for qnfit tutorials: Example 6 Sum of 2 normal cdfs
qnfit.tf1  Quadratic in Expert mode for qnfit
qnfit.tf2  Reversible Michaelis-Menten data in Expert mode for qnfit
qnfit.tf3  Linear function of 3 variables in Expert mode for qnfit
qnfit_ode.tf1  Michaelis-Menten substrate depletion data in Expert mode for qnfit
qnfit_ode.tf2  Von Bertalanffy growth data in Expert mode for qnfit
qnfit_ode.tf3  Von Bertalanffy growth decay data in Expert mode for qnfit
rainfall.tf1  Rainfall in England and Wales from 1766 to 2015
rffit.tf1  2:2 Rational function data for rffit
rffit.tf2  1:2 Rational function data for rffit
rffit.tf3  2:2 Rational function data for rffit
rffit.tf4  2:3 Rational function data for rffit
rffit.tf5  4:4 Rational function data for rffit (2 turning points)
rffit.tf6  3:4 Rational function data for rffit (3 turning points)
rffit.tf7  rffit6 with triplicates and 7.5% relative error
robust.tf1  Normal.tf1 with 5 outliers
rtest.tf1  Residuals for runs test in rtest
sffit.tf1  Exact data for 1 site in sffit
sffit.tf2  Random error added to sffit.tf1 by adderr
sffit.tf3  Exact data for 2 sites in sffit
sffit.tf4  Random error added to sffit.tf3 by adderr
simplot.tf1  Error-bar data for **simplot**
simplot.tf2  Best-fit 1:1 to simplot.tf1 for **simplot**
simplot.tf3  Best-fit 2:2 to simplot.tf1 for **simplot**
spiral.tf1  Creates a 3 dimensional curve in **simplot**
spiral.tf2  Creates a 3 dimensional curve in **simplot**
spline.tf1  Spline coefficients for **spline-e02baf.tf1**
spline.tf2  Spline coefficients for **spline-compare.tf1**
spline.tf3  Spline coefficients for **spline-compare.tf2**
strata.tf1  Data for stratified binomial logistic regression
surface.tf1  Creates a surface in **simplot**
surface.tf2  Creates a surface in **simplot**
surface.tf3  Creates a surface in **simplot**
surface.tf4  Creates a surface in **simplot**
survive.tf1  Survival data for **gcfit** in mode 3
survive.tf2  Survival data to pair with survive.tf1
survive.tf3  Survival data for **gcfit** in mode 3
survive.tf4  Survival data to pair with survive.tf3
survive.tf5  Survival data for **gcfit** in mode 3
survive.tf6  Survival data to pair with survive.tf5
swarm.tf1  Data with error in x and y
times.tf1  Data for time series analysis in **simstat**
trinom.tf1  Trinomial contour plots in **binomial**
trinom.tf2  Trinomial contour plots in **binomial**
trinom.tf3  Trinomial contour plots in **binomial**
ttest.tf1  Fifty numbers from a \[ t \] distribution with \[ \nu = 10 \]
ttest.tf2  \[ t \] test data for **ttest** or **simstat**
ttest.tf3  Data paired with ttest.tf2
ttest.tf4  \[ t \] test data for **ttest** or **simstat**
ttest.tf5  Data paired with ttest.tf4
ttest.tf6  Data for \[ t \] test on rows of a matrix
tukeyq.tf1  matrix for ANOVA then Tukey Q test
ukmap.tf1  coordinates for K-means clustering
ukmap.tf2  starting centroids for ukmap.tf2
ukmap.tf3  uk coastal outline coordinates
vector.tf1  Vector (5 by 1) consistent with matrix.tf1
vector.tf2  Vector (7 by 1) consistent with matrix.tf2
vector.tf3  Vector (4 by 1) consistent with matrix.tf3
vfield.tf1  vector field file (4 columns)
vfield.tf2  vector field file (9 columns, i.e. a biplot)
weibull.tf1  Survival data for **gcfit** in mode 2
wilcoxon.tf1  Data for Wilcoxon signed ranks paired with wilcoxon.tf2
wilcoxon.tf2  Data for Wilcoxon signed ranks paired with wilcoxon.tf1
zeros.tf1  Zeros of the Riemann zeta function
zigzag.tf1  Zig-zag data to illustrate clipping to boundaries

### 1.3.2 Library files (Data)

<table>
<thead>
<tr>
<th>File</th>
<th>Description</th>
</tr>
</thead>
<tbody>
<tr>
<td>anova1.TFL</td>
<td>1-way ANOVA in <strong>ttest</strong> or <strong>simstat</strong></td>
</tr>
<tr>
<td>consec3.TFL</td>
<td>Data for fitting by <strong>qnnfit</strong> using <strong>consec3.mod</strong></td>
</tr>
<tr>
<td>consec4.TFL</td>
<td>Used by <strong>deqsol</strong> for 4 differential equations [ A=B=C=D ]</td>
</tr>
<tr>
<td>consec5.TFL</td>
<td>Used by <strong>deqsol</strong> for 5 differential equations [ A=B=C=D=E ]</td>
</tr>
<tr>
<td>convolv3.TFL</td>
<td>Data for fitting by <strong>qnnfit</strong> using <strong>convolv3.mod</strong></td>
</tr>
<tr>
<td>deqsol.TFL</td>
<td>Curve fitting data for <strong>deqsol</strong> (Identical to deqsol.tf1)</td>
</tr>
<tr>
<td>editps.TFL</td>
<td>PostScript files for EDITPS</td>
</tr>
</tbody>
</table>
epidemic.TFL Data for fitting epidemic differential equations
images.TFL PostScript files for EDITPS
inhibit.TFL Data for plotting mixed inhibition results
ncorr.TFL Nonparametric correlation data for rtest or simstat
simfig1.TFL Creates figure 1 in simplot
simfig2.TFL Creates figure 2 in simplot
simfig3.TFL Creates figure 3 in simplot
simfig4.TFL Creates figure 4 in simplot
simplot.TFL Identical to simfig1.TFL
spiral.TFL Creates a spiral in simplot
qnfit.TFL Parameter limits library file for qnfit
line3.TFL Data for fitting three lines simultaneously by qnfit

1.3.3 Test files (Models in reverse Polish)
camalot.mod Model for Logarithmic Spiral as used in Camalots
cheby.mod Model for Chebyshev expansion
consec3.mod Model for irreversible chemical kinetics A to B to C
cconvolve.mod Model for a convolution between an exponential and gamma function
convolv3.mod Version of convolve.mod for all components
dble_exp.mod Chemical kinetic double exponential model
d01fcf.mod Model with four variables for integration
dellipse.mod Model for an ellipse in makdat/simplot/usermod
dfamily2d.mod Two dimensional family of diffusion equations
dfamily3d.mod Three dimensional family of diffusion equations
dhelix.mod Model for a helix in makdat/simplot/usermod
diff.mod Model illustrating logical commands
dimpulse.mod Model illustrating 5 single impulse functions
dline3.mod Model for 3 lines in qnfit
doptimum.mod Model for optimizing Rosenbrock’s 2-dimensional test function in usermod
dperiodic.mod Model illustrating 7 periodic impulse functions
drose.mod Model for a rose in makdat/simplot/usermod
dtangent.mod Tangent to logarithmic spiral defined in camalot.mod
dtwister.mod Projection of a space curve onto coordinate planes
dupdown.mod Model that swaps definition at a cross-over point
dupdownup.mod Model that swaps definition at two cross-over points
duser1.mod Model illustrating arbitrary models
deqmat.tf1 How to transform a system of differential equations
deqmat.tf2 How to transform a system of differential equations
deqmod1.tf1 1 DE Michaelis-Menten substrate depletion
deqmod1.tf2 1 DE Michaelis-Menten product accumulation
deqmod1.tf3 1 DE Generalised substrate depletion
deqmod1.tf4 1 DE Generalised product accumulation
deqmod1.tf5 1 DE Membrane transport corrected for osmosis
deqmod1.tf6 1 DE von Bertalanffy allometric growth
deqmod2.tf1 2 DE Order 2 equation expressed as two equations
deqmod2.tf2 2 DE Lotka-Volterra predator-prey model
deqmod2.tf3 2 DE Competing species ecological model
deqmod3.tf1 3 DE Epidemic model (with Jacobian)
deqmod3.tf2 3 DE Epidemic model (without Jacobian)
deqmod4.tf1 4 DE Comprehensive Michaelis-Menten reversible model
deqpar1.tf1 Parameters for deqmod1.tf1
deqpar1.tf2 Parameters for deqmod1.tf2
deqpar1.tf3 Parameters for deqmod1.tf3
1.3.4 Test files (Models using expressions)

- **camalot_e.mod** Model for Logarithmic Spiral as used in Camalots
- **convolv3_e.mod** Version of **convolve.mod** for all components
- **deqmod2_e.tf1** Model for 2 differential equations
- **ellipse_e.mod** Model for an ellipse
- **helix_e.mod** Model for a helix
- **line3_e.mod** Model for 3 lines
- **optimum_e.mod** Model for optimizing Rosenbrock’s 2-dimensional test function
- **qnfit_model.tf1** Model for **qnfit** tutorials: Example 1 Quadratic
- **qnfit_model.tf2** Model for **qnfit** tutorials: Example 2 2D linear
- **qnfit_model.tf3** Model for **qnfit** tutorials: Example 3 3D linear
- **qnfit_model.tf4** Model for **qnfit** tutorials: Example 4 Sum of 2 MM curves
- **qnfit_model.tf5** Model for **qnfit** tutorials: Example 5 B in A->B>C
- **qnfit_model.tf6** Model for **qnfit** tutorials: Example 6 Sum of 2 normal pdfs
- **qnfit_model.tf7** Model for **qnfit** tutorials: Example 7 Sum of 2 normal cdfs
- **rose_e.mod** Model for a eight-leaved rose
- **usermod1_e.tf1** Function of 1 variable: line
- **usermod1_e.tf2** Function of 1 variable: quadratic
- **usermod1_e.tf3** Function of 1 variable: cubic
- **usermod1_e.tf4** Function of 1 variable: 2:2 rational function
usermod1_e.tf5 Function of 1 variable: one exponential
usermod1_e.tf6 Function of 1 variable: two exponentials
usermod1_e.tf7 Function of 1 variable: normal integral
usermod1_e.tf8 Function of 1 variable: capillary diffusion
usermod1_e.tf9 Function of 1 variable: damped simple harmonic motion
usermod2_e.tf1 Function of 2 variables: linear
usermod3_e.tf1 Function of 3 variables: linear
usermod4_e.tf1 Function of 4 variables: integrand for D01FCF
usermodd_e.tf1 Differential equation
usermodn_e.tf1 Four functions for plotting
usermodn_e.tf2 Two functions of 2 variables
usermodn_e.tf3 Three functions of 3 variables
usermodn_e.tf4 Nine functions of 9 variables
usermods_e.tf1 Special functions with one argument
usermods_e.tf2 Special functions with two arguments
usermods_e.tf3 Special functions with three arguments
deqmod1_e.tf1 1 DE Michaelis-Menten substrate depletion
deqmod1_e.tf2 1 DE Michaelis-Menten product accumulation
deqmod1_e.tf3 1 DE Generalised substrate depletion
deqmod1_e.tf4 1 DE Generalised product accumulation
deqmod1_e.tf5 1 DE Membrane transport corrected for osmosis
deqmod1_e.tf6 1 DE von Bertalanffy allometric growth
deqmod2_e.tf1 2 DE Order 2 equation expressed as two equations
deqmod2_e.tf2 2 DE Lotka-Volterra predator-prey model
deqmod2_e.tf3 2 DE Competing species ecological model
deqmod3_e.tf1 3 DE Epidemic model (with Jacobian)
deqmod3_e.tf2 3 DE Epidemic model (without Jacobian)
deqmod4_e.tf1 4 DE Comprehensive Michaelis-Menten reversible model

1.3.5 Miscellaneous data files

<table>
<thead>
<tr>
<th>File</th>
<th>Description</th>
</tr>
</thead>
<tbody>
<tr>
<td>cheby.data</td>
<td>Data required by cheby.mod</td>
</tr>
<tr>
<td>consec3_A.data</td>
<td>Data for component A in consec3.mod</td>
</tr>
<tr>
<td>consec3_B.data</td>
<td>Data for component B in consec3.mod</td>
</tr>
<tr>
<td>consec3_C.data</td>
<td>Data for component C in consec3.mod</td>
</tr>
<tr>
<td>convolv3.data</td>
<td>Data for convolv3.mod</td>
</tr>
<tr>
<td>inhibit?.data</td>
<td>Data for inhibit.tfl</td>
</tr>
<tr>
<td>line?.data</td>
<td>line1.data, line2.data and line3.data for line3.tfl</td>
</tr>
<tr>
<td>simfig3?.data</td>
<td>Data for simfig3.tfl</td>
</tr>
<tr>
<td>simfig4?.data</td>
<td>Data for simfig4.tfl</td>
</tr>
<tr>
<td>y?.data</td>
<td>y1.data, y2.data and y3.data for epidemic.tfl</td>
</tr>
</tbody>
</table>

1.3.6 Graphics configuration and metafiles

These files can be created on demand from program simplot in order to save plotting parameters from the current plot for subsequent re-use.

<table>
<thead>
<tr>
<th>File</th>
<th>Description</th>
</tr>
</thead>
<tbody>
<tr>
<td>logodds.cfg</td>
<td>Configure a logodds plot</td>
</tr>
<tr>
<td>logoddsratios.cfg</td>
<td>Configure a logoddsratios plot</td>
</tr>
<tr>
<td>metafile.tf1</td>
<td>Metafile for multiple plots</td>
</tr>
<tr>
<td>metafile.tf2</td>
<td>Metafile for a double plot</td>
</tr>
<tr>
<td>metafile.tf3</td>
<td>Metafile for a barchart</td>
</tr>
<tr>
<td>metafile.tf4</td>
<td>Metafile for a piechart</td>
</tr>
</tbody>
</table>
1.3.7 Parameter limits files

These files consist of lowest possible values, starting estimates and highest possible values for parameters used by \textit{qnfit} and \textit{deqsol} for constraining parameters during curve fitting. They are usually referenced by library files such as \textit{qnfit.tfl}. See, for example, positive.plf, negative.plf and unconstrained.plf.

1.3.8 Error message files

When programs like \textit{deqsol}, \textit{makdat} and \textit{qnfit} start to execute they open special files like \texttt{w\_deqsol.txt} and \texttt{w\_qnfit.txt} to receive all messages generated during the current curve fitting and solving of differential equations. Advanced \textsc{SimFtT} users can inspect these files and other files like \texttt{iterate.txt} to get more details about any singularities encountered during iterations. If any serious problems are encountered using \textit{deqsol} or \textit{qnfit}, you can consult the appropriate *.txt file for more information.

1.3.9 PostScript example files

\begin{itemize}
  \item \texttt{pscodes.ps} PostScript octal codes
  \item \texttt{psfragx.ps} Illustrating psfragx.tex/psfragx.ps
  \item \texttt{simfig1.ps} Example
  \item \texttt{simfig2.ps} Example
  \item \texttt{simfig3.ps} Example
  \item \texttt{simfig4.ps} Example
  \item \texttt{simfonts.ps} Standard PostScript fonts
  \item \texttt{ms\_office.ps} Using MS Excel and Word
  \item \texttt{pspecial.i} Example PS specials (i = 1 to 10)
  \item \texttt{*\_eps} Assorted Encapsulated PostScript files
\end{itemize}

1.3.10 \textsc{SimFtT} configuration files

These files are created automatically by \textsc{SimFtT} and should not be edited manually unless you know exactly what you are doing, e.g., setting the PostScript color palette.

\begin{itemize}
  \item \texttt{g\_recent.cfg} Recent graphics files
  \item \texttt{l\_simfit.cfg} This stores information for configuring the Linux version
  \item \texttt{pspecial.cfg} Configuration file for PostScript specials
  \item \texttt{w\_clpbrd.cfg} This holds the last file number x as in clipboard_x.txt
  \item \texttt{w\_colors.cfg} Colors for simple graphs
  \item \texttt{w\_filter.cfg} This contains the current search patterns used to configure the file selection and creation controls
  \item \texttt{w\_fsizes.cfg} This holds the graphics font sizes
  \item \texttt{w\_ffests.cfg} This holds the last NPTS, NPAR, WSSQ values used for F tests
  \item \texttt{w\_graphs.cfg} This holds the graph configuration parameters
\end{itemize}
1.3.11 Default files

These files save details of changes made to the SimFIT defaults from several programs.

- **w_labels.cfg**: Stores default plotting labels
- **w_module.cfg**: Stores file names of executable modules
- **w_params.cfg**: Stores default editing parameters
- **w_symbol.cfg**: Stores default plotting symbols

1.3.12 Temporary files

These next two files are deleted then re-written during each SimFIT session. You may wish to save them to disk after a session as a permanent record of files analyzed and created.

- **w_in.tmp**: Stores the list of files accessed during the latest SimFIT session
- **w_out.tmp**: Stores the list of files created during the latest SimFIT session

The results log file `$result.tmp` is created anew each time a program is started that performs calculations, so it overwrites any previous results. You can save results retrospectively either by renaming this file, or else you can configure SimFIT to ask you for a file name instead of creating this particular results file. SimFIT also creates a number of temporary files with names like `$000008.tmp` which should be deleted. If you have an abnormal exit from SimFIT, the current results file may be such a file and, in such circumstances, you may wish to save it to disk. SimFIT sometimes makes other temporary files, such as `$simfit.tmp` with the name of the current program, but you can always presume that it is safe to delete any such files.

1.3.13 NAG library files (contents of list.nag)

Models
- `c05adf.mod`: 1 function of 1 variable
- `c05adf_e.mod`: 1 function of 1 variable
- `c05nbf.mod`: 9 functions of 9 variables
c05nbf_e.mod 9 functions of 9 variables
d01ajf.mod 1 function of 1 variable
d01ajf_e.mod 1 function of 1 variable
d01eaf.mod 10 functions of 4 variables
d01eaf_e.mod 10 functions of 4 variables
d01fcf.mod 1 function of 4 variables
d01fcf_e.mod 1 function of 4 variables
e04fyf.mod 1 function of 3 variables
e04fyf_e.mod 1 function of 3 variables
Data
c02agf.tf1 Zeros of a polynomial
e02adf.tf1 Polynomial data
e02baf.tf1 Data for fixed knot spline fitting
e02baf.tf2 Spline knots and coefficients
e02bef.tf1 Data for automatic knot spline fitting
e04fyf.tf1 Data for curve fitting using e04fyf.mod
f01abf.tf1 Inverse: symposdef matrix
f01baf.tf1 Pseudo inverse of a matrix
f02ddf.tf1 A for Ax = (lambda)Bx
f02ddf.tf2 B for Ax = (lambda)Bx
f02wef.tf1 Singular value decomposition
f02wef.tf2 Singular value decomposition
f03aaf.tf1 Determinant by LU
f03aef.tf1 Determinant by Cholesky
f07ddf.tf1 Cholesky factorisation
f08kaf.tf1 Singular value decomposition
f08kaf.tf2 Singular value decomposition
g02baf.tf1 Correlation: Pearson
g02bnf.tf1 Correlation: Kendall/Spearman
g02caf.tf1 Unweighted linear regression
g02daf.tf1 Multiple linear regression
g02gaf.tf1 GLM normal errors
g02gbf.tf1 GLM binomial errors
g02gcf.tf1 GLM Poisson errors
g02gdf.tf1 GLM gamma errors
g02haf.tf1 Robust regression (M-estimates)
g02laf.tf1 Partial Least squares X-predictor data
g02laf.tf2 Partial Least Squares Y-response data
g02laf.tf3 Partial Least Squares Z-predictor data
g02wef.tf1 Singular value decomposition
g02wef.tf2 Singular value decomposition
g03aaf.tf1 Principal components
g03acf.tf1 Canonical variates
g03adtf.tf1 Canonical correlation
g03baf.tf1 Matrix for Orthomax/Varimax rotation
g03bcf.tf1 X-matrix for procrustes analysis
g03bcf.tf2 Y-matrix for procrustes analysis
g03caf.tf1 Correlation matrix for factor analysis
g03ccf.tf1 Correlation matrix for factor analysis
g03daf.tf1 Discriminant analysis
g03dbf.tf1 Discriminant analysis
g03dcf.tf1 Discriminant analysis
g03eaf.tf1 Data for distance matrix: calculation