Simfit

Simulation, fitting, statistics, and plotting.

William G. Bardsley

https://simfit.uk

https://simfit.org.uk

https://simfit.silverfrost.com

Contents

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., exponentail) 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
barcht3d.tf1	Creates a 3 dimensional barchart in **simplot**
barcht3d.tf2	Creates a 3 dimensional barchart in **simplot**
barcht3d.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 x given y with calcurve.tf1
chisqd.tf1	Fifty numbers from a chi-square distribution with $\nu = 10$
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 **rstest** or **simstat**
column2.tf2	Vector for nonparametric correlation in **rstest** or **simstat**
column2.tf3	Vector for nonparametric correlation in **rstest** 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
csadat.tf1	Example of the preliminary flow cytometry format for **csadat**
csadat.tf2	Example of the preliminary flow cytometry format for **csadat**
csafit.tf1	Geometric type data with 15% stretch for **csafit**
csafit.tf2	Arithmetic type data with 5% translation for **csafit**
csafit.tf3	Mixed type data for **csafit**
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**
diversity.tf1	Shannon-Brillouin indices of diversity data for **simstat**
editfl.tf1	Data for editing by **editfl**
editfl.tf2	Data for editing by **editfl**
editfl.tf3	Data for editing by **editfl**
editfl.tf4	Data for editing by **editfl**
editmt.tf1	Data for editing by **editmt**
editmt.tf2	Data for editing by **editmt**
editmt.tf3	Data for editing by **editmt**
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 dicovery rate calculations in **simstat**
ftest.tf1	Fifty numbers from the F distribution with $m = 2, n = 5$
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
gcfit.tf7	Logistic decay data by reversing gcfit.tf2
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 in text format for editing by **maksim**
maksim.tf2	Matrix in CSV format with no labels for editing by **maksim**
maksim.tf3	Matrix in CSV format with row and column labels for editing by **maksim**
maksim_1.html	Matrix in W3C compliant format for editing by **maksim**
maksim_2.html	Matrix in HTML with all closure tags for editing by **maksim**
maksim_3.html	Matrix in HTML with no closure tags 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**
pls_x.tf1	Partial least squares X matrix in **simstat**
pls_y.tf1	Partial least squares Y matrix in **simstat**
pls_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 Bertallanffy growth data in EXPERT mode for **qnfit**
qnfit_ode.tf3	Von Bertallanffy growthdecay data in EXPERT mode for **qnfit**
rainfall.tf1	Rainfall in England and Wales from 1766 to 2015
recurrent.tf1	Data for y(1) in the recurrent epidemic scheme for **deqsol**
recurrent.tf2	Data for y(2) in the recurrent epidemic scheme for **deqsol**
recurrent.tf3	Data for y(3) in the recurrent epidemic scheme for **deqsol**
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
rstest.tf1	Residuals for runs test in **rstest**
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**
surface.tf5	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)

anova1.TFL	1-way ANOVA in **ftest** or **simstat**
consec3.TFL	Data for fitting by **qnfit** using `consec3.mod`
consec4.TFL	Used by **deqsol** for 4 differential equations A=B=C=D
consec5.TFL	Used by **deqsol** for 5 differential equations A=B=C=D=E
convolv3.TFL	Data for fitting by **qnfit** using `convolv3.mod`
deqsol.TFL	Curve fitting data for **deqsol** (Identical to deqsol.tf1)
editps.TFL	PostScript files for EDITPS
epidemic.TFL	Data for fitting epidemic differential equations
images.TFL	PostScript files for EDITPS
inhibit.TFL	Data for plotting mixed inhibition results
npcorr.TFL	Nonparametric correlation data for **rstest** or **simstat**
recurrent.TFL	Data for fitting the recurrent epidemic scheme in **deqsol**
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
convolve.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
ellipse.mod	Model for an ellipse in **makdat/simplot/usermod**
family2d.mod	Two dimensional family of diffusion equations
family3d.mod	Three dimensional family of diffusion equations
helix.mod	Model for a helix in **makdat/simplot/usermod**
if.mod	Model illustrating logical commands
impulse.mod	Model illustrating 5 single impulse functions
line3.mod	Model for 3 lines in **qnfit**
optimum.mod	Model for optimizing Rosenbrock's 2-dimensional test function in **usermod**
periodic.mod	Model illustrating 7 periodic impulse functions
rose.mod	Model for a rose in **makdat/simplot/usermod**
tangent.mod	Tangent to logarithmic spiral defined in camalot.mod
twister.mod	Projection of a space curve onto coordinate planes
updown.mod	Model that swaps definition at a cross-over point
updownup.mod	Model that swaps definition at two cross-over points
user1.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 Bertalannfy 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 Jcobian)
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
deqpar1.tf4	Parameters for deqmod1.tf4
deqpar1.tf5	Parameters for deqmod1.tf5
deqpar1.tf6	Parameters for deqmod1.tf6
deqpar2.tf1	Parameters for deqmod2.tf1
deqpar2.tf2	Parameters for deqmod2.tf2
deqpar2.tf3	Parameters for deqmod2.tf3
deqpar4.tf1	Parameters for deqmod4.tf1
usermod1.tf1	Function of 1 variable: line
usermod1.tf2	Function of 1 variable: quadratic
usermod1.tf3	Function of 1 variable: cubic
usermod1.tf4	Function of 1 variable: 2:2 rational function
usermod1.tf5	Function of 1 variable: one exponential
usermod1.tf6	Function of 1 variable: two exponentials
usermod1.tf7	Function of 1 variable: normal integral
usermod1.tf8	Function of 1 variable: capillary diffusion
usermod1.tf9	Function of 1 variable: damped simple harmonic motion
usermod2.tf1	Function of 2 variables: linear
usermod3.tf1	Function of 3 variables: linear
usermod4.tf1	Function of 4 variables: integrand for D01FCF
usermodd.tf1	Differential equation for **usermod**
usermodn.tf1	Four functions for plotting by **usermod**
usermodn.tf2	Two functions of 2 variables for **usermod**
usermodn.tf3	Three functions of 3 variables for **usermod**
usermodn.tf4	Nine functions of 9 variables for **usermod**
usermods.tf1	Special functions with one argument
usermods.tf2	Special functions with two arguments
usermods.tf3	Special functions with three arguments
usermodx.tf1	Using a sub-model for function evaluation
usermodx.tf2	Using a sub-model for quadrature
usermodx.tf3	Using a sub-model for root-finding
usermodx.tf4	Using three sub-models for root-finding of an integral
usermodx.tf5	Using a sub-model to evaluate a multiple integral

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
gauss3_e.mod	Model for a sum of three Gaussians
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 Bertalannfy 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 Jcobian)
deqmod3_e.tf2	3 DE Epidemic model (without Jacobian)
deqmod3_e.tf3	3 DE Recurrent Epidemic model (with Jacobian)
deqmod4_e.tf1	4 DE Comprehensive Michaelis-Menten reversible model

1.3.5 Miscellaneous data files

cheby.data	Data required by `cheby.mod`
consec3_A.data	Data for component A in `consec3.mod`
consec3_B.data	Data for component B in `consec3.mod`
consec3_C.data	Data for component C in `consec3.mod`
convolv3.data	Data for `convolv3.mod`
inhibit?.data	Data for `inhibit.tfl`
line?.data	line1.data, line2.data and line3.data for line3.tfl
simfig3?.data	Data for `simfig3.tfl`
simfig4?.data	Data for `simfig4.tfl`
y?.data	y1.data, y2.data and y3.data for `epidemic.tfl`

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.

logodds.cfg	Configure a logodds plot
logoddsratios.cfg	Configure a logoddsratios plot
metafile.tf1	Metafile for multiple plots
metafile.tf2	Metafile for a double plot
metafile.tf3	Metafile for a barchart
metafile.tf4	Metafile for a piechart
metafile.tf5	Metafile for a labels plot
metafile.tf6	Metafile for a vector field plot
metafile.tf7	Metafile for a biplot
metafile.tf8	Metafile for a dendrogram
metafile.tf9	Metafile for logodds plot
w_simfig1.cfg	Configures **simplot** to use simfig1.tfl
w_simfig2.cfg	Configures **simplot** to use simfig2.tfl
w_simfig3.cfg	Configures **simplot** to use simfig3.tfl
w_simfig4.cfg	Configures **simplot** to use simfig4.tfl

1.3.7 Parameter limits files

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

1.3.8 Error message files

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

1.3.9 PostScript example files

pscodes.ps	PostScript octal codes
psgfragx.ps	Illustrating psfragex.tex/psfragex.ps1
simfig1.ps	Example
simfig2.ps	Example
simfig3.ps	Example
simfig4.ps	Example
simfonts.ps	Standard PostScript fonts
ms_office.ps	Using MS Excel and Word
pspecial.i	Example PS specials (i = 1 to 10)
*.eps	Assorted Encapsulated PostScript files

1.3.10 SIMFIT configuration files

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

g_recent.cfg	Recent graphics files
l_simfit.cfg	This stores information for configuring the Linux version
pspecial.cfg	Configuration file for PostScript specials
w_clpbrd.cfg	This holds the last file number x as in clipboard_x.txt
w_colors.cfg	Colors for simple graphs
w_filter.cfg	This contains the current search patterns used to configure
	the file selection and creation controls
w_fsizes.cfg	This holds the graphics font sizes
w_ftests.cfg	This holds the last NPTS, NPAR, WSSQ values used for F tests
w_graphs.cfg	This holds the graph configuration parameters
w_input.cfg	This holds the last filenames used for data input
w_labels.cfg	This holds the labels and other bar and pie chart details
w_matrix.cfg	This holds the last file number x as in matrix_x.txt
w_modules.cfg	This holds the names of current modules
w_output.cfg	This holds the last filenames used for data output
w_params.cfg	Current parameters for editing data sets
w_pathto.cfg	Paths
w_ps.cfg	This stores all the PostScript configuration details
w_result.cfg	This holds the filename of the latest results file
w_simfit.cfg	This stores all the important details needed to run SimFIT
	from the program manager w_simfit.exe
w_symbol.cfg	Symbol and Line types
w_txtcfg.cfg	Formats the SimFIT text editor interface
w_vector.cfg	This holds the last file number x as in vector_x.txt
a_recent.cfg	Recently selected project files (all types)
c_recent.cfg	Recently selected project files (covariance matrices)
f_recent.cfg	Recently selected project files (curve fitting)
g_recent.cfg	Recently selected project files (graphics)
m_recent.cfg	Recently selected project files (matrix))
p_recent.cfg	Recently selected project files (PostScript)
v_recent.cfg	Recently selected project files (vector)

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 f$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 f$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 f$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
f01blf.tf1	Pseudo inverse of a matrix
f02fdf.tf1	A for Ax = (lambda)Bx
f02fdf.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
f07fdf.tf1	Cholesky factorisation
f08kff.tf1	Singular value decomposition
f08kff.tf2	Singular value decomposition
g02baf.tf1	Correlation: Pearson
g02bnf.tf1	Correlation: Kendall/Spearman
g02bny.tf1	Partial correlation matrix
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

g03adf.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
g03ecf.tf1	Data for distance matrix: clustering
g03eff.tf1	K-means clustering
g03eff.tf2	K-means clustering
g03faf.tf1	Distance matrix for classical metric scaling
g03ehf.tf1	Data for distance matrix: dendrogram plot
g03ejf.tf1	Data for distance matrix: cluster indicators
g04adf.tf1	ANOVA
g04aef.tfl	ANOVA library file
g04caf.tf1	ANOVA (factorial)
g07bef.tf1	Weibull fitting
g08acf.tf1	Median test
g08acf.tf2	Median test
g08aef.tf1	ANOVA (Friedman)
g08aff.tfl	ANOVA (Kruskall-Wallis)
g08agf.tf1	Wilcoxon signed ranks test
g08agf.tf2	Wilcoxon signed ranks test
g08ahf.tf1	Mann-Whitney U test
g08ahf.tf2	Mann-Whitney U test
g08baf.tf1	Mood and David dispersion tests
g08baf.tf2	Mood and David dispersion tests
g08cbf.tf1	Kolmogorov-Smirnov 1-sample test
g08daf.tf1	Kendall coefficient of concordance
g08eaf.tf1	1000 U(0,1) psedo-random numbers
g08raf.tf1	Regression on ranks
g08rbf.tf1	Regression on ranks
g10abf.tf1	Data for cross validation spline fitting
g10caf.tf1	Data for T4253H smoothing
g11caf.tf1	Stratified logistic regression
g12aaf.tf1	Survival analysis
g12aaf.tf2	Survival analysis
g12baf.tf1	Cox regression
g13dmf.tf1	Auto- and cross-correlation matrices
j06sbf.tf1	Time series