```
function
[FitResults,GOF,baseline,coeff,residual,xi,yi,BootResults]=peakfit(signal,center,window,NumPeaks,p
eakshape,extra,NumTrials,start,autozero,fixedparameters,plots,bipolar,minwidth,DELTA,clipheight)
 %A command-line peak fitting program for time-series signals, written as a
 %self-contained Matlab function in a single m-file. Uses a non-linear
 %optimization algorithm to decompose a complex, overlapping-peak signal
 %into its component parts. The objective is to determine whether your
 %signal can be represented as the sum of fundamental underlying peaks
 %shapes. Accepts signals of any length, including those with non-integer
 %and non-uniform x-values. Fits any number of peaks of any of 33 curve
 %shapes. This is a command line version, usable from a remote terminal. It
 %is capable of making multiple trial fits with sightly different starting
 %values (whose variability is controled by the 14th input argument) and
 %taking the one with the lowest mean fit error (example 6). It can
 %estimate the standard deviation of peak parameters from a single signal
 %using the bootstrap method (example 10.(
%
 %Version 7.1: March, 2015, adds peak shapes with three unconstrained
 %iterated variables: 30=voigt (variable alpha), 31=ExpGaussian (variable
 %time constant), 32=Pearson (variable shape factor), 34=Gaussian/
 %Lorentzian blend (variable percent). See Examples 25-28 below.
%
 %For more details, see
 %http://terpconnect.umd.edu/~toh/spectrum/CurveFittingC.html and
 %http://terpconnect.umd.edu/~toh/spectrum/InteractivePeakFitter.htm
%
 %peakfit(signal       ;(
 %Performs an iterative least-squares fit of a single Gaussian peak to the
```

```
 %data matrix "signal", which has x values in column 1 and Y values in
 %column 2 (e.g. [x y([
%
 %peakfit(signal,center,window;(
 %Fits a single Gaussian peak to a portion of the matrix "signal". The
 %portion is centered on the x-value "center" and has width "window" (in x
 %units.(
 %
 %peakfit(signal,center,window,NumPeaks;(
" %NumPeaks" = number of peaks in the model (default is 1 if not
 %specified). No limit to maximum number of peaks in version 3.1
 %
 %peakfit(signal,center,window,NumPeaks,peakshape ;(
" %peakshape" specifies the peak shape of the model: (1=Gaussian (default,(
=٢ %Lorentzian, 3=logistic distribution, 4=Pearson, 5=exponentionally
 %broadened Gaussian; 6=equal-width Gaussians; 7=Equal-width Lorentzians;
=٨ %exponentionally broadened equal-width Gaussian, 9=exponential pulse,
=١٠ %up-sigmoid (logistic function), 11=Fixed-width Gaussian,
=١٢ %Fixed-width Lorentzian; 13=Gaussian/ Lorentzian blend; 14=Bifurcated
 %Gaussian, 15=Breit-Wigner-Fano, 16=Fixed-position Gaussians;
=١٧ %Fixed-position Lorentzians; 18=exponentionally broadened Lorentzian;
=١٩ %alpha function; 20=Voigt profile; 21=triangular; 22=multiple shapes;
=٢٣ %down-sigmoid; 25=lognormal; 26=slope; 27=Gaussian first derivative ;
=٢٨ %polynomial; 29=piecewise linear; 30=variable-alpha Voigt; 31=variable
 %time constant ExpGaussian; 32=variable Pearson; 33=variable
 %Gaussian/Lorentzian blend
%
 %peakfit(signal,center,window,NumPeaks,peakshape,extra (
```

```
' %extra' specifies the value of 'extra', used only in the Voigt, Pearson,
 %exponentionally broadened Gaussian, Gaussian/Lorentzian blend, and
 %bifurcated Gaussian and Lorentzian shapes to fine-tune the peak shape.
 %
 %peakfit(signal,center,window,NumPeaks,peakshape,extra,NumTrials;(
 %Performs "NumTrials" trial fits and selects the best one (with lowest
 %fitting error). NumTrials can be any positive integer (default is 1.(
%
 %peakfit(signal,center,window,NumPeaks,peakshape,extra,NumTrials,start(
 %Specifies the first guesses vector "firstguess" for the peak positions
 %and widths. Must be expressed as a vector , in square brackets, e.g.
 %start=[position1 width1 position2 width2[...
 %
 %peakfit(signal,center,window,NumPeaks,peakshape,extra,NumTrials,start,autozero (
' %autozero' sets the baseline correction mode:
 %autozero=0 (default) does not subtract baseline from data segment ;
 %autozero=1 interpolates a linear baseline from the edges of the data
        %segment and subtracts it from the signal (assumes that the
        %peak returns to the baseline at the edges of the signal ;(
 %autozero=2 is like mode 1 except that it computes a quadratic curved baseline ;
 %autozero=3 compensates for a flat baseline without reference to the
        %signal itself (best if the peak does not return to the
        %baseline at the edges of the signal.(
%
 %peakfit(signal,center,window,NumPeaks,peakshape,extra,NumTrials,start...,
 %autozero,fixedparameters(
' %fixedparameters' specifies fixed values for widths (shapes 10, 11) or
 %positions (shapes 16, 17(
```

```
 %
 %peakfit(signal,center,window,NumPeaks,peakshape,extra,NumTrials,start...,
 %autozero,fixedparameters,plots(
' %plots' controls graphic plotting: 0=no plot; 1=plots draw as usual (default(
 %
 %peakfit(signal,center,window,NumPeaks,peakshape,extra,NumTrials,start...,
 %autozero,fixedparameters,plots,bipolar(
' %bipolar' = 0 constrain peaks heights to be positions; 'bipolar' = 1
 %allows positive ands negative peak heights.
%
 %peakfit(signal,center,window,NumPeaks,peakshape,extra,NumTrials,start...,
 %autozero,fixedparameters,plots,bipolar,minwidth(
' %minwidth' sets the minmimum allowed peak width. The default if not
 %specified is equal to the x-axis interval. Must be a vector of minimum
 %widths, one value for each peak, if the multiple peak shape is chosen ,
 %as in example 17 and 18.
%
 %peakfit(signal,center,window,NumPeaks,peakshape,extra,NumTrials,start...,
 %autozero,fixedparameters,plots,bipolar,minwidth(
'  %DELTA' (14th input argument) controls the restart variance when
  %NumTrials>1. Default value is 1.0. Larger values give more variance.
  %Version 5.8 and later only .
] %FitResults,FitError]=peakfit(signal,center,window...) Returns the
 %FitResults vector in the order peak number, peak position, peak height,
 %peak width, and peak area), and the FitError (the percent RMS
 %difference between the data and the model in the selected segment of that
 %data) of the best fit.
%
```

```
] %FitResults,LowestError,BestStart,xi,yi,BootResults]=peakfit(signal(...,
 %Prints out parameter error estimates for each peak (bootstrap method.(
%
 %Optional output parameters
.١ %FitResults: a table of model peak parameters, one row for each peak,
   %listing Peak number, Peak position, Height, Width, and Peak area.
.٢ %GOF: Goodness of Fit, a vector containing the rms fitting error of the
   %best trial fit and the R-squared (coefficient of determination.(
.٣ %Baseline, the polynomial coefficients of  the baseline in linear
   %and quadratic baseline modes (1 and 2) or the value of the constant
   %baseline in flat baseline mode.
.٣ %coeff: Coefficients for the polynomial fit (shape 28 only; for other
   %shapes, coeff=0(
.٥ %residual: the difference between the data and the best fit.
.٦ %xi: vector containing 600 interploated x-values for the model peaks .
.٧ %yi: matrix containing the y values of each model peak at each xi .
   %Type plot(xi,yi(1,:)) to plot peak 1 or plot(xi,yi) to plot all peaks
.٨ %BootResults: a table of bootstrap precision results for a each peak
   %and peak parameter.
 %
 %Example 1 :
 << %x=[0:.1:10]';y=exp(-(x-5).^2);peakfit([x y([
 %Fits exp(-x)^2 with a single Gaussian peak model.
%
       %Peak number  Peak position   Height     Width      Peak area
١٫٧٧٢٥       ١٫٦٦٥        ١            ٥            ١            %
%
 << %y=[0 1 2 4 6 7 6 4 2 1 0 ];x=1:length(y;(
```

<< %peakfit([x;y],length(y)/2,length(y),0,0,0,0,0,0(

%Fits small set of manually entered y data to a single Gaussian peak model.

%

%Example 2:

%x=[0:.01:10];y=exp(-(x-5).^2)+randn(size(x));peakfit([x;y([

%Measurement of very noisy peak with signal-to-noise ratio = 1.

%ans=

۱٫۷۷۱۶ ۱٫۷۹۴۸ ۰٫۹۲۷۲ ۵٫۰۲۷۹ ۱ %

%

%Example 3:

%x=[0:.1:10];y=exp(-(x-5).^2)+.5*exp(-(x-3).^2)+.1*randn(size(x;((

%peakfit([x' y'],0,0,2(

%Fits a noisy two-peak signal with a double Gaussian model (NumPeaks=2.(

%ans=

۰٫۸۶۵۰۴ ۱٫۶۴۲ ۰٫۴۹۴۸۹ ۳٫۰۰۰۱ ۱ %

۱٫۷۶۹۶ ۱٫۶۵۹۷ ۱٫۰۰۱۶ ۴٫۹۹۲۷ ۲ %

%

%Example 4:

<< %x=1:100;y=ones(size(x))./(1+(x-50).^2);peakfit(y,0,0,1,2(

%Fit Lorentzian (peakshape=2) located at x=50, height=1, width=2.

%ans=

۳٫۱۰۷۹ ۱٫۹۹۷۱ ۰٫۹۹۹۷۴ ۵۰ ۱ %

%

%Example 5 :

<< %x=[0:.005:1];y=humps(x);peakfit([x' y'],.3,.7,1,4,3;(

%Fits a portion of the humps function, 0.7 units wide and centered on

%x=0.3, with a single (NumPeaks=1) Pearson function (peakshape=4) with

%extra=3 (controls shape of Pearson function.(

```
%
 %Example 6 :
 << %x=[0:.005:1];y=(humps(x)+humps(x-.13)).^3;smatrix=[x' y;['
] << %FitResults,FitError]=peakfit(smatrix,.4,.7,2,1,0,10(
 %Creates a data matrix 'smatrix', fits a portion to a two-peak Gaussian
 %model, takes the best of 10 trials.  Returns FitResults and FitError.
 %FitResults=
٢٫٠١٢٥  ٠٫٣١٠٥۶      ١            %e+006     0.11057  2.3689e+005
٢٫٢۴٠٣  ٠٫۴١٥٢٩      ٢            %e+006     0.12033  2.8696e+005
 %FitError=
١٫١٨٩٩        %
%
 %Example 7:
 << %peakfit([x' y'],.4,.7,2,1,0,10,[.3 .1 .5 .1;([
 %As above, but specifies the first-guess position and width of the two
 %peaks, in the order [position1 width1 position2 width2[
%
 %Example 8: (Version 4 only(
 %Demonstration of the four autozero modes, for a single Gaussian on flat
  %baseline, with position=10, height=1, and width=1.66. Autozero mode
  %is specified by the 9th input argument (0,1,2, or 3.(
 << %x=8:.05:12;y=1+exp(-(x-10).^2;(
] << %FitResults,FitError]=peakfit([x;y],0,0,1,1,0,1,0,0(
 %Autozero=0 means to ignore the baseline (default mode if not specified(
 %FitResults=
٥٫٧۶۴١      ٣٫۶١٢      ١٫٨٥۶١      ١٠          ١           %
 %FitError=
٥٫٣٨٧        %
```

] << %FitResults,FitError]=peakfit([x;y],0,0,1,1,0,1,0,1(

%Autozero=1 subtracts linear baseline from edge to edge.

%Does not work well because signal does not return to baseline at edges.

%FitResults=

١٫٥٩١٦ ١٫٥٥٩ ٠٫٩٦١٥٣ ٩٫٩٩٨٤ ١ %

%FitError=

١٫٩٨٠١ %

] << %FitResults,FitError]=peakfit([x;y],0,0,1,1,0,1,0,2(

%Autozero=1 subtracts quadratic baseline from edge to edge.

%Does not work well because signal does not return to baseline at edges.

%FitResults=

١٫٢٥٠٣ ١٫٤٣٨٤ ٠٫٨١٧٤٩ ٩٫٩٩٩٦ ١ %

%FitError=

١٫٨٢٠٤ %

%Autozero=3: Flat baseline mode, measures baseline by regression

] << %FitResults,Baseline,FitError]=peakfit([x;y],0,0,1,1,0,1,0,3(

%FitResults=

١٫٧٦٤٥ ١٫٦٦٥٣ ١٫٠٠٠١ ١٠ ١ %

%Baseline=

٠٫٠٠٣٧٠٥٦ %

%FitError=

٠٫٩٩٩٨٥ %

%

%Example 9:

%x=[0:.1:10];y=exp(-(x-5).^2)+.5*exp(-(x-3).^2)+.1*randn(size(x;((

] %FitResults,FitError]=peakfit([x' y'],0,0,2,11,0,0,0,0,1.666(

%Same as example 3, fit with fixed-width Gaussian (shape 11), width=1.666

%

```
 %Example 10: (Version 3 or later; Prints out parameter error estimates(
 %x=0:.05:9;y=exp(-(x-5).^2)+.5*exp(-(x-3).^2)+.01*randn(1,length(x;((
] %FitResults,LowestError,residuals,xi,yi,BootstrapErrors]=peakfit([x;y],0,0,2,6,0,1,0,0,0;(
%
 %Example 11: (Version 3.2 or later(
 %x=[0:.005:1];y=humps(x);[FitResults,FitError]=peakfit([x' y'],0.54,0.93,2,13,15,10,0,0,0 (
%
 %FitResults=
۲۳٫۰۶۴       ۰٫۱۹۱۳۱       ۱۹۰٫۴۱       ۰٫۳۰۰۷۸       ۱            %
۶٫۱۹۹۹       ۰٫۳۳۴۴۸       ۳۹٫۵۵۲       ۰٫۸۹۷۸۸       ۲            %
 %FitError =
۰٫۳۴۵۰۲       %
 %Fits both peaks of the Humps function with a Gaussian/Lorentzian blend
) %shape 13) that is 15% Gaussian (Extra=15.(
 %
 %Example 12:  (Version 3.2 or later(
 << %x=[0:.1:10];y=exp(-(x-4).^2)+.5*exp(-(x-5).^2)+.01*randn(size(x;((
] << %FitResults,FitError]=peakfit([x' y'],0,0,1,14,45,10,0,0,0 (
 %FitResults=
۲٫۶۷۲۳       ۴٫۰۷۷       ۱٫۲۳۱۵       ۴٫۲۰۲۸       ۱            %
 %FitError=
۰٫۸۴۴۶۱       %
 %Fit a slightly asymmetrical peak with a bifurcated Gaussian (shape 14(
 %
 %Example 13:  (Version 3.3 or later(
 << %x=[0:.1:10]';y=exp(-(x-5).^2);peakfit([x y],0,0,1,1,0,0,0,0,0,0(
 %Example 1 without plotting (11th input argument = 0, default is 1(
 %
```

```
 %Example 14:  (Version 3.9 or later(
 %Exponentially broadened Lorentzian with position=9, height=1.
 %x=[0:.1:20 ;[
 %L=lorentzian(x,9,1;(
 %L1=ExpBroaden(L',-10)+0.02.*randn(size(x;'((
] %FitResults,FitError]=peakfit([x;L1'],0,0,1,18,10(
%
 %Example 15: Fitting the humps function with two Voigt profiles, flat
 %baseline mode
] %FitResults,FitError]=peakfit(humps(0:.01:2),71,140,2,20,1.7,1,[31 4.7 90 8.8],3(
%FitResults=
٢٥٥٠/١       ۴/۶٧٨۵       ٩۶/٧۶٢       ٣١/٠۴٧       ١            %
١٠٨٩/۵       ٨/٨٢۵٣       ٢٢/٩٣۵       ٩٠/٠٩        ٢            %
 %FitError=
٠/٨٠۵٠١       %
%
 %Example 16: (Version 4.3 or later) Set +/- mode to 1 (bipolar(
 << %x=[0:.1:10];y=exp(-(x-5).^2)-.5*exp(-(x-3).^2)+.1*randn(size(x;((
 << %peakfit([x' y'],0,0,2,1,0,1,0,0,0,1,1(
 %FitResults=
٠/٩٣۶٩-      ١/۶٢         ٠/۵۴٣٣-      ٣/١۶٣۶       ١            %
١/٩٠٢٩       ١/٨۴۵۶       ٠/٩۶٨۵٩      ۴/٩۴٨٧       ٢            %
 %FitError=
٨/٢٧۵٧        %
%
 %Example 17: Version 5 or later. Fits humps function to a model consisting
 %of one Pearson (shape=4, extra=3) and one Gaussian (shape=1), flat
 %baseline mode=3, NumTrials=10.
```

```
%x=[0:.005:1.2];y=humps(x);[FitResults,FitError]=peakfit([x' y'],0,0,2,[2 1],[0 0([
%FitResults=
١٧٫٠٨٥      ٠٫٢٧٨٩٢      ٨٤٫٦٧١      ٠٫٣٠١٥٤      ١          %
٢٫٥٣٩٩      ٠٫٢٠٨٢٥      ١١٫٥٤٥      ٠٫٨٨٥٢٢      ٢          %
%Baseline=
٠٫٩٠١        %
%FitError=
١٠٫٤٥٧       %
%
%Example 18: 5 peaks, 5 different shapes, all heights = 1, widths = 3.
%x=0:.1:60;
%y=modelpeaks2(x,[1 2 3 4 5],[1 1 1 1 1],[10 20 30 40 50...,[
*٠١.+([٢٠- ٢ ٠ ٠ ٠],[٣ ٣ ٣ ٣ ٣] %randn(size(x;((
%peakfit([x' y'],0,0,5,[1 2 3 4 5],[0 0 0 2 -20([
%
%Example 19: Minimum width constraint (13th input argument(
%x=1:30;y=gaussian(x,15,8)+.05*randn(size(x;((
%No constraint:
%peakfit([x;y],0,0,5,1,0,10,0,0,0,1,0,0;(
%Widths constrained to values above 7:
%peakfit([x;y],0,0,5,1,0,10,0,0,0,1,0,7;(
%
%Example 20: Noise test with peak height = RMS noise = 1.
%x=[-5:.02:5];y=exp(-(x).^2)+randn(size(x));P=peakfit([x;y],0,0,1,1,0,10,0,0,0,1,1;(
%
%Example 21: Gaussian peak on strong sloped straight-line baseline, 2-peak
%fit with variable-slope straight line (shape 26, peakfit version 6 only.(
<< %x=8:.05:12;y=x+exp(-(x-10).^2;(
```

```
] << %FitResults,FitError]=peakfit([x;y],0,0,2,[1 26],[1 1],1,0(
 %FitResults           =
١/٧۶۴٢       ١/۶۶۵١       ١           ١٠          ١           %
۴٠/٠۴۵       ٠/٠۵         ٠/٢٢٢٩٧      ۴/۴٨۵       ٢           %
 %FitError =0.093
%
 %Example 22: Segmented linear fit (Shape 29, peakfit version 6 only:(
 %x=[0.9:.005:1.7];y=humps(x;(
 %peakfit([x' y'],0,0,9,29,0,10,0,0,0,1,1(
%
 %Example 23: Polynomial fit (Shape 27, peakfit version 6 only(
 %x=[0.3:.005:1.7];y=humps(x);y=y+cumsum(y;(
 %peakfit([x' y'],0,0,4,1,6,10,0,0,0,1,1(
%
 %Example 24: Effect of quantization of independent (x) and dependent (y) variables.
 %x=.5+round([2:.02:7.5]);y=exp(-(x-5).^2)+randn(size(x))/10;peakfit([x;y([
 %x=[2:.01:8];y=exp(-(x-5).^2)+.1.*randn(size(x));y=.1.*round(10.*y);peakfit([x;y([
%
 %Example 25: Variable-alpha Voigt functions, shape 30. (Version 7 and
 %above only). FitResults has an added 6th column for the measured alphas
 %of each peak.
 %x=[0:.005:1.3];y=humps(x);[FitResults,FitError]=peakfit([x' y'],0,0,2,30,15,10(
 %FitResults=
٢/٣١٩۴       ٢۴/۵۶٣       ٠/٠٣۵٨٠٩     ٩۵/٨٩۶       ٠/٣٠١۵۴      ١       %
٠/٢٧٨١۵      ٧/٢۶٣۴       ٠/٨٩١٩۴      ١٩/٣٣۶       ٢/٣١٩۴       ٢       %
 %FitError=
٠/٩٩٨٨۶      ٠/٨۴٣٣١       %
%
```

%Example 26: Variable time constant exponentially braodened Gaussian

%functions, shape 31. (Version 7 and above only). FitResults has an added

۶ %th column for the measured time constant of each peak.

] %FitResults,FitError]=peakfit(DataMatrix3,1860.5,364,2,31,32.9731,5,[1810 60 30 1910 60 30([

%FitResults=

۳۲/۷۸۱ ۱۱۹/۰۱ ۶۰/۱۶۹ ۱/۸۵۸۱ ۱۸۰۰/۶ ۱ %

۳۳/۴۴۳ ۳۰/۷۹ ۱۹۰۰/۴ ۰/۴۸۴۹۱ ۳۲/۷۸۱ ۲ %

%FitError=

۰/۹۹۹۹۹ ۰/۰۷۶۶۵۱ %

%

%Example 27 Pearson variable shape, PeakShape=32,(Version 7 and above

%only). Requires modelpeaks2 function in path.

%x=1:.1:30;y=modelpeaks2(x,[4 4],[1 1],[10 20],[5 5],[1 10;([

] %FitResults,FitError]=peakfit([x;y],0,0,2,32,10,5(

%

%Example 28 Gaussian/Lorentzian blend variable shape, PeakShape=33

) %Version 7 and above only). Requires modelpeaks2 function in path.

%x=1:.1:30;y=modelpeaks2(x,[13 13],[1 1],[10 20],[3 3],[20 80;([

] %FitResults,FitError]=peakfit([x;y],0,0,2,33,0,5(

%

%Example 29: Fixed-position Gaussian (shape 16), positions=[3 5 .[

%x=0:.1:10;y=exp(-(x-5).^2)+.5*exp(-(x-3).^2)+.1*randn(size(x;((

] %FitResults,FitError]=peakfit([x' y'],0,0,2,16,0,0,0,0,[3 5([

%

```
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%LIABILITY, WHETHER IN AN ACTION OF CONTRACT, TORT OR OTHERWISE, ARISING FROM,
%OUT OF OR IN CONNECTION WITH THE SOFTWARE OR THE USE OR OTHER DEALINGS IN
%THE SOFTWARE.
%
global AA xxx PEAKHEIGHTS FIXEDPARAMETERS AUTOZERO delta BIPOLAR CLIPHEIGHT
format short g
format compact
warning off all
NumArgOut=nargout;
datasize=size(signal;(
if datasize(1)<datasize(2),signal=signal';end
datasize=size(signal;(
if datasize(2)==1, %  Must be isignal(Y-vector(
    X=1:length(signal); % Create an independent variable vector
    Y=signal;
else
```

```
 %     Must be isignal(DataMatrix(
    X=signal(:,1); % Split matrix argument
    Y=signal(:,2;(
end
X=reshape(X,1,length(X)); % Adjust X and Y vector shape to 1 x n (rather than n x 1(
Y=reshape(Y,1,length(Y;((
 %If necessary, flip the data vectors so that X increases
if X(1)>X(length(X,((
    disp('X-axis flipped('.
    X=fliplr(X;(
    Y=fliplr(Y;(
end

 %Isolate desired segment from data set for curve fitting
if nargin==1 || nargin==2,center=(max(X)-min(X))/2;window=max(X)-min(X);end
 %Y=Y-min(Y;(
xoffset=0;
n1=val2ind(X,center-window/2;(
n2=val2ind(X,center+window/2;(
if window==0,n1=1;n2=length(X);end
xx=X(n1:n2)-xoffset;
yy=Y(n1:n2;(
ShapeString='Gaussian;'
coeff=0;
CLIPHEIGHT=max(Y;(
LOGPLOT=0;
 %Define values of any missing arguments
```

```
%
)signal,center,window,NumPeaks,peakshape,extra,NumTrials,start,autozero,fixedparameters,plots,bipolar,minwidth,DELTA(

switch nargin

    case 1

        NumPeaks=1;

        peakshape=1;

        extra=0;

        NumTrials=1;

        xx=X;yy=Y;

        start=calcstart(xx,NumPeaks,xoffset;(

        AUTOZERO=0;

        plots=1;

        BIPOLAR=0;

        MINWIDTH=xx(2)-xx(1;(

        delta=1;

        CLIPHEIGHT=max(Y;(

    case 2

        NumPeaks=1;

        peakshape=1;

        extra=0;

        NumTrials=1;

        xx=signal;yy=center;

        start=calcstart(xx,NumPeaks,xoffset;(

        AUTOZERO=0;

        plots=1;

        BIPOLAR=0;

        MINWIDTH=xx(2)-xx(1;(
```

```
    delta=1;
    CLIPHEIGHT=max(Y;(
case 3
    NumPeaks=1;
    peakshape=1;
    extra=0;
    NumTrials=1;
    start=calcstart(xx,NumPeaks,xoffset;(
    AUTOZERO=0;
    FIXEDPARAMETERS=0;
    plots=1;
    BIPOLAR=0;
    MINWIDTH=xx(2)-xx(1;(
    delta=1;
    CLIPHEIGHT=max(Y;(
case 4 % Numpeaks specified in arguments
    peakshape=1;
    extra=0;
    NumTrials=1;
    start=calcstart(xx,NumPeaks,xoffset;(
    AUTOZERO=0;
    FIXEDPARAMETERS=0;
    plots=1;
    BIPOLAR=0;
    MINWIDTH=xx(2)-xx(1;(
    delta=1;
    CLIPHEIGHT=max(Y;(
```

```
case 5 % Numpeaks, peakshape specified in arguments
    extra=zeros(1,NumPeaks;(
    NumTrials=1;
    start=calcstart(xx,NumPeaks,xoffset;(
    AUTOZERO=0;
    FIXEDPARAMETERS=0;
    plots=1;
    BIPOLAR=0;
    MINWIDTH=zeros(size(peakshape))+(xx(2)-xx(1;((
    delta=1;
    CLIPHEIGHT=max(Y;(
case 6
    NumTrials=1;
    start=calcstart(xx,NumPeaks,xoffset;(
    AUTOZERO=0;
    FIXEDPARAMETERS=0;
    plots=1;
    BIPOLAR=0;
    MINWIDTH=zeros(size(peakshape))+(xx(2)-xx(1;((
    delta=1;
case 7
    start=calcstart(xx,NumPeaks,xoffset;(
    AUTOZERO=0;
    FIXEDPARAMETERS=0;
    plots=1;
    BIPOLAR=0;
    MINWIDTH=zeros(size(peakshape))+(xx(2)-xx(1;((
```

```
    delta=1;
    CLIPHEIGHT=max(Y;(
case 8
    AUTOZERO=0;
    FIXEDPARAMETERS=0;
    plots=1;
    BIPOLAR=0;
    MINWIDTH=zeros(size(peakshape))+(xx(2)-xx(1;((
    delta=1;
    CLIPHEIGHT=max(Y;(
case 9
    AUTOZERO=autozero;
    FIXEDPARAMETERS=0;
    plots=1;
    BIPOLAR=0;
    MINWIDTH=zeros(size(peakshape))+(xx(2)-xx(1;((
    delta=1;
case 10
    AUTOZERO=autozero;
    FIXEDPARAMETERS=fixedparameters;
    plots=1;
    BIPOLAR=0;
    MINWIDTH=zeros(size(peakshape))+(xx(2)-xx(1;((
    delta=1;
case 11
    AUTOZERO=autozero;
    FIXEDPARAMETERS=fixedparameters;
```

```
    BIPOLAR=0;
    MINWIDTH=zeros(size(peakshape))+(xx(2)-xx(1;((
    delta=1;
    CLIPHEIGHT=max(Y;(
case 12
    AUTOZERO=autozero;
    FIXEDPARAMETERS=fixedparameters;
    BIPOLAR=bipolar;
    MINWIDTH=zeros(size(peakshape))+(xx(2)-xx(1;((
    delta=1;
    CLIPHEIGHT=max(Y;(
case 13
    AUTOZERO=autozero;
    FIXEDPARAMETERS=fixedparameters;
    BIPOLAR=bipolar;
    MINWIDTH=minwidth;
    delta=1;
case 14
    AUTOZERO=autozero;
    FIXEDPARAMETERS=fixedparameters;
    BIPOLAR=bipolar;
    MINWIDTH=minwidth;
    delta=DELTA;
    CLIPHEIGHT=max(Y;(
case 15
    AUTOZERO=autozero;
    FIXEDPARAMETERS=fixedparameters;
```

```
        BIPOLAR=bipolar;
        MINWIDTH=minwidth;
        delta=DELTA;
        CLIPHEIGHT=clipheight;
    otherwise
end % switch nargin

 %Saturation Code, skips points greater than set maximum
if CLIPHEIGHT<max(Y,(
    apnt=1;
    for pnt=1:length(xx,(
        if yy(pnt)<CLIPHEIGHT,
            axx(apnt)=xx(pnt;(
            ayy(apnt)=yy(pnt;(
            apnt=apnt+1;
        end
    end
    xx=axx;yy=ayy;
end
 %Default values for placeholder zeros1
if NumTrials==0;NumTrials=1;end
if isscalar(peakshape,(
else
 %    disp('peakshape is vector;('
    shapesvector=peakshape;
    NumPeaks=length(peakshape;(
    peakshape=22;
```

```
end
if peakshape==0;peakshape=1;end
if NumPeaks==0;NumPeaks=1;end
if start==0;start=calcstart(xx,NumPeaks,xoffset);end
if FIXEDPARAMETERS==0, FIXEDPARAMETERS=length(xx)/10;end
if peakshape==16;FIXEDPOSITIONS=fixedparameters;end
if peakshape==17;FIXEDPOSITIONS=fixedparameters;end
if AUTOZERO>3,AUTOZERO=3,end
if AUTOZERO<0,AUTOZERO=0,end
Heights=zeros(1,NumPeaks;(
FitResults=zeros(NumPeaks,6;(

 % %Remove linear baseline from data segment if AUTOZERO==1
baseline=0;
bkgcoef=0;
bkgsize=round(length(xx)/10;(
if bkgsize<2,bkgsize=2;end
lxx=length(xx;(
if AUTOZERO==1, % linear autozero operation
    XX1=xx(1:round(lxx/bkgsize;((
    XX2=xx((lxx-round(lxx/bkgsize)):lxx;(
    Y1=yy(1:(round(length(xx)/bkgsize;(((
    Y2=yy((lxx-round(lxx/bkgsize)):lxx;(
    bkgcoef=polyfit([XX1,XX2],[Y1,Y2],1);  % Fit straight line to sub-group of points
    bkg=polyval(bkgcoef,xx;(
    yy=yy-bkg;
end % if
```

```
if AUTOZERO==2, % Quadratic autozero operation
    XX1=xx(1:round(lxx/bkgsize;((
    XX2=xx((lxx-round(lxx/bkgsize)):lxx;(
    Y1=yy(1:round(length(xx)/bkgsize;((
    Y2=yy((lxx-round(lxx/bkgsize)):lxx;(
    bkgcoef=polyfit([XX1,XX2],[Y1,Y2],2);  % Fit parabola to sub-group of points
    bkg=polyval(bkgcoef,xx;(
    yy=yy-bkg;
end % if autozero

PEAKHEIGHTS=zeros(1,NumPeaks;(
n=length(xx;(
newstart=start;
 %Assign ShapStrings
switch peakshape(1(
    case 1
        ShapeString='Gaussian;'
    case 2
        ShapeString='Lorentzian;'
    case 3
        ShapeString='Logistic;'
    case 4
        ShapeString='Pearson;'
    case 5
        ShapeString='ExpGaussian;'
    case 6
        ShapeString='Equal width Gaussians;'
```

```
case 7
    ShapeString='Equal width Lorentzians;'
case 8
    ShapeString='Exp. equal width Gaussians;'
case 9
    ShapeString='Exponential Pulse;'
case 10
    ShapeString='Up Sigmoid (logistic function;'(
case 23
    ShapeString='Down Sigmoid (logistic function  ;'(
case 11
    ShapeString='Fixed-width Gaussian;'
case 12
    ShapeString='Fixed-width Lorentzian;'
case 13
    ShapeString='Gaussian/Lorentzian blend;'
case 14
    ShapeString='BiGaussian     ;'
case 15
    ShapeString='Breit-Wigner-Fano    ;'
case 16
    ShapeString='Fixed-position Gaussians;'
case 17
    ShapeString='Fixed-position Lorentzians;'
case 18
    ShapeString='Exp. Lorentzian;'
case 19
```

```
    ShapeString='Alpha function;'
case 20
    ShapeString='Voigt (equal alphas;'(
case 21
    ShapeString='triangular;'
case 22
    ShapeString=num2str(shapesvector;(
case 24
    ShapeString='Negative Binomial Distribution;'
case 25
    ShapeString='Lognormal Distribution;'
case 26
    ShapeString='slope;'
case 27
    ShapeString='First derivative;'
case 28
    ShapeString='Polynomial;'
case 29
    ShapeString='Segmented linear;'
case 30
    ShapeString='Voigt (variable alphas;'(
case 31
    ShapeString='ExpGaussian (var. time constant;'(
case 32
    ShapeString='Pearson (var. shape constant;'(
case 33
    ShapeString='Variable Gaussian/Lorentzian;'
```

```
    otherwise
end % switch peakshape

 %Perform peak fitting for selected peak shape using fminsearch function
options = optimset('TolX',.001,'Display','off','MaxFunEvals',1000;(
LowestError=1000; % or any big number greater than largest error expected
FitParameters=zeros(1,NumPeaks.*2 ;(
BestStart=zeros(1,NumPeaks.*2 ;(
height=zeros(1,NumPeaks ;(
bestmodel=zeros(size(yy;((

for k=1:NumTrials ,
 %     StartMatrix(k,:)=newstart;
 %     disp(['Trial number ' num2str(k) ] ) % optionally prints the current trial number as progress indicator
    switch peakshape(1(
        case 1
            TrialParameters=fminsearch(@(lambda)(fitgaussian(lambda,xx,yy)),newstart,options;(
            for Peak=1:NumPeaks;
                if TrialParameters(2*Peak)<MINWIDTH,
                    TrialParameters(2*Peak)=MINWIDTH;
                end
            end
        case 2
            TrialParameters=fminsearch(@(lambda)(fitlorentzian(lambda,xx,yy)),newstart,options;(
            for Peak=1:NumPeaks;
                if TrialParameters(2*Peak)<MINWIDTH,
                    TrialParameters(2*Peak)=MINWIDTH;
```

```
            end
        end
    case 3
        TrialParameters=fminsearch(@(lambda)(fitlogistic(lambda,xx,yy)),newstart,options;(
        for Peak=1:NumPeaks;
            if TrialParameters(2*Peak)<MINWIDTH,
                TrialParameters(2*Peak)=MINWIDTH;
            end
        end
    case 4
        TrialParameters=fminsearch(@(lambda)(fitpearson(lambda,xx,yy,extra)),newstart,options;(
        for Peak=1:NumPeaks;
            if TrialParameters(2*Peak)<MINWIDTH,
                TrialParameters(2*Peak)=MINWIDTH;
            end
        end
    case 5
        zxx=[zeros(size(xx)) xx zeros(size(xx;[ ((
        zyy=[zeros(size(yy)) yy zeros(size(yy;[ ((
        TrialParameters=fminsearch(@(lambda)(fitexpgaussian(lambda,zxx,zyy,-
extra)),newstart,options;(
        for Peak=1:NumPeaks;
            if TrialParameters(2*Peak)<MINWIDTH,
                TrialParameters(2*Peak)=MINWIDTH;
            end
        end
    case 6
        cwnewstart(1)=newstart(1;(
```

```
        for pc=2:NumPeaks,
            cwnewstart(pc)=newstart(2.*pc-1;(
        end
        cwnewstart(NumPeaks+1)=(max(xx)-min(xx))/5;
        TrialParameters=fminsearch(@(lambda)(fitewgaussian(lambda,xx,yy)),cwnewstart,options;(
        for Peak=1:NumPeaks;
            if TrialParameters(NumPeaks+1)<MINWIDTH,
                TrialParameters(NumPeaks+1)=MINWIDTH;
            end
        end
    case 7
        cwnewstart(1)=newstart(1;(
        for pc=2:NumPeaks,
            cwnewstart(pc)=newstart(2.*pc-1;(
        end
        cwnewstart(NumPeaks+1)=(max(xx)-min(xx))/5;

TrialParameters=fminsearch(@(lambda)(fitewlorentzian(lambda,xx,yy)),cwnewstart,options;(
        for Peak=1:NumPeaks;
            if TrialParameters(NumPeaks+1)<MINWIDTH,
                TrialParameters(NumPeaks+1)=MINWIDTH;
            end
        end
    case 8
        cwnewstart(1)=newstart(1;(
        for pc=2:NumPeaks,
            cwnewstart(pc)=newstart(2.*pc-1;(
        end
```

```
        cwnewstart(NumPeaks+1)=(max(xx)-min(xx))/5;
        TrialParameters=fminsearch(@(lambda)(fitexpewgaussian(lambda,xx,yy,-
extra)),cwnewstart,options;(
        for Peak=1:NumPeaks;
            if TrialParameters(NumPeaks+1)<MINWIDTH,
                TrialParameters(NumPeaks+1)=MINWIDTH;
            end
        end
    case 9
        TrialParameters=fminsearch(@(lambda)(fitexppulse(lambda,xx,yy)),newstart,options;(
        for Peak=1:NumPeaks;
            if TrialParameters(2*Peak)<MINWIDTH,
                TrialParameters(2*Peak)=MINWIDTH;
            end
        end
    case 10
        TrialParameters=fminsearch(@(lambda)(fitupsigmoid(lambda,xx,yy)),newstart,options;(
        for Peak=1:NumPeaks;
            if TrialParameters(2*Peak)<MINWIDTH,
                TrialParameters(2*Peak)=MINWIDTH;
            end
        end
    case 23
        TrialParameters=fminsearch(@(lambda)(fitdownsigmoid(lambda,xx,yy)),newstart,options;(
        for Peak=1:NumPeaks;
            if TrialParameters(2*Peak)<MINWIDTH,
                TrialParameters(2*Peak)=MINWIDTH;
            end
```

```
    end
  case 11
    fixedstart;[]=
    for pc=1:NumPeaks,
      fixedstart(pc)=min(xx)+pc.*(max(xx)-min(xx))./(NumPeaks+1;(
    end
    TrialParameters=fminsearch(@(lambda)(FitFWGaussian(lambda,xx,yy)),fixedstart,options;(
  case 12
    fixedstart;[]=
    for pc=1:NumPeaks,
      fixedstart(pc)=min(xx)+pc.*(max(xx)-min(xx))./(NumPeaks+1;(
    end
    TrialParameters=fminsearch(@(lambda)(FitFWLorentzian(lambda,xx,yy)),fixedstart,options;(
  case 13
    TrialParameters=fminsearch(@(lambda)(fitGL(lambda,xx,yy,extra)),newstart,options;(
    for Peak=1:NumPeaks;
      if TrialParameters(2*Peak)<MINWIDTH,
        TrialParameters(2*Peak)=MINWIDTH;
      end
    end
  case 14
TrialParameters=fminsearch(@(lambda)(fitBiGaussian(lambda,xx,yy,extra)),newstart,options;(
    for Peak=1:NumPeaks;
      if TrialParameters(2*Peak)<MINWIDTH,
        TrialParameters(2*Peak)=MINWIDTH;
      end
    end
```

```
case 15
    TrialParameters=fminsearch(@(lambda)(fitBWF(lambda,xx,yy,extra)),newstart,options;(
    for Peak=1:NumPeaks;
        if TrialParameters(2*Peak)<MINWIDTH,
            TrialParameters(2*Peak)=MINWIDTH;
        end
    end
case 16
    fixedstart;[]=
    for pc=1:NumPeaks,
        fixedstart(pc)=(max(xx)-min(xx))./(NumPeaks+1;(
        fixedstart(pc)=fixedstart(pc)+.1*(rand-.5).*fixedstart(pc;(
    end
    TrialParameters=fminsearch(@(lambda)(FitFPGaussian(lambda,xx,yy)),fixedstart,options;(
    for Peak=1:NumPeaks;
        if TrialParameters(Peak)<MINWIDTH,
            TrialParameters(Peak)=MINWIDTH;
        end
    end
case 17
    fixedstart;[]=
    for pc=1:NumPeaks,
        fixedstart(pc)=(max(xx)-min(xx))./(NumPeaks+1;(
        fixedstart(pc)=fixedstart(pc)+.1*(rand-.5).*fixedstart(pc;(
    end
    TrialParameters=fminsearch(@(lambda)(FitFPLorentzian(lambda,xx,yy)),fixedstart,options;(
    for Peak=1:NumPeaks;
```

```
            if TrialParameters(Peak)<MINWIDTH,
                TrialParameters(Peak)=MINWIDTH;
            end
        end
    case 18
        zxx=[zeros(size(xx)) xx zeros(size(xx;[ ((
        zyy=[ones(size(yy)).*yy(1) yy zeros(size(yy)).*yy(length(yy;[ ((
        TrialParameters=fminsearch(@(lambda)(fitexplorentzian(lambda,zxx,zyy,-
extra)),newstart,options;(
        for Peak=1:NumPeaks;
            if TrialParameters(2*Peak)<MINWIDTH,
                TrialParameters(2*Peak)=MINWIDTH;
            end
        end
    case 19
        TrialParameters=fminsearch(@(lambda)(fitalphafunction(lambda,xx,yy)),newstart,options;(
        for Peak=1:NumPeaks;
            if TrialParameters(2*Peak)<MINWIDTH,
                TrialParameters(2*Peak)=MINWIDTH;
            end
        end
    case 20
        TrialParameters=fminsearch(@(lambda)(fitvoigt(lambda,xx,yy,extra)),newstart,options;(
        for Peak=1:NumPeaks;
            if TrialParameters(2*Peak)<MINWIDTH,
                TrialParameters(2*Peak)=MINWIDTH;
            end
        end
```

```
    case 21
        TrialParameters=fminsearch(@(lambda)(fittriangular(lambda,xx,yy)),newstart,options;(
        for Peak=1:NumPeaks;
            if TrialParameters(2*Peak)<MINWIDTH,
                TrialParameters(2*Peak)=MINWIDTH;
            end
        end
    case 22

TrialParameters=fminsearch(@(lambda)(fitmultiple(lambda,xx,yy,shapesvector,extra)),newstart,opti
ons;(
        for Peak=1:NumPeaks;
            if TrialParameters(2*Peak)<MINWIDTH(Peak,(
                TrialParameters(2*Peak)=MINWIDTH(Peak;(
            end
        end
    case 24
        TrialParameters=fminsearch(@(lambda)(fitnbinpdf(lambda,xx,yy)),newstart,options;(
        for Peak=1:NumPeaks;
            if TrialParameters(2*Peak)<MINWIDTH,
                TrialParameters(2*Peak)=MINWIDTH;
            end
        end
    case 25
        TrialParameters=fminsearch(@(lambda)(fitlognpdf(lambda,xx,yy)),newstart,options;(
        for Peak=1:NumPeaks;
            if TrialParameters(2*Peak)<MINWIDTH,
                TrialParameters(2*Peak)=MINWIDTH;
```

```
        end
    end
case 26
    TrialParameters=fminsearch(@(lambda)(fitlinslope(lambda,xx,yy)),polyfit(xx,yy,1),options;(
     coeff=TrialParameters;
case 27
    TrialParameters=fminsearch(@(lambda)(fitd1gauss(lambda,xx,yy)),newstart,options;(
case 28
    coeff=fitpolynomial(xx,yy,extra;(
    TrialParameters=coeff;
case 29
    cnewstart(1)=newstart(1;(
    for pc=2:NumPeaks,
        cnewstart(pc)=newstart(2.*pc-1)+(delta*(rand-.5)/50;(
    end
    TrialParameters=fminsearch(@(lambda)(fitsegmented(lambda,xx,yy)),cnewstart,options;(
case 30
    nn=max(xx)-min(xx;(
    start;[]=
    startpos=[nn/(NumPeaks+1):nn/(NumPeaks+1):nn-(nn/(NumPeaks+1))]+min(xx;(
    for marker=1:NumPeaks,
        markx=startpos(marker)+ xoffset;
        start=[start markx nn/5 extra;[
    end % for marker
     newstart=start;
    for parameter=1:3:3*NumPeaks,
        newstart(parameter)=newstart(parameter)*(1+randn/100;(
```

```
            newstart(parameter+1)=newstart(parameter+1)*(1+randn/20;(
            newstart(parameter+2)=newstart(parameter+1)*(1+randn/20;(
        end
        TrialParameters=fminsearch(@(lambda)(fitvoigtv(lambda,xx,yy)),newstart;(
    case 31
        nn=max(xx)-min(xx;(
        start;[]=
        startpos=[nn/(NumPeaks+1):nn/(NumPeaks+1):nn-(nn/(NumPeaks+1))]+min(xx;(
        for marker=1:NumPeaks,
            markx=startpos(marker)+ xoffset;
            start=[start markx nn/5 extra;[
        end % for marker
         newstart=start;
        for parameter=1:3:3*NumPeaks,
            newstart(parameter)=newstart(parameter)*(1+randn/100;(
            newstart(parameter+1)=newstart(parameter+1)*(1+randn/20;(
            newstart(parameter+2)=newstart(parameter+1)*(1+randn/20;(
        end
%           newstart=newstart
        zxx=[zeros(size(xx)) xx zeros(size(xx;[ ((
        zyy=[ones(size(yy)).*yy(1) yy zeros(size(yy)).*yy(length(yy;[ ((
        TrialParameters=fminsearch(@(lambda)(fitexpgaussianv(lambda,zxx,zyy)),newstart;(
    case 32
        nn=max(xx)-min(xx;(
        start;[]=
        startpos=[nn/(NumPeaks+1):nn/(NumPeaks+1):nn-(nn/(NumPeaks+1))]+min(xx;(
        for marker=1:NumPeaks,
```

```
        markx=startpos(marker)+ xoffset;
        start=[start markx nn/5 extra;[
    end % for marker
     newstart=start;
    for parameter=1:3:3*NumPeaks,
        newstart(parameter)=newstart(parameter)*(1+randn/100;(
        newstart(parameter+1)=newstart(parameter+1)*(1+randn/20;(
        newstart(parameter+2)=newstart(parameter+1)*(1+randn/20;(
    end
%         newstart=newstart
    TrialParameters=fminsearch(@(lambda)(fitpearsonv(lambda,xx,yy)),newstart;(
  case 33
     nn=max(xx)-min(xx;(
    start;[]=
    startpos=[nn/(NumPeaks+1):nn/(NumPeaks+1):nn-(nn/(NumPeaks+1))]+min(xx;(
    for marker=1:NumPeaks,
        markx=startpos(marker)+ xoffset;
        start=[start markx nn/5 extra;[
    end % for marker
     newstart=start;
    for parameter=1:3:3*NumPeaks,
        newstart(parameter)=newstart(parameter)*(1+randn/100;(
        newstart(parameter+1)=newstart(parameter+1)*(1+randn/20;(
        newstart(parameter+2)=newstart(parameter+1)*(1+randn/20;(
    end
%         newstart=newstart
    TrialParameters=fminsearch(@(lambda)(fitGLv(lambda,xx,yy)),newstart;(
```

```
        otherwise
    end % switch peakshape

 %Construct model from Trial parameters
A=zeros(NumPeaks,n;(
for m=1:NumPeaks,
    switch peakshape(1(
        case 1
            A(m,:)=gaussian(xx,TrialParameters(2*m-1),TrialParameters(2*m;((
        case 2
            A(m,:)=lorentzian(xx,TrialParameters(2*m-1),TrialParameters(2*m;((
        case 3
            A(m,:)=logistic(xx,TrialParameters(2*m-1),TrialParameters(2*m;((
        case 4
            A(m,:)=pearson(xx,TrialParameters(2*m-1),TrialParameters(2*m),extra;(
        case 5
            A(m,:)=expgaussian(xx,TrialParameters(2*m-1),TrialParameters(2*m),-extra;'(
        case 6
            A(m,:)=gaussian(xx,TrialParameters(m),TrialParameters(NumPeaks+1;((
        case 7
            A(m,:)=lorentzian(xx,TrialParameters(m),TrialParameters(NumPeaks+1;((
        case 8
            A(m,:)=expgaussian(xx,TrialParameters(m),TrialParameters(NumPeaks+1),-extra;'(
        case 9
            A(m,:)=exppulse(xx,TrialParameters(2*m-1),TrialParameters(2*m;((
        case 10
            A(m,:)=upsigmoid(xx,TrialParameters(2*m-1),TrialParameters(2*m;((
```

```
        case 11
            A(m,:)=gaussian(xx,TrialParameters(m),FIXEDPARAMETERS;(
        case 12
            A(m,:)=lorentzian(xx,TrialParameters(m),FIXEDPARAMETERS;(
        case 13
            A(m,:)=GL(xx,TrialParameters(2*m-1),TrialParameters(2*m),extra;(
        case 14
            A(m,:)=BiGaussian(xx,TrialParameters(2*m-1),TrialParameters(2*m),extra;(
        case 15
            A(m,:)=BWF(xx,TrialParameters(2*m-1),TrialParameters(2*m),extra        ;(
        case 16
            A(m,:)=gaussian(xx,FIXEDPOSITIONS(m),TrialParameters(m;((
        case 17
            A(m,:)=lorentzian(xx,FIXEDPOSITIONS(m),TrialParameters(m;((
        case 18
            A(m,:)=explorentzian(xx,TrialParameters(2*m-1),TrialParameters(2*m),-extra;'(
        case 19
            A(m,:)=alphafunction(xx,TrialParameters(2*m-1),TrialParameters(2*m;((
        case 20
            A(m,:)=voigt(xx,TrialParameters(2*m-1),TrialParameters(2*m),extra        ;(
        case 21
            A(m,:)=triangular(xx,TrialParameters(2*m-1),TrialParameters(2*m;((
        case 22
            A(m,:)=peakfunction(shapesvector(m),xx,TrialParameters(2*m-
1),TrialParameters(2*m),extra(m        ;((
        case 23
            A(m,:)=downsigmoid(xx,TrialParameters(2*m-1),TrialParameters(2*m        ;((
        case 24
```

```
            A(m,:)=nbinpdf(xx,TrialParameters(2*m-1),TrialParameters(2*m;((
        case 25
            A(m,:)=lognormal(xx,TrialParameters(2*m-1),TrialParameters(2*m;((
        case 26
            A(m,:)=linslope(xx,TrialParameters(2*m-1),TrialParameters(2*m;((
        case 27
            A(m,:)=d1gauss(xx,TrialParameters(2*m-1),TrialParameters(2*m;((
        case 28
            A(m,:)=polynomial(xx,coeff;(
        case 29
            A(m,:)=segmented(xx,yy,PEAKHEIGHTS;(
        case 30
            A(m,:)=voigt(xx,TrialParameters(3*m-2),TrialParameters(3*m-1),TrialParameters(3*m      ;((

        case 31
            A(m,:)=expgaussian(xx,TrialParameters(3*m-2),TrialParameters(3*m-1),-
TrialParameters(3*m        ;((
        case 32
            A(m,:)=pearson(xx,TrialParameters(3*m-2),TrialParameters(3*m-1),TrialParameters(3*m  ;((

        case 33
            A(m,:)=GL(xx,TrialParameters(3*m-2),TrialParameters(3*m-1),TrialParameters(3*m        ;((
        otherwise
    end % switch
    for parameter=1:2:2*NumPeaks,
        newstart(parameter)=newstart(parameter)*(1+delta*(rand-.5)/500;(
        newstart(parameter+1)=newstart(parameter+1)*(1+delta*(rand-.5)/100;(
    end
end % for NumPeaks
```

```
 %Multiplies each row by the corresponding amplitude and adds them up
if peakshape(1)==29, % Segmented linear
    model=segmented(xx,yy,PEAKHEIGHTS;(
    TrialParameters=PEAKHEIGHTS;
    Heights=ones(size(PEAKHEIGHTS;((
else
    if AUTOZERO==3,
        baseline=PEAKHEIGHTS(1;(
        Heights=PEAKHEIGHTS(2:1+NumPeaks;(
        model=Heights'*A+baseline;
    else
          %size(PEAKHEIGHTS) % error check
          %size(A(
        model=PEAKHEIGHTS'*A;
        Heights=PEAKHEIGHTS;
        baseline=0;
    end
end
if peakshape(1)==28, % polynomial;
    model=polynomial(xx,coeff;(
    TrialParameters=PEAKHEIGHTS;
    Heights=ones(size(PEAKHEIGHTS;((
end
 %Compare trial model to data segment and compute the fit error
    MeanFitError=100*norm(yy-model)./(sqrt(n)*max(yy;((
 %  Take only the single fit that has the lowest MeanFitError
```

```
  if MeanFitError<LowestError ,
      if min(Heights)>=-BIPOLAR*10^100,  % Consider only fits with positive peak heights
        LowestError=MeanFitError;  % Assign LowestError to the lowest MeanFitError
        FitParameters=TrialParameters;  % Assign FitParameters to the fit with the lowest
MeanFitError
        BestStart=newstart; % Assign BestStart to the start with the lowest MeanFitError
        height=Heights; % Assign height to the PEAKHEIGHTS with the lowest MeanFitError
        bestmodel=model; % Assign bestmodel to the model with the lowest MeanFitError
      end % if min(PEAKHEIGHTS)>0
  end % if MeanFitError<LowestError
  %ErrorVector(k)=MeanFitError;
end % for k (NumTrials(
    Rsquared=1-(norm(yy-bestmodel)./norm(yy-mean(yy;(((
    SStot=sum((yy-mean(yy)).^2;(
    SSres=sum((yy-bestmodel).^2;(
    Rsquared=1-(SSres./SStot;(
    GOF=[LowestError Rsquared;[
 %Uncomment following 4 lines to monitor trail fit starts and errors.
 %StartMatrix=StartMatrix;
 %ErrorVector=ErrorVector;
 %matrix=[StartMatrix ErrorVector['
 %std(StartMatrix(
 %Construct model from best-fit parameters
AA=zeros(NumPeaks,600;(
xxx=linspace(min(xx),max(xx),600;(
 %xxx=linspace(min(xx)-length(xx),max(xx)+length(xx),200;(
for m=1:NumPeaks,
   switch peakshape(1(
```

```
    case 1
        AA(m,:)=gaussian(xxx,FitParameters(2*m-1),FitParameters(2*m;((
    case 2
        AA(m,:)=lorentzian(xxx,FitParameters(2*m-1),FitParameters(2*m;((
    case 3
        AA(m,:)=logistic(xxx,FitParameters(2*m-1),FitParameters(2*m;((
    case 4
        AA(m,:)=pearson(xxx,FitParameters(2*m-1),FitParameters(2*m),extra;(
    case 5
        AA(m,:)=expgaussian(xxx,FitParameters(2*m-1),FitParameters(2*m),-
extra*length(xxx)./length(xx;'((
    case 6
        AA(m,:)=gaussian(xxx,FitParameters(m),FitParameters(NumPeaks+1;((
    case 7
        AA(m,:)=lorentzian(xxx,FitParameters(m),FitParameters(NumPeaks+1;((
    case 8
        AA(m,:)=expgaussian(xxx,FitParameters(m),FitParameters(NumPeaks+1),-
extra*length(xxx)./length(xx;'((
    case 9
        AA(m,:)=exppulse(xxx,FitParameters(2*m-1),FitParameters(2*m  ;((
    case 10
        AA(m,:)=upsigmoid(xxx,FitParameters(2*m-1),FitParameters(2*m   ;((
    case 11
        AA(m,:)=gaussian(xxx,FitParameters(m),FIXEDPARAMETERS;(
    case 12
        AA(m,:)=lorentzian(xxx,FitParameters(m),FIXEDPARAMETERS;(
    case 13
        AA(m,:)=GL(xxx,FitParameters(2*m-1),FitParameters(2*m),extra;(
```

```
    case 14
        AA(m,:)=BiGaussian(xxx,FitParameters(2*m-1),FitParameters(2*m),extra       ;(
    case 15
        AA(m,:)=BWF(xxx,FitParameters(2*m-1),FitParameters(2*m),extra       ;(
    case 16
        AA(m,:)=gaussian(xxx,FIXEDPOSITIONS(m),FitParameters(m;((
    case 17
        AA(m,:)=lorentzian(xxx,FIXEDPOSITIONS(m),FitParameters(m;((
    case 18
        AA(m,:)=explorentzian(xxx,FitParameters(2*m-1),FitParameters(2*m),-
extra*length(xxx)./length(xx;'((
    case 19
        AA(m,:)=alphafunction(xxx,FitParameters(2*m-1),FitParameters(2*m;((
    case 20
        AA(m,:)=voigt(xxx,FitParameters(2*m-1),FitParameters(2*m),extra       ;(
    case 21
        AA(m,:)=triangular(xxx,FitParameters(2*m-1),FitParameters(2*m;((
    case 22
        AA(m,:)=peakfunction(shapesvector(m),xxx,FitParameters(2*m-
1),FitParameters(2*m),extra(m         ;((
    case 23
        AA(m,:)=downsigmoid(xxx,FitParameters(2*m-1),FitParameters(2*m  ;((
    case 24
        AA(m,:)=nbinpdf(xxx,FitParameters(2*m-1),FitParameters(2*m    ;((
    case 25
        AA(m,:)=lognormal(xxx,FitParameters(2*m-1),FitParameters(2*m    ;((
    case 26
        AA(m,:)=linslope(xxx,FitParameters(2*m-1),FitParameters(2*m   ;((
```

```
    case 27
        AA(m,:)=d1gauss(xxx,FitParameters(2*m-1),FitParameters(2*m  ;((
    case 28
        AA(m,:)=polynomial(xxx,coeff;(
    case 29
    case 30
        AA(m,:)=voigt(xxx,FitParameters(3*m-2),FitParameters(3*m-1),FitParameters(3*m        ;((
    case 31
        AA(m,:)=expgaussian(xxx,FitParameters(3*m-2),FitParameters(3*m-1),-
FitParameters(3*m)*length(xxx)./length(xx        ;((
    case 32
        AA(m,:)=pearson(xxx,FitParameters(3*m-2),FitParameters(3*m-1),FitParameters(3*m        ;((
    case 33
        AA(m,:)=GL(xxx,FitParameters(3*m-2),FitParameters(3*m-1),FitParameters(3*m ;((
       otherwise
  end % switch
end % for NumPeaks

 %Multiplies each row by the corresponding amplitude and adds them up
if peakshape(1)==29, % Segmented linear
    mmodel=segmented(xx,yy,PEAKHEIGHTS;(
    baseline=0;
else
    heightsize=size(height;('
    AAsize=size(AA;(
    if heightsize(2)==AAsize(1,(
        mmodel=height'*AA+baseline;
    else
```

```
        mmodel=height*AA+baseline;
    end
end
 %Top half of the figure shows original signal and the fitted model.
if plots,
    subplot(2,1,1);plot(xx+xoffset,yy,'b.'); % Plot the original signal in blue dots
    hold on
end
if peakshape(1)==28, % Polynomial
     yi=polynomial(xxx,coeff;(
else
    for m=1:NumPeaks,
        if plots, plot(xxx+xoffset,height(m)*AA(m,:)+baseline,'g'),end  % Plot the individual component peaks in green lines
        area(m)=trapz(xxx+xoffset,height(m)*AA(m,:)); % Compute the area of each component peak using trapezoidal method
        yi(m,:)=height(m)*AA(m,:); % Place y values of individual model peaks into matrix yi
    end
end
xi=xxx+xoffset; % Place the x-values of the individual model peaks into xi

if plots,
 %     Mark starting peak positions with vertical dashed magenta lines
    if peakshape(1)==16||peakshape(1)==17
    else
        if peakshape(1)==29, % Segmented linear
            subplot(2,1,1);plot([PEAKHEIGHTS' PEAKHEIGHTS'],[0 max(yy)],'m('--
        else
```

```
        for marker=1:NumPeaks,
            markx=BestStart((2*marker)-1;(
            subplot(2,1,1);plot([markx+xoffset markx+xoffset],[0 max(yy)],'m('--
        end % for
    end
end % if peakshape

%    Plot the total model (sum of component peaks) in red lines
if peakshape(1)==29, % Segmented linear
    mmodel=segmented(xx,yy,PEAKHEIGHTS;(
   plot(xx+xoffset,mmodel,'r  ;('
else
   plot(xxx+xoffset,mmodel,'r  ;('
end
hold off;
lyy=min(yy;(
uyy=max(yy)+(max(yy)-min(yy))/10;
if BIPOLAR,
    axis([min(xx) max(xx) lyy uyy;([
    ylabel('+ - mode('
else
    axis([min(xx) max(xx) 0 uyy;([
    ylabel('+ mode('
end
switch AUTOZERO,
    case 0
        title(['peakfit.m Version 7   No baseline correction([']
```

```
        case 1
            title(['peakfit.m Version 7   Linear baseline subtraction(['
        case 2
            title(['peakfit.m Version 7   Quadratic subtraction baseline(['
        case 3
            title(['peakfit.m Version 7   Flat baseline correction(['
    end


    switch peakshape(1(
        case {4,20{
            xlabel(['Peaks = ' num2str(NumPeaks) '     Shape = ' ShapeString '     Min. Width = '
num2str(MINWIDTH) '     Shape Constant = ' num2str(extra)  '     Error = '
num2str(round(1000*LowestError)/1000) '%   R2 = ' num2str(round(100000*Rsquared)/100000( [ (
        case {5,8,18{
            xlabel(['Peaks = ' num2str(NumPeaks) '     Shape = ' ShapeString '     Min. Width = '
num2str(MINWIDTH) '     Time Constant = ' num2str(extra)   '     Error = '
num2str(round(1000*LowestError)/1000) '%   R2 = ' num2str(round(100000*Rsquared)/100000( [   (
        case 13
            xlabel(['Peaks = ' num2str(NumPeaks) '     Shape = ' ShapeString '     Min. Width = '
num2str(MINWIDTH) '     % Gaussian = ' num2str(extra)   '     Error = '
num2str(round(1000*LowestError)/1000) '%   R2 = ' num2str(round(100000*Rsquared)/100000( [   (
        case {14,15,22{
            xlabel(['Peaks = ' num2str(NumPeaks) '     Shape = ' ShapeString '     Min. Width = '
num2str(MINWIDTH) '     extra = ' num2str(extra)  '     Error = '
num2str(round(1000*LowestError)/1000) '%   R2 = ' num2str(round(100000*Rsquared)/100000( [ (
        case 28
            xlabel(['Shape = ' ShapeString '     Order = ' num2str(extra)  '     Error = '
num2str(round(1000*LowestError)/1000) '%  R2 = ' num2str(round(1000*LowestError)/1000( [ (
        otherwise
            if peakshape(1)==29, % Segmented linear
```

```
            xlabel(['Breakpoints = ' num2str(NumPeaks) '    Shape = ' ShapeString  '    Error = '
num2str(round(1000*LowestError)/1000) '%  R2 = ' num2str(round(100000*Rsquared)/100000( [ (

        else

            xlabel(['Peaks = ' num2str(NumPeaks) '    Shape = ' ShapeString '    Min. Width = '
num2str(MINWIDTH)  '    Error = ' num2str(round(1000*LowestError)/1000) '%  R2 = '
num2str(round(100000*Rsquared)/100000( [ (

        end % if peakshape(1)==29

    end % switch peakshape(1(


 %    Bottom half of the figure shows the residuals and displays RMS error

 %    between original signal and model

    residual=yy-bestmodel;

    subplot(2,1,2);plot(xx+xoffset,residual,'r('.

    axis([min(xx)+xoffset max(xx)+xoffset min(residual) max(residual;([(

    xlabel('Residual Plot('

    if NumTrials>1,

      title(['Best of ' num2str(NumTrials) ' fits([']

    else

      title(['Single fit([']

    end

end % if plots


 %Put results into a matrix FitResults, one row for each peak, showing peak index number,

 %position, amplitude, and width.

FitResults=zeros(NumPeaks,6;(

switch peakshape(1,(

    case {6,7,8}, % equal-width peak models only

       for m=1:NumPeaks,

          if m==1,
```

```
            FitResults=[[round(m) FitParameters(m)+xoffset height(m)
abs(FitParameters(NumPeaks+1)) area(m;[[(

        else

            FitResults=[FitResults ; [round(m) FitParameters(m)+xoffset height(m)
abs(FitParameters(NumPeaks+1)) area(m;[[(

        end

    end

case {11,12}, % Fixed-width shapes only

    for m=1:NumPeaks,

        if m==1,

            FitResults=[[round(m) FitParameters(m)+xoffset height(m) FIXEDPARAMETERS area(m;[[(

        else

            FitResults=[FitResults ; [round(m) FitParameters(m)+xoffset height(m) FIXEDPARAMETERS
area(m;[[(

        end

    end

case {16,17}, % Fixed-position shapes only

    for m=1:NumPeaks,

        if m==1,

            FitResults=[round(m) FIXEDPOSITIONS(m) height(m) FitParameters(m) area(m;[(

        else

            FitResults=[FitResults ; [round(m) FIXEDPOSITIONS(m) height(m) FitParameters(m)
area(m;[[(

        end

    end

case 28,   % Simple polynomial fit

    FitResults=PEAKHEIGHTS;

case 29, % Segmented linear fit

    FitResults=PEAKHEIGHTS;
```

```
    case {30,31,32,33} % Special case of shapes with 3 iterated variables
        for m=1:NumPeaks,
            if m==1,
                FitResults=[round(m) FitParameters(3*m-2) height(m) abs(FitParameters(3*m-1)) area(m)
FitParameters(3*m;[(
            else
                FitResults=[FitResults ; [round(m) FitParameters(3*m-2) height(m)
abs(FitParameters(3*m-1)) area(m)] FitParameters(3*m;[(
            end
        end
    otherwise % Normal shapes with 2 iterated variables
        for m=1:NumPeaks,
            if m==1,
                FitResults=[round(m) FitParameters(2*m-1)+xoffset height(m) abs(FitParameters(2*m))
area(m;[(
            else
                FitResults=[FitResults ; [round(m) FitParameters(2*m-1)+xoffset height(m)
abs(FitParameters(2*m)) area(m;[[(
            end % if m==1
        end % for m=1:NumPeaks,
end % switch peakshape(1(


 %Display Fit Results on lower graph
if plots,
 %    Display Fit Results on lower  graph
    subplot(2,1,2;(
    startx=min(xx)+(max(xx)-min(xx))./20;
    dxx=(max(xx)-min(xx))./10;
    dyy=((max(residual)-min(residual))./10;(
```

```
    starty=max(residual)-dyy;
    FigureSize=get(gcf,'Position;('
    switch peakshape(1(
        case {9,19,11}  % Pulse and sigmoid shapes only
            text(startx,starty+dyy/2,['Peak #         tau1         Height         tau2         Area;( ['
        case 28, % Polynomial
            text(startx,starty+dyy/2,['Polynomial coefficients;( ['
        case 29 % Segmented linear
             text(startx,starty+dyy/2,['x-axis breakpoints;( ['
        case {30,31,32,33} % Special case of shapes with 3 iterated variables
            text(startx,starty+dyy/2,['Peak #         Position       Height       Width          Area      Shape
factor            ;( ['
        otherwise
            text(startx,starty+dyy/2,['Peak #         Position       Height       Width          Area;( ['
    end
 %     Display FitResults using sprintf
    if peakshape(1)==28||peakshape(1)==29, % Polynomial or segmented linear
        for number=1:length(FitResults,(
            column=1;
            itemstring=sprintf('%0.4g',FitResults(number;((
            xposition=startx+(1.7.*dxx.*(column-1).*(600./FigureSize(3;(((
            yposition=starty-number.*dyy.*(400./FigureSize(4;((
            text(xposition,yposition,['              ' itemstring;([
        end
    else
        for peaknumber=1:NumPeaks,
            for column=1:5,
                itemstring=sprintf('%0.4g',FitResults(peaknumber,column;((
```

```
            xposition=startx+(1.7.*dxx.*(column-1).*(600./FigureSize(3;(((
            yposition=starty-peaknumber.*dyy.*(400./FigureSize(4;((
            text(xposition,yposition,itemstring;(
        end
    end
    xposition=startx;
    yposition=starty-(peaknumber+1).*dyy.*(400./FigureSize(4;((
    if AUTOZERO==3,
        text(xposition,yposition,[ 'Baseline= ' num2str(baseline;([ (
    end % if AUTOZERO
end % if peakshape(1(
if peakshape(1)==30 || peakshape(1)==31 || peakshape(1)==32 || peakshape(1)==33,
    for peaknumber=1:NumPeaks,
        column=6;
        itemstring=sprintf('%0.4g',FitParameters(3*peaknumber;((
        xposition=startx+(1.7.*dxx.*(column-1).*(600./FigureSize(3;(((
        yposition=starty-peaknumber.*dyy.*(400./FigureSize(4;((
        text(xposition,yposition,itemstring;(
    end
end
end % if plots

if NumArgOut==8,
    if plots,disp('Computing bootstrap sampling statistics.....'),end
    BootstrapResultsMatrix=zeros(6,100,NumPeaks;(
    BootstrapErrorMatrix=zeros(1,100,NumPeaks;(
    clear bx by
```

```
    tic;
    for trial=1:100,
        n=1;
        bx=xx;
        by=yy;
        while n<length(xx)-1,
            if rand>.5,
                bx(n)=xx(n+1;(
                by(n)=yy(n+1;(
            end
            n=n+1;
        end
        bx=bx+xoffset;

]FitResults,BootFitError]=fitpeaks(bx,by,NumPeaks,peakshape,extra,NumTrials,start,AUTOZERO,FIXE
DPARAMETERS;(
        for peak=1:NumPeaks,
            switch peakshape(1(
                case {30,31,32,33{
                    BootstrapResultsMatrix(1:6,trial,peak)=FitResults(peak,1:6;(
                otherwise
                    BootstrapResultsMatrix(1:5,trial,peak)=FitResults(peak,1:5;(
            end
            BootstrapErrorMatrix(:,trial,peak)=BootFitError;
        end
    end
    if plots,toc;end
    for peak=1:NumPeaks,
```

```
        if plots,
            disp(' ')
            disp(['Peak #',num2str(peak) '      Position   Height    Width     Area    Shape Factor;(['
        end % if plots
        BootstrapMean=mean(real(BootstrapResultsMatrix(:,:,peak;(('(
        BootstrapSTD=std(BootstrapResultsMatrix(:,:,peak;('(
        BootstrapIQR=iqr(BootstrapResultsMatrix(:,:,peak;('(
        PercentRSD=100.*BootstrapSTD./BootstrapMean;
        PercentIQR=100.*BootstrapIQR./BootstrapMean;
        BootstrapMean=BootstrapMean(2:6;(
        BootstrapSTD=BootstrapSTD(2:6;(
        BootstrapIQR=BootstrapIQR(2:6;(
        PercentRSD=PercentRSD(2:6;(
        PercentIQR=PercentIQR(2:6;(
        if plots,
            disp(['Bootstrap Mean: ', num2str(BootstrapMean([(
            disp(['Bootstrap STD:  ', num2str(BootstrapSTD([(
            disp(['Bootstrap IQR:  ', num2str(BootstrapIQR([(
            disp(['Percent RSD:    ', num2str(PercentRSD([(
            disp(['Percent IQR:    ', num2str(PercentIQR([(
        end % if plots
        BootResults(peak,:)=[BootstrapMean BootstrapSTD PercentRSD BootstrapIQR PercentIQR;[
    end % peak=1:NumPeaks,
end % if NumArgOut==8,
if AUTOZERO==3;
else
    baseline=bkgcoef;
```

```
end

------------------------------------------------------------------- %

function
[FitResults,LowestError]=fitpeaks(xx,yy,NumPeaks,peakshape,extra,NumTrials,start,AUTOZERO,fixed
parameters(

 %Based on peakfit Version 3: June, 2012 .

global PEAKHEIGHTS FIXEDPARAMETERS AUTOZERO BIPOLAR MINWIDTH coeff

format short g

format compact

warning off all

FIXEDPARAMETERS=fixedparameters;

xoffset=0;

if start==0;start=calcstart(xx,NumPeaks,xoffset);end

PEAKHEIGHTS=zeros(1,NumPeaks;(

n=length(xx;(

newstart=start;

coeff=0;

LOGPLOT=0;


 %Perform peak fitting for selected peak shape using fminsearch function

options = optimset('TolX',.001,'Display','off','MaxFunEvals',1000;(

LowestError=1000; % or any big number greater than largest error expected

FitParameters=zeros(1,NumPeaks.*2 ;(

BestStart=zeros(1,NumPeaks.*2 ;(

height=zeros(1,NumPeaks ;(

bestmodel=zeros(size(yy;((

for k=1:NumTrials,

 %    StartVector=newstart
```

```
switch peakshape(1(
    case 1
        TrialParameters=fminsearch(@(lambda)(fitgaussian(lambda,xx,yy)),newstart,options;(
        for Peak=1:NumPeaks;
            if TrialParameters(2*Peak)<MINWIDTH,
                TrialParameters(2*Peak)=MINWIDTH;
            end
        end
    case 2
        TrialParameters=fminsearch(@(lambda)(fitlorentzian(lambda,xx,yy)),newstart,options;(
        for Peak=1:NumPeaks;
            if TrialParameters(2*Peak)<MINWIDTH,
                TrialParameters(2*Peak)=MINWIDTH;
            end
        end
    case 3
        TrialParameters=fminsearch(@(lambda)(fitlogistic(lambda,xx,yy)),newstart,options;(
        for Peak=1:NumPeaks;
            if TrialParameters(2*Peak)<MINWIDTH,
                TrialParameters(2*Peak)=MINWIDTH;
            end
        end
    case 4
        TrialParameters=fminsearch(@(lambda)(fitpearson(lambda,xx,yy,extra)),newstart,options;(
        for Peak=1:NumPeaks;
            if TrialParameters(2*Peak)<MINWIDTH,
                TrialParameters(2*Peak)=MINWIDTH;
```

```
            end
        end
    case 5
        zxx=[zeros(size(xx)) xx zeros(size(xx;[ ((
        zyy=[zeros(size(yy)) yy zeros(size(yy;[ ((
        TrialParameters=fminsearch(@(lambda)(fitexpgaussian(lambda,zxx,zyy,-
extra)),newstart,options;(
        for Peak=1:NumPeaks;
            if TrialParameters(2*Peak)<MINWIDTH,
                TrialParameters(2*Peak)=MINWIDTH;
            end
        end
    case 6
        cwnewstart(1)=newstart(1;(
        for pc=2:NumPeaks,
            cwnewstart(pc)=newstart(2.*pc-1;(
        end
        cwnewstart(NumPeaks+1)=(max(xx)-min(xx))/5;
        TrialParameters=fminsearch(@(lambda)(fitewgaussian(lambda,xx,yy)),cwnewstart,options;(
        for Peak=1:NumPeaks;
            if TrialParameters(NumPeaks+1)<MINWIDTH,
                TrialParameters(NumPeaks+1)=MINWIDTH;
            end
        end
    case 7
        cwnewstart(1)=newstart(1;(
        for pc=2:NumPeaks,
            cwnewstart(pc)=newstart(2.*pc-1;(
```

```
        end
        cwnewstart(NumPeaks+1)=(max(xx)-min(xx))/5;

TrialParameters=fminsearch(@(lambda)(fitewlorentzian(lambda,xx,yy)),cwnewstart,options;(
        for Peak=1:NumPeaks;
            if TrialParameters(NumPeaks+1)<MINWIDTH,
                TrialParameters(NumPeaks+1)=MINWIDTH;
            end
        end
    case 8
        cwnewstart(1)=newstart(1;(
        for pc=2:NumPeaks,
            cwnewstart(pc)=newstart(2.*pc-1;(
        end
        cwnewstart(NumPeaks+1)=(max(xx)-min(xx))/5;
        TrialParameters=fminsearch(@(lambda)(fitexpewgaussian(lambda,xx,yy,-
extra)),cwnewstart,options;(
        for Peak=1:NumPeaks;
            if TrialParameters(NumPeaks+1)<MINWIDTH,
                TrialParameters(NumPeaks+1)=MINWIDTH;
            end
        end
    case 9
        TrialParameters=fminsearch(@(lambda)(fitexppulse(lambda,xx,yy)),newstart,options;(
        for Peak=1:NumPeaks;
            if TrialParameters(2*Peak)<MINWIDTH,
                TrialParameters(2*Peak)=MINWIDTH;
            end
```

```
    end
case 10
    TrialParameters=fminsearch(@(lambda)(fitupsigmoid(lambda,xx,yy)),newstar,optionst;(
    for Peak=1:NumPeaks;
        if TrialParameters(2*Peak)<MINWIDTH,
            TrialParameters(2*Peak)=MINWIDTH;
        end
    end
case 11
    fixedstart;[]=
    for pc=1:NumPeaks,
        fixedstart(pc)=min(xx)+pc.*(max(xx)-min(xx))./(NumPeaks+1;(
    end
    TrialParameters=fminsearch(@(lambda)(FitFWGaussian(lambda,xx,yy)),fixedstart,options;(
    for Peak=1:NumPeaks;
        if TrialParameters(2*Peak)<MINWIDTH,
            TrialParameters(2*Peak)=MINWIDTH;
        end
    end
case 12
    fixedstart;[]=
    for pc=1:NumPeaks,
        fixedstart(pc)=min(xx)+pc.*(max(xx)-min(xx))./(NumPeaks+1;(
    end
    TrialParameters=fminsearch(@(lambda)(FitFWLorentzian(lambda,xx,yy)),fixedstart,options;(
    for Peak=1:NumPeaks;
        if TrialParameters(2*Peak)<MINWIDTH,
```

```
            TrialParameters(2*Peak)=MINWIDTH;
        end
    end
case 13
    TrialParameters=fminsearch(@(lambda)(fitGL(lambda,xx,yy,extra)),newstart,options;(
    for Peak=1:NumPeaks;
        if TrialParameters(2*Peak)<MINWIDTH,
            TrialParameters(2*Peak)=MINWIDTH;
        end
    end
case 14

TrialParameters=fminsearch(@(lambda)(fitBiGaussian(lambda,xx,yy,extra)),newstart,options;(
    for Peak=1:NumPeaks;
        if TrialParameters(2*Peak)<MINWIDTH,
            TrialParameters(2*Peak)=MINWIDTH;
        end
    end
case 15
    TrialParameters=fminsearch(@(lambda)(fitBWF(lambda,xx,yy,extra)),newstart,options;(
    for Peak=1:NumPeaks;
        if TrialParameters(2*Peak)<MINWIDTH,
            TrialParameters(2*Peak)=MINWIDTH;
        end
    end
case 16
    fixedstart;[]=
    for pc=1:NumPeaks,
```

```
            fixedstart(pc)=(max(xx)-min(xx))./(NumPeaks+1;(
        end
        TrialParameters=fminsearch(@(lambda)(FitFPGaussian(lambda,xx,yy)),fixedstart,options;(
        for Peak=1:NumPeaks;
            if TrialParameters(Peak)<MINWIDTH,
                TrialParameters(Peak)=MINWIDTH;
            end
        end
    case 17
        fixedstart;[]=
        for pc=1:NumPeaks,
            fixedstart(pc)=(max(xx)-min(xx))./(NumPeaks+1;(
        end
        TrialParameters=fminsearch(@(lambda)(FitFPLorentzian(lambda,xx,yy)),fixedstart,options;(
        for Peak=1:NumPeaks;
            if TrialParameters(Peak)<MINWIDTH,
                TrialParameters(Peak)=MINWIDTH;
            end
        end
    case 18
        zxx=[zeros(size(xx)) xx zeros(size(xx;[ ((
        zyy=[zeros(size(yy)) yy zeros(size(yy;[ ((
        TrialParameters=fminsearch(@(lambda)(fitexplorentzian(lambda,zxx,zyy,-
extra)),newstart,options;(
    case 19
        TrialParameters=fminsearch(@(lambda)(alphafunction(lambda,xx,yy)),newstart,options;(
        for Peak=1:NumPeaks;
            if TrialParameters(2*Peak)<MINWIDTH,
```

```
            TrialParameters(2*Peak)=MINWIDTH;
        end
    end
case 20
    TrialParameters=fminsearch(@(lambda)(fitvoigt(lambda,xx,yy,extra)),newstart,options;(
    for Peak=1:NumPeaks;
        if TrialParameters(2*Peak)<MINWIDTH,
            TrialParameters(2*Peak)=MINWIDTH;
        end
    end
case 21
    TrialParameters=fminsearch(@(lambda)(fittriangular(lambda,xx,yy)),newstart,options;(
    for Peak=1:NumPeaks;
        if TrialParameters(2*Peak)<MINWIDTH,
            TrialParameters(2*Peak)=MINWIDTH;
        end
    end
case 22

TrialParameters=fminsearch(@(lambda)(fitmultiple(lambda,xx,yy,shapesvector,extra)),newstart,opti
ons;(
    for Peak=1:NumPeaks;
        if TrialParameters(2*Peak)<MINWIDTH(Peak,(
            TrialParameters(2*Peak)=MINWIDTH(Peak;(
        end
    end
case 23
    TrialParameters=fminsearch(@(lambda)(fitdownsigmoid(lambda,xx,yy)),newstar,optionst;(
```

```
    for Peak=1:NumPeaks;
        if TrialParameters(2*Peak)<MINWIDTH,
            TrialParameters(2*Peak)=MINWIDTH;
        end
    end
case 24
    TrialParameters=fminsearch(@(lambda)(fitnbinpdf(lambda,xx,yy)),newstart,options;(
    for Peak=1:NumPeaks;
        if TrialParameters(2*Peak)<MINWIDTH,
            TrialParameters(2*Peak)=MINWIDTH;
        end
    end
case 25
    TrialParameters=fminsearch(@(lambda)(fitlognpdf(lambda,xx,yy)),newstart,options;(
    for Peak=1:NumPeaks;
        if TrialParameters(2*Peak)<MINWIDTH,
            TrialParameters(2*Peak)=MINWIDTH;
        end
    end
case 26
    TrialParameters=fminsearch(@(lambda)(fitlinslope(lambda,xx,yy)),polyfit(xx,yy,1),options;(
coeff=TrialParameters;
case 27
    TrialParameters=fminsearch(@(lambda)(fitd1gauss(lambda,xx,yy)),newstart,options;(
    for Peak=1:NumPeaks;
        if TrialParameters(2*Peak)<MINWIDTH,
            TrialParameters(2*Peak)=MINWIDTH;
```

```
            end
        end
    case 28
        TrialParameters=fitpolynomial(xx,yy,extra;(
    case 29
        TrialParameters=fminsearch(@(lambda)(fitsegmented(lambda,xx,yy)),newstart,options;(
    case 30
        TrialParameters=fminsearch(@(lambda)(fitvoigtv(lambda,xx,yy)),newstart;(
    case 31
        zxx=[zeros(size(xx)) xx zeros(size(xx;[ ((
        zyy=[zeros(size(yy)) yy zeros(size(yy;[ ((
        TrialParameters=fminsearch(@(lambda)(fitexpgaussianv(lambda,zxx,zyy)),newstart;(
    case 32
        TrialParameters=fminsearch(@(lambda)(fitpearsonv(lambda,xx,yy)),newstart;(
    case 33
        TrialParameters=fminsearch(@(lambda)(fitGLv(lambda,xx,yy)),newstart;(
    otherwise
  end % switch peakshape

for peaks=1:NumPeaks,
   peakindex=2*peaks-1;
   newstart(peakindex)=start(peakindex)-xoffset;
end

 %   Construct model from Trial parameters
  A=zeros(NumPeaks,n;(
  for m=1:NumPeaks,
```

```
switch peakshape(1(
    case 1
        A(m,:)=gaussian(xx,TrialParameters(2*m-1),TrialParameters(2*m;((
    case 2
        A(m,:)=lorentzian(xx,TrialParameters(2*m-1),TrialParameters(2*m;((
    case 3
        A(m,:)=logistic(xx,TrialParameters(2*m-1),TrialParameters(2*m;((
    case 4
        A(m,:)=pearson(xx,TrialParameters(2*m-1),TrialParameters(2*m),extra;(
    case 5
        A(m,:)=expgaussian(xx,TrialParameters(2*m-1),TrialParameters(2*m),-extra;'(
    case 6
        A(m,:)=gaussian(xx,TrialParameters(m),TrialParameters(NumPeaks+1;((
    case 7
        A(m,:)=lorentzian(xx,TrialParameters(m),TrialParameters(NumPeaks+1;((
    case 8
        A(m,:)=expgaussian(xx,TrialParameters(m),TrialParameters(NumPeaks+1),-extra;'(
    case 9
        A(m,:)=exppulse(xx,TrialParameters(2*m-1),TrialParameters(2*m;((
    case 10
        A(m,:)=upsigmoid(xx,TrialParameters(2*m-1),TrialParameters(2*m;((
    case 11
        A(m,:)=gaussian(xx,TrialParameters(m),FIXEDPARAMETERS;(
    case 12
        A(m,:)=lorentzian(xx,TrialParameters(m),FIXEDPARAMETERS;(
    case 13
        A(m,:)=GL(xx,TrialParameters(2*m-1),TrialParameters(2*m),extra;(
```

```
        case 14
            A(m,:)=BiGaussian(xx,TrialParameters(2*m-1),TrialParameters(2*m),extra;(
        case 15
            A(m,:)=BWF(xx,TrialParameters(2*m-1),TrialParameters(2*m),extra;(
        case 16
            A(m,:)=gaussian(xx,FIXEDPOSITIONS(m),TrialParameters(m;((
        case 17
            A(m,:)=lorentzian(xx,FIXEDPOSITIONS(m),TrialParameters(m;((
        case 18
            A(m,:)=explorentzian(xx,TrialParameters(2*m-1),TrialParameters(2*m),-extra;'(
        case 19
            A(m,:)=alphafunction(xx,TrialParameters(2*m-1),TrialParameters(2*m;((
        case 20
            A(m,:)=voigt(xx,TrialParameters(2*m-1),TrialParameters(2*m),extra;(
        case 21
            A(m,:)=triangular(xx,TrialParameters(2*m-1),TrialParameters(2*m;((
        case 22
            A(m,:)=peakfunction(shapesvector(m),xx,TrialParameters(2*m-
1),TrialParameters(2*m),extra(m;((
        case 23
            A(m,:)=downsigmoid(xx,TrialParameters(2*m-1),TrialParameters(2*m      ;((
        case 24
            A(m,:)=nbinpdf(xx,TrialParameters(2*m-1),TrialParameters(2*m;((
        case 25
            A(m,:)=lognormal(xx,TrialParameters(2*m-1),TrialParameters(2*m;((
        case 26
            A(m,:)=linslope(xx,TrialParameters(2*m-1),TrialParameters(2*m;((
        case 27
```

```
            A(m,:)=d1gauss(xx,TrialParameters(2*m-1),TrialParameters(2*m       ;((
        case 28
            A(m,:)=polynomial(xx,TrialParameters(2*m-1),TrialParameters(2*m       ;((
        case 29
            A(m,:)=segmented(xx,yy,PEAKHEIGHTS;(
        case 30
            A(m,:)=voigt(xx,TrialParameters(3*m-2),TrialParameters(3*m-1),TrialParameters(3*m  ;((

        case 31
            A(m,:)=expgaussian(xx,TrialParameters(3*m-2),TrialParameters(3*m-
1),TrialParameters(3*m        ;((
        case 32
            A(m,:)=pearson(xx,TrialParameters(3*m-2),TrialParameters(3*m-
1),TrialParameters(3*m        ;((
        case 33
            A(m,:)=GL(xx,TrialParameters(3*m-2),TrialParameters(3*m-1),TrialParameters(3*m;((
    end % switch
end % for

%   Multiplies each row by the corresponding amplitude and adds them up
if peakshape(1)==29, % Segmented linear
    model=segmented(xx,yy,PEAKHEIGHTS;(
    TrialParameters=coeff;
    Heights=ones(size(coeff;((
else
    if AUTOZERO==3,
        baseline=PEAKHEIGHTS(1;(
        Heights=PEAKHEIGHTS(2:1+NumPeaks;(
        model=Heights'*A+baseline;
```

```
        else
            model=PEAKHEIGHTS'*A;
            Heights=PEAKHEIGHTS;
            baseline=0;
        end
    end

 %    Compare trial model to data segment and compute the fit error
    MeanFitError=100*norm(yy-model)./(sqrt(n)*max(yy;((
 %    Take only the single fit that has the lowest MeanFitError
    if MeanFitError<LowestError,
        if min(Heights)>=-BIPOLAR*10^100,  % Consider only fits with positive peak heights
            LowestError=MeanFitError;  % Assign LowestError to the lowest MeanFitError
            FitParameters=TrialParameters;  % Assign FitParameters to the fit with the lowest
MeanFitError
            height=Heights; % Assign height to the PEAKHEIGHTS with the lowest MeanFitError
        end % if min(PEAKHEIGHTS)>0
    end % if MeanFitError<LowestError
end % for k (NumTrials(
    Rsquared=1-(norm(yy-bestmodel)./norm(yy-mean(yy;(((
    SStot=sum((yy-mean(yy)).^2;(
    SSres=sum((yy-bestmodel).^2;(
    Rsquared=1-(SSres./SStot;(
    GOF=[LowestError Rsquared;[
for m=1:NumPeaks,
    area(m)=trapz(xx+xoffset,height(m)*A(m,:)); % Compute the area of each component peak using
trapezoidal method
end
```

```
 %Put results into a matrix FitResults, one row for each peak, showing peak index number,
 %position, amplitude, and width.
FitResults=zeros(NumPeaks,6;(
switch peakshape(1,(
    case {6,7,8}, % equal-width peak models only
        for m=1:NumPeaks,
            if m==1,
                FitResults=[[round(m) FitParameters(m)+xoffset height(m)
abs(FitParameters(NumPeaks+1)) area(m;[[(
            else
                FitResults=[FitResults ; [round(m) FitParameters(m)+xoffset height(m)
abs(FitParameters(NumPeaks+1)) area(m;[[(
            end
        end
    case {11,12}, % Fixed-width shapes only
        for m=1:NumPeaks,
            if m==1,
                FitResults=[[round(m) FitParameters(m)+xoffset height(m) FIXEDPARAMETERS area(m;[[(
            else
                FitResults=[FitResults ; [round(m) FitParameters(m)+xoffset height(m) FIXEDPARAMETERS
area(m;[[(
            end
        end
    case {16,17}, % Fixed-position shapes only
        for m=1:NumPeaks,
            if m==1,
                FitResults=[round(m) FIXEDPOSITIONS(m) height(m) FitParameters(m) area(m;[(
            else
```

```
            FitResults=[FitResults ; [round(m) FIXEDPOSITIONS(m) height(m) FitParameters(m)
area(m;[[(

        end

    end

case 28,   % Simple polynomial fit

    FitResults=PEAKHEIGHTS;

case 29, % Segmented linear fit

    FitResults=PEAKHEIGHTS;

case {30,31,32,33} % Special case of shapes with 3 iterated variables

    for m=1:NumPeaks,

        if m==1,

            FitResults=[round(m) FitParameters(3*m-2) height(m) abs(FitParameters(3*m-1)) area(m)
FitParameters(3*m;[(

        else

            FitResults=[FitResults ; [round(m) FitParameters(3*m-2) height(m)
abs(FitParameters(3*m-1)) area(m) FitParameters(3*m;[[(

        end

    end

otherwise % Normal shapes with 2 iterated variables

    for m=1:NumPeaks,

        if m==1,

            FitResults=[round(m) FitParameters(2*m-1)+xoffset height(m) abs(FitParameters(2*m))
area(m;[(

        else

            FitResults=[FitResults ; [round(m) FitParameters(2*m-1)+xoffset height(m)
abs(FitParameters(2*m)) area(m;[[(

        end % if m==1

    end % for m=1:NumPeaks,

end % switch peakshape(1(
```

```
---------------------------------------------------------------- %
function start=calcstart(xx,NumPeaks,xoffset(
  n=max(xx)-min(xx;(
  start;[]=
  startpos=[n/(NumPeaks+1):n/(NumPeaks+1):n-(n/(NumPeaks+1))]+min(xx;(
  for marker=1:NumPeaks,
      markx=startpos(marker)+ xoffset;
      start=[start markx n/ (3.*NumPeaks;[(
  end % for marker
---------------------- ---------------------------------------- %
function [index,closestval]=val2ind(x,val(
 %Returns the index and the value of the element of vector x that is closest to val
 %If more than one element is equally close, returns vectors of indicies and values
 %Tom O'Haver (toh@umd.edu) October 2006
 %Examples: If x=[1 2 4 3 5 9 6 4 5 3 1], then val2ind(x,6)=7 and val2ind(x,5.1)=[5 9[
] %indices values]=val2ind(x,3.3) returns indices = [4 10] and values = [3 3[
dif=abs(x-val;(
index=find((dif-min(dif))==0;(
closestval=x(index;(
---------------------------------------------------------------- %
function err = fitgaussian(lambda,t,y(
 %Fitting function for a Gaussian band signal.
global PEAKHEIGHTS AUTOZERO BIPOLAR LOGPLOT
numpeaks=round(length(lambda)/2;(
A = zeros(length(t),numpeaks;(
for j = 1:numpeaks,
    %if lambda(2*j)<MINWIDTH,lambda(2*j)=MINWIDTH;end
    A(:,j) = gaussian(t,lambda(2*j-1),lambda(2*j;'((
```

```
end
if AUTOZERO==3,A=[ones(size(y))' A];end
if BIPOLAR,PEAKHEIGHTS=A\y';else PEAKHEIGHTS=abs(A\y');end
z = A*PEAKHEIGHTS;
if LOGPLOT,
    err = norm(log10(z)-log10(y;('(
else
    err = norm(z-y;('
end
---------------------------------------------------------------------  %
function err = fitewgaussian(lambda,t,y(
 %Fitting function for a Gaussian band signal with equal peak widths.
global PEAKHEIGHTS AUTOZERO BIPOLAR LOGPLOT
numpeaks=round(length(lambda)-1;(
A = zeros(length(t),numpeaks;(
for j = 1:numpeaks,
    A(:,j) = gaussian(t,lambda(j),lambda(numpeaks+1;'((
end
if AUTOZERO==3,A=[ones(size(y))' A];end
if BIPOLAR,PEAKHEIGHTS=A\y';else PEAKHEIGHTS=abs(A\y');end
z = A*PEAKHEIGHTS;
if LOGPLOT,
    err = norm(log10(z)-log10(y;('(
else
    err = norm(z-y;('
end
---------------------------------------------------------------------  %
```

```
function err = FitFWGaussian(lambda,t,y(
%       Fitting function for a fixed width Gaussian
global PEAKHEIGHTS AUTOZERO FIXEDPARAMETERS BIPOLAR LOGPLOT
numpeaks=round(length(lambda;((
A = zeros(length(t),numpeaks;(
for j = 1:numpeaks,
    A(:,j) = gaussian(t,lambda(j),FIXEDPARAMETERS;'(
end
if AUTOZERO==3,A=[ones(size(y))' A];end
if BIPOLAR,PEAKHEIGHTS=A\y';else PEAKHEIGHTS=abs(A\y');end
z = A*PEAKHEIGHTS;
if LOGPLOT,
    err = norm(log10(z)-log10(y;('(
else
    err = norm(z-y;('
end
---------------------------------------------------------------------  %
function err = FitFPGaussian(lambda,t,y(
%       Fitting function for fixed-position Gaussians
global PEAKHEIGHTS AUTOZERO FIXEDPARAMETERS BIPOLAR LOGPLOT
numpeaks=round(length(lambda;((
A = zeros(length(t),numpeaks;(
for j = 1:numpeaks,
    A(:,j) = gaussian(t,FIXEDPARAMETERS(j), lambda(j;'((
end
if AUTOZERO==3,A=[ones(size(y))' A];end
if BIPOLAR,PEAKHEIGHTS=A\y';else PEAKHEIGHTS=abs(A\y');end
```

```
z = A*PEAKHEIGHTS;
if LOGPLOT,
    err = norm(log10(z)-log10(y;('(
else
    err = norm(z-y;('
end
---------------------------------------------------------------- %
function err = FitFPLorentzian(lambda,t,y(
%       Fitting function for fixed-position Lorentzians
global PEAKHEIGHTS AUTOZERO FIXEDPARAMETERS BIPOLAR
numpeaks=round(length(lambda;((
A = zeros(length(t),numpeaks;(
for j = 1:numpeaks,
    A(:,j) = lorentzian(t,FIXEDPARAMETERS(j), lambda(j;'((
end
if AUTOZERO==3,A=[ones(size(y))' A];end
if BIPOLAR,PEAKHEIGHTS=A\y';else PEAKHEIGHTS=abs(A\y');end
z = A*PEAKHEIGHTS;
err = norm(z-y;('
---------------------------------------------------------- ---------- %
function err = FitFWLorentzian(lambda,t,y(
%       Fitting function for fixed width Lorentzian
global PEAKHEIGHTS AUTOZERO FIXEDPARAMETERS BIPOLAR LOGPLOT
numpeaks=round(length(lambda;((
A = zeros(length(t),numpeaks;(
for j = 1:numpeaks,
    A(:,j) = lorentzian(t,lambda(j),FIXEDPARAMETERS;'(
```

```
end
if AUTOZERO==3,A=[ones(size(y))' A];end
if BIPOLAR,PEAKHEIGHTS=A\y';else PEAKHEIGHTS=abs(A\y');end
z = A*PEAKHEIGHTS;
if LOGPLOT,
    err = norm(log10(z)-log10(y;('(
else
    err = norm(z-y;('
end
---------------------------------------------------------------------  %
function err = fitewlorentzian(lambda,t,y(
 %Fitting function for a Lorentzian band signal with equal peak widths.
global PEAKHEIGHTS AUTOZERO BIPOLAR LOGPLOT
numpeaks=round(length(lambda)-1;(
A = zeros(length(t),numpeaks;(
for j = 1:numpeaks,
    A(:,j) = lorentzian(t,lambda(j),lambda(numpeaks+1;'((
end
if AUTOZERO==3,A=[ones(size(y))' A];end
if BIPOLAR,PEAKHEIGHTS=A\y';else PEAKHEIGHTS=abs(A\y');end
z = A*PEAKHEIGHTS;
if LOGPLOT,
    err = norm(log10(z)-log10(y;('(
else
    err = norm(z-y;('
end
---------------------------------------------------------------------  %
```

```
function g = gaussian(x,pos,wid(
  %gaussian(X,pos,wid) = gaussian peak centered on pos, half-width=wid
  %X may be scalar, vector, or matrix, pos and wid both scalar
 %Examples: gaussian([0 1 2],1,2) gives result [0.5000    1.0000    0.5000[
 %plot(gaussian([1:100],50,20)) displays gaussian band centered at 50 with width 20.
g = exp(-((x-pos)./(0.6005615.*wid)).^2;(
---------------------------------------------------------------------  %
function err = fitlorentzian(lambda,t,y(
%       Fitting function for single lorentzian, lambda(1)=position, lambda(2)=width
%       Fitgauss assumes a lorentzian function
global PEAKHEIGHTS AUTOZERO BIPOLAR LOGPLOT
A = zeros(length(t),round(length(lambda)/2;((
for j = 1:length(lambda)/2,
    A(:,j) = lorentzian(t,lambda(2*j-1),lambda(2*j;'((
end
if AUTOZERO==3,A=[ones(size(y))' A];end
if BIPOLAR,PEAKHEIGHTS=A\y';else PEAKHEIGHTS=abs(A\y');end
z = A*PEAKHEIGHTS;
if LOGPLOT,
    err = norm(log10(z)-log10(y;('(
else
    err = norm(z-y;('
end
---------------------------------------------------------------------  %
function g = lorentzian(x,position,width(
 %lorentzian(x,position,width) Lorentzian function.
 %where x may be scalar, vector, or matrix
```

```
 %position and width scalar
 %T. C. O'Haver, 1988
 %Example: lorentzian([1 2 3],2,2) gives result [0.5 1 0.5[
g=ones(size(x))./(1+((x-position)./(0.5.*width)).^2;(
---------------------------------------------------------------------  %
function err = fitlogistic(lambda,t,y(
%       Fitting function for logistic, lambda(1)=position, lambda(2)=width
%       between the data and the values computed by the current
%       function of lambda.  Fitlogistic assumes a logistic function
  %T. C. O'Haver, May 2006
global PEAKHEIGHTS AUTOZERO BIPOLAR LOGPLOT
A = zeros(length(t),round(length(lambda)/2;((
for j = 1:length(lambda)/2,
    A(:,j) = logistic(t,lambda(2*j-1),lambda(2*j;'((
end
if AUTOZERO==3,A=[ones(size(y))' A];end
if BIPOLAR,PEAKHEIGHTS=A\y';else PEAKHEIGHTS=abs(A\y');end
z = A*PEAKHEIGHTS;
if LOGPLOT,
    err = norm(log10(z)-log10(y;('(
else
    err = norm(z-y;('
end
---------------------------------------------------------------------  %
function g = logistic(x,pos,wid(
 %logistic function.  pos=position; wid=half-width (both scalar(
 %logistic(x,pos,wid), where x may be scalar, vector, or matrix
```

```
 %pos=position; wid=half-width (both scalar(
 %T. C. O'Haver, 1991
n = exp(-((x-pos)/(.477.*wid)) .^2;(
g = (2.*n)./(1+n;(
---------------------------------------------------------------------  %
function err = fittriangular(lambda,t,y(
%       Fitting function for triangular, lambda(1)=position, lambda(2)=width
%       between the data and the values computed by the current
%       function of lambda.  Fittriangular assumes a triangular function
  %T. C. O'Haver, May 2006
global PEAKHEIGHTS AUTOZERO BIPOLAR LOGPLOT
A = zeros(length(t),round(length(lambda)/2;((
for j = 1:length(lambda)/2,
    A(:,j) = triangular(t,lambda(2*j-1),lambda(2*j;'((
end
if AUTOZERO==3,A=[ones(size(y))' A];end
if BIPOLAR,PEAKHEIGHTS=A\y';else PEAKHEIGHTS=abs(A\y');end
z = A*PEAKHEIGHTS;
if LOGPLOT,
    err = norm(log10(z)-log10(y;('(
else
    err = norm(z-y;('
end
---------------------------------------------------------------------  %
function g = triangular(x,pos,wid(
%triangle function.  pos=position; wid=half-width (both scalar(
%trianglar(x,pos,wid), where x may be scalar or vector,
```

```
%pos=position; wid=half-width (both scalar(
 %T. C. O'Haver, 1991
 %Example
 %x=[0:.1:10];plot(x,trianglar(x,5.5,2.3('.',(
g=1-(1./wid) .*abs(x-pos;(
for i=1:length(x  ,(
if g(i)<0,g(i)=0;end
end
---------------------------------------------------------------------  %
function err = fitpearson(lambda,t,y,shapeconstant(
   %Fitting functions for a Pearson 7 band signal.
 %T. C. O'Haver (toh@umd.edu),   Version 1.3, October 23, 2006.
global PEAKHEIGHTS AUTOZERO BIPOLAR LOGPLOT
A = zeros(length(t),round(length(lambda)/2;((
for j = 1:length(lambda)/2,
    A(:,j) = pearson(t,lambda(2*j-1),lambda(2*j),shapeconstant;'(
end
if AUTOZERO==3,A=[ones(size(y))' A];end
if BIPOLAR,PEAKHEIGHTS=A\y';else PEAKHEIGHTS=abs(A\y');end
z = A*PEAKHEIGHTS;
if LOGPLOT,
    err = norm(log10(z)-log10(y;('(
else
    err = norm(z-y;('
end
---------------------------------------------------------------------  %
function err = fitpearsonv(lambda,t,y(
```

```
 %Fitting functions for pearson function with independently variable
 %percent Gaussian
 %T. C. O'Haver (toh@umd.edu), 2015.
global PEAKHEIGHTS AUTOZERO BIPOLAR LOGPLOT
A = zeros(length(t),round(length(lambda)/3;((
for j = 1:length(lambda)/3,
    A(:,j) = pearson(t,lambda(3*j-2),lambda(3*j-1),lambda(3*j;'((
end
if AUTOZERO==3,A=[ones(size(y))' A];end
if BIPOLAR,PEAKHEIGHTS=A\y';else PEAKHEIGHTS=abs(A\y');end
z = A*PEAKHEIGHTS;
if LOGPLOT,
    err = norm(log10(z)-log10(y;('(
else
    err = norm(z-y;('
end
-------------------------------------------------------------------  %
function g = pearson(x,pos,wid,m(
 %Pearson VII function .
 %g = pearson7(x,pos,wid,m) where x may be scalar, vector, or matrix
 %pos=position; wid=half-width (both scalar(
 %m=some number
  %T. C. O'Haver, 1990
g=ones(size(x))./(1+((x-pos)./((0.5.^(2/m)).*wid)).^2).^m;
-------------------------------------------------------------------  %
function err = fitexpgaussian(lambda,t,y,timeconstant(
   %Fitting functions for a exponentially-broadened Gaussian band signal.
```

```
  %T. C. O'Haver, October 23, 2006.
global PEAKHEIGHTS AUTOZERO BIPOLAR LOGPLOT
A = zeros(length(t),round(length(lambda)/2;((
for j = 1:length(lambda)/2,
    A(:,j) = expgaussian(t,lambda(2*j-1),lambda(2*j),timeconstant;(
end
if AUTOZERO==3,A=[ones(size(y))' A];end
if BIPOLAR,PEAKHEIGHTS=A\y';else PEAKHEIGHTS=abs(A\y');end
z = A*PEAKHEIGHTS;
if LOGPLOT,
    err = norm(log10(z)-log10(y;('(
else
    err = norm(z-y;('
end
---------------------------------------------------------------------  %
function err = fitexplorentzian(lambda,t,y,timeconstant(
   %Fitting functions for a exponentially-broadened lorentzian band signal.
  %T. C. O'Haver, 2013.
global PEAKHEIGHTS AUTOZERO BIPOLAR LOGPLOT
A = zeros(length(t),round(length(lambda)/2;((
for j = 1:length(lambda)/2,
    A(:,j) = explorentzian(t,lambda(2*j-1),lambda(2*j),timeconstant;(
end
if AUTOZERO==3,A=[ones(size(y))' A];end
if BIPOLAR,PEAKHEIGHTS=A\y';else PEAKHEIGHTS=abs(A\y');end
z = A*PEAKHEIGHTS;
if LOGPLOT,
```

```
    err = norm(log10(z)-log10(y;('(
else
    err = norm(z-y;('
end
---------------------------------------------------------------------  %
function err = fitexpewgaussian(lambda,t,y,timeconstant(
 %Fitting function for exponentially-broadened Gaussian bands with equal peak widths.
global PEAKHEIGHTS AUTOZERO BIPOLAR LOGPLOT
numpeaks=round(length(lambda)-1;(
A = zeros(length(t),numpeaks;(
for j = 1:numpeaks,
    A(:,j) = expgaussian(t,lambda(j),lambda(numpeaks+1),timeconstant;(
end
if AUTOZERO==3,A=[ones(size(y))' A];end
if BIPOLAR,PEAKHEIGHTS=A\y';else PEAKHEIGHTS=abs(A\y');end
z = A*PEAKHEIGHTS;
if LOGPLOT,
    err = norm(log10(z)-log10(y;('(
else
    err = norm(z-y;('
end
---------------------------------------------------------------------  %
function err = fitexpgaussianv(lambda,t,y(
 %Fitting functions for  exponentially-broadened Gaussians with
 %independently variable time constants
 %T. C. O'Haver (toh@umd.edu), 2015.
global PEAKHEIGHTS AUTOZERO BIPOLAR LOGPLOT
```

```
A = zeros(length(t),round(length(lambda)/3;((
for j = 1:length(lambda)/3,
    A(:,j) = expgaussian(t,lambda(3*j-2),lambda(3*j-1),-lambda(3*j;'((
end
if AUTOZERO==3,A=[ones(size(y))' A];end
if BIPOLAR,PEAKHEIGHTS=A\y';else PEAKHEIGHTS=abs(A\y');end
z = A*PEAKHEIGHTS;
if LOGPLOT,
    err = norm(log10(z)-log10(y;('(
else
    err = norm(z-y;('
end
---------------------------------------------------------------------  %
function g = expgaussian(x,pos,wid,timeconstant(
  %Exponentially-broadened gaussian(x,pos,wid) = gaussian peak centered on pos, half-width=wid
  %x may be scalar, vector, or matrix, pos and wid both scalar
  %T. C. O'Haver, 2006
g = exp(-((x-pos)./(0.6005615.*wid)) .^2;(
g = ExpBroaden(g',timeconstant;(
---------------------------------------------------------------------  %
function g = explorentzian(x,pos,wid,timeconstant(
  %Exponentially-broadened lorentzian(x,pos,wid) = lorentzian peak centered on pos, half-
width=wid
  %x may be scalar, vector, or matrix, pos and wid both scalar
  %T. C. O'Haver, 2013
g = ones(size(x))./(1+((x-pos)./(0.5.*wid)).^2;(
g = ExpBroaden(g',timeconstant;(
---------------------------------------------------------------------  %
```

```
function yb = ExpBroaden(y,t(
 %ExpBroaden(y,t) zero pads y and convolutes result by an exponential decay
 %of time constant t by multiplying Fourier transforms and inverse
 %transforming the result.
hly=round(length(y)./2;(
ey=[y(1).*ones(1,hly)';y;y(length(y)).*ones(1,hly;['(
 %figure(2);plot(ey);figure(1;(
fy=fft(ey;(
a=exp(-(1:length(fy))./t;(
fa=fft(a;(
fy1=fy.*fa;'
ybz=real(ifft(fy1))./sum(a;(
yb=ybz(hly+2:length(ybz)-hly+1;(
---------------------------------------------------------------- %
function err = fitexppulse(tau,x,y(
 %Iterative fit of the sum of exponential pulses
 %of the form Height.*exp(-tau1.*x).*(1-exp(-tau2.*x(((
global PEAKHEIGHTS AUTOZERO BIPOLAR LOGPLOT
A = zeros(length(x),round(length(tau)/2;((
for j = 1:length(tau)/2,
    A(:,j) = exppulse(x,tau(2*j-1),tau(2*j;((
end
if AUTOZERO==3,A=[ones(size(y))' A];end
if BIPOLAR,PEAKHEIGHTS=A\y';else PEAKHEIGHTS=abs(A\y');end
z = A*PEAKHEIGHTS;
if LOGPLOT,
    err = norm(log10(z)-log10(y;('(
```

```
else
    err = norm(z-y;('
end
---------- %
function g = exppulse(x,t1,t2(
 %Exponential pulse of the form
 %g = (x-spoint)./pos.*exp(1-(x-spoint)./pos;(
e=(x-t1)./t2;
p = 4*exp(-e).*(1-exp(-e;((
p=p .* (p>0;(
g = p;'
---------- %
function err = fitalphafunction(tau,x,y(
 %Iterative fit of the sum of alpha funciton
 %of the form Height.*exp(-tau1.*x).*(1-exp(-tau2.*x(((
global PEAKHEIGHTS AUTOZERO BIPOLAR LOGPLOT
A = zeros(length(x),round(length(tau)/2;((
for j = 1:length(tau)/2,
    A(:,j) = alphafunction(x,tau(2*j-1),tau(2*j;((
end
if AUTOZERO==3,A=[ones(size(y))' A];end
if BIPOLAR,PEAKHEIGHTS=A\y';else PEAKHEIGHTS=abs(A\y');end
z = A*PEAKHEIGHTS;
if LOGPLOT,
    err = norm(log10(z)-log10(y;('(
else
    err = norm(z-y;('
```

```
end
---------------------------------------------------------------------  %
function g = alphafunction(x,pos,spoint(
 %alpha function.  pos=position; wid=half-width (both scalar(
 %alphafunction(x,pos,wid), where x may be scalar, vector, or matrix
 %pos=position; wid=half-width (both scalar(
 %Taekyung Kwon, July 2013
g = (x-spoint)./pos.*exp(1-(x-spoint)./pos;(
for m=1:length(x);if g(m)<0;g(m)=0;end;end
---------------------------------------------------------------------  %
function err = fitdownsigmoid(tau,x,y(
 %Fitting function for iterative fit to the sum of
 %downward moving sigmiods
global PEAKHEIGHTS AUTOZERO BIPOLAR LOGPLOT
A = zeros(length(x),round(length(tau)/2;((
for j = 1:length(tau)/2,
    A(:,j) = downsigmoid(x,tau(2*j-1),tau(2*j;((
end
if AUTOZERO==3,A=[ones(size(y))' A];end
if BIPOLAR,PEAKHEIGHTS=A\y';else PEAKHEIGHTS=abs(A\y');end
z = A*PEAKHEIGHTS;
if LOGPLOT,
    err = norm(log10(z)-log10(y;('(
else
    err = norm(z-y;('
end
---------------------------------------------------------------------  %
function err = fitupsigmoid(tau,x,y(
```

```
 %Fitting function for iterative fit to the sum of
 %upwards moving sigmiods
global PEAKHEIGHTS AUTOZERO BIPOLAR LOGPLOT
A = zeros(length(x),round(length(tau)/2;((
for j = 1:length(tau)/2,
    A(:,j) = upsigmoid(x,tau(2*j-1),tau(2*j;((
end
if AUTOZERO==3,A=[ones(size(y))' A];end
if BIPOLAR,PEAKHEIGHTS=A\y';else PEAKHEIGHTS=abs(A\y');end
z = A*PEAKHEIGHTS;
if LOGPLOT,
    err = norm(log10(z)-log10(y;('(
else
    err = norm(z-y;('
end
---------------------------------------------------------------------  %
function g=downsigmoid(x,t1,t2(
 % down step sigmoid
g=.5-.5*erf(real((x-t1)/sqrt(2*t2;(((
---------------------------------------------------------------------  %
function g=upsigmoid(x,t1,t2(
 %up step sigmoid
g=1/2 + 1/2* erf(real((x-t1)/sqrt(2*t2 ;(((
---------------------------------------------------------------------  %
function err = fitGL(lambda,t,y,shapeconstant(
   %Fitting functions for Gaussian/Lorentzian blend.
 %T. C. O'Haver (toh@umd.edu), 2012.
global PEAKHEIGHTS AUTOZERO BIPOLAR LOGPLOT
```

```
A = zeros(length(t),round(length(lambda)/2;((
for j = 1:length(lambda)/2,
    A(:,j) = GL(t,lambda(2*j-1),lambda(2*j),shapeconstant;'(
end
if AUTOZERO==3,A=[ones(size(y))' A];end
if BIPOLAR,PEAKHEIGHTS=A\y';else PEAKHEIGHTS=abs(A\y');end
z = A*PEAKHEIGHTS;
if LOGPLOT,
    err = norm(log10(z)-log10(y;('(
else
    err = norm(z-y;('
end
---------- ---------- %
function err = fitGLv(lambda,t,y(
 %Fitting functions for Gaussian/Lorentzian blend function with
 %independently variable percent Gaussian
 %T. C. O'Haver (toh@umd.edu), 2015.
global PEAKHEIGHTS AUTOZERO BIPOLAR LOGPLOT
A = zeros(length(t),round(length(lambda)/3;((
for j = 1:length(lambda)/3,
    A(:,j) = GL(t,lambda(3*j-2),lambda(3*j-1),lambda(3*j;'((
end
if AUTOZERO==3,A=[ones(size(y))' A];end
if BIPOLAR,PEAKHEIGHTS=A\y';else PEAKHEIGHTS=abs(A\y');end
z = A*PEAKHEIGHTS;
if LOGPLOT,
    err = norm(log10(z)-log10(y;('(
```

```
else
    err = norm(z-y;('
end
------------------------------------------------------------------  %
function g = GL(x,pos,wid,m(
 %Gaussian/Lorentzian blend. m = percent Gaussian character
 %pos=position; wid=half-width
 %m = percent Gaussian character.
  %T. C. O'Haver, 2012
 %sizex=size(x(
 %sizepos=size(pos(
 %sizewid=size(wid(
 %sizem=size(m(
g=2.*((m/100).*gaussian(x,pos,wid)+(1-(m(1)/100)).*lorentzian(x,pos,wid))/2;
------------------------------------------------------------------  %
function err = fitvoigt(lambda,t,y,shapeconstant(
 %Fitting functions for Voigt profile function
 %T. C. O'Haver (toh@umd.edu), 2013.
global PEAKHEIGHTS AUTOZERO BIPOLAR LOGPLOT
A = zeros(length(t),round(length(lambda)/2;((
for j = 1:length(lambda)/2,
    A(:,j) = voigt(t,lambda(2*j-1),lambda(2*j),shapeconstant;'(
end
if AUTOZERO==3,A=[ones(size(y))' A];end
if BIPOLAR,PEAKHEIGHTS=A\y';else PEAKHEIGHTS=abs(A\y');end
z = A*PEAKHEIGHTS;
if LOGPLOT,
```

```
    err = norm(log10(z)-log10(y;('(
else
    err = norm(z-y;('
end
---------------------------------------------------------------------  %
function err = fitvoigtv(lambda,t,y(
 %Fitting functions for Voigt profile function with independently variable
 %alphas
 %T. C. O'Haver (toh@umd.edu), 2015.
global PEAKHEIGHTS AUTOZERO BIPOLAR LOGPLOT
A = zeros(length(t),round(length(lambda)/3;((
for j = 1:length(lambda)/3,
    A(:,j) = voigt(t,lambda(3*j-2),lambda(3*j-1),lambda(3*j;'((
end
if AUTOZERO==3,A=[ones(size(y))' A];end
if BIPOLAR,PEAKHEIGHTS=A\y';else PEAKHEIGHTS=abs(A\y');end
z = A*PEAKHEIGHTS;
if LOGPLOT,
    err = norm(log10(z)-log10(y;('(
else
    err = norm(z-y;('
end
---------------------------------------------------------------------  %
function g=voigt(xx,pos,gD,alpha(
 %Voigt profile function. xx is the independent variable (energy,
 %wavelength, etc), gD is the Doppler (Gaussian) width, and alpha is the
 %shape constant (ratio of the Lorentzian width gL to the Doppler width gD.
```

```
 %Based on Chong Tao's "Voigt lineshape spectrum simulation ,"

 %File ID: #26707

 %alpha=alpha

gL=alpha.*gD;

gV = 0.5346*gL + sqrt(0.2166*gL.^2 + gD.^2;(

x = gL/gV;

y = abs(xx-pos)/gV;

g = 1/(2*gV*(1.065 + 0.447*x + 0.058*x^2))*((1-x)*exp(-0.693.*y.^2) + (x./(1+y.^2)) + 0.016*(1-
x)*x*(exp(-0.0841.*y.^2.25)-1./(1 + 0.021.*y.^2.25;(((

g=g./max(g;(

---------------------------------------------------------------------  %

function err = fitBiGaussian(lambda,t,y,shapeconstant(

   %Fitting functions for BiGaussian.

 %T. C. O'Haver (toh@umd.edu),  2012.

global PEAKHEIGHTS AUTOZERO BIPOLAR LOGPLOT

A = zeros(length(t),round(length(lambda)/2;((

for j = 1:length(lambda)/2,

    A(:,j) = BiGaussian(t,lambda(2*j-1),lambda(2*j),shapeconstant;'(

end

if AUTOZERO==3,A=[ones(size(y))' A];end

if BIPOLAR,PEAKHEIGHTS=A\y';else PEAKHEIGHTS=abs(A\y');end

z = A*PEAKHEIGHTS;

if LOGPLOT,

    err = norm(log10(z)-log10(y;('(

else

    err = norm(z-y;('

end

---------------------------------------------------------------------  %
```

```
function g = BiGaussian(x,pos,wid,m(
 %BiGaussian (different widths on leading edge and trailing edge.(
 %pos=position; wid=width
 %m determines shape; symmetrical if m=50.
  %T. C. O'Haver, 2012
lx=length(x;(
hx=val2ind(x,pos;(
g(1:hx)=gaussian(x(1:hx),pos,wid*(m/100;((
g(hx+1:lx)=gaussian(x(hx+1:lx),pos,wid*(1-m/100;((
---------------------------------------------------------------------  %
function err = fitBWF(lambda,t,y,shapeconstant(
   %Fitting function for Breit-Wigner-Fano.
 %T. C. O'Haver (toh@umd.edu),  2014.
global PEAKHEIGHTS AUTOZERO BIPOLAR LOGPLOT
A = zeros(length(t),round(length(lambda)/2;((
for j = 1:length(lambda)/2,
    A(:,j) = BWF(t,lambda(2*j-1),lambda(2*j),shapeconstant;'(
end
if AUTOZERO==3,A=[ones(size(y))' A];end
if BIPOLAR,PEAKHEIGHTS=A\y';else PEAKHEIGHTS=abs(A\y');end
z = A*PEAKHEIGHTS;
if LOGPLOT,
    err = norm(log10(z)-log10(y;('(
else
    err = norm(z-y;('
end
---------------------------------------------------------------------  %
```

```
function g = BWF(x,pos,wid,m(
 %BWF (Breit-Wigner-Fano) http://en.wikipedia.org/wiki/Fano_resonance
 %pos=position; wid=width; m=Fano factor
  %T. C. O'Haver, 2014
y=((m*wid/2+x-pos).^2)./(((wid/2).^2)+(x-pos).^2;(
 %y=((1+(x-pos./(m.*wid))).^2)./(1+((x-pos)./wid).^2;(
g=y./max(y;(
---------------------------------------------------------------------  %
function err = fitnbinpdf(tau,x,y(
 %Fitting function for iterative fit to the sum of
 %Negative Binomial Distributions
) %http://www.mathworks.com/help/stats/negative-binomial-distribution.html(
global PEAKHEIGHTS AUTOZERO BIPOLAR LOGPLOT
A = zeros(length(x),round(length(tau)/2;((
for j = 1:length(tau)/2,
    A(:,j) = nbinpdf(x,tau(2*j-1),tau(2*j;((
end
if AUTOZERO==3,A=[ones(size(y))' A];end
if BIPOLAR,PEAKHEIGHTS=A\y';else PEAKHEIGHTS=abs(A\y');end
z = A*PEAKHEIGHTS;
if LOGPLOT,
    err = norm(log10(z)-log10(y;('(
else
    err = norm(z-y;('
end
---------------------------------------------------------------------  %
function err = fitlognpdf(tau,x,y(
```

```
 %Fitting function for iterative fit to the sum of
 %Lognormal Distributions
) %http://www.mathworks.com/help/stats/lognormal-distribution.html(
global PEAKHEIGHTS AUTOZERO BIPOLAR LOGPLOT
A = zeros(length(x),round(length(tau)/2;((
for j = 1:length(tau)/2,
    A(:,j) = lognormal(x,tau(2*j-1),tau(2*j;((
end
if AUTOZERO==3,A=[ones(size(y))' A];end
if BIPOLAR,PEAKHEIGHTS=A\y';else PEAKHEIGHTS=abs(A\y');end
z = A*PEAKHEIGHTS;
if LOGPLOT,
    err = norm(log10(z)-log10(y;('(
else
    err = norm(z-y;('
end
---------------------------------------------------------------------  %
function g = lognormal(x,pos,wid(
 %lognormal function.  pos=position; wid=half-width (both scalar(
 %lognormal(x,pos,wid), where x may be scalar, vector, or matrix
 %pos=position; wid=half-width (both scalar(
 %T. C. O'Haver, 1991
g = exp(-(log(x/pos)/(0.01.*wid)) .^2;(
---------------------------------------------------------------------  %
function err = fitsine(tau,x,y(
 %Fitting function for iterative fit to the sum of
 %sine waves (alpha test, NRFPT(
```

```
global PEAKHEIGHTS AUTOZERO BIPOLAR LOGPLOT
A = zeros(length(x),round(length(tau)/2;((
for j = 1:length(tau)/2,
    A(:,j) = sine(x,tau(2*j-1),tau(2*j;((
end
if AUTOZERO==3,A=[ones(size(y))' A];end
if BIPOLAR,PEAKHEIGHTS=A\y';else PEAKHEIGHTS=abs(A\y');end
z = A*PEAKHEIGHTS;
if LOGPLOT,
    err = norm(log10(z)-log10(y;('(
else
    err = norm(z-y;('
end
---------------------------------------------------------------------  %
function g=sine(x,f,phase (
 %Sine wave (alpha test(
g=sin(2*pi*f*(x+phase;((
---------------------------------------------------------------------  %
function err = fitd1gauss(lambda,t,y(
   %Fitting functions for the first derivative of a Gaussian
  %T. C. O'Haver, 2014
global PEAKHEIGHTS AUTOZERO BIPOLAR
A = zeros(length(t),round(length(lambda)/2;((
for j = 1:length(lambda)/2,
    A(:,j) = d1gauss(t,lambda(2*j-1),lambda(2*j;'((
end
if AUTOZERO==3,A=[ones(size(y))' A];end
```

```
if BIPOLAR,PEAKHEIGHTS=A\y';else PEAKHEIGHTS=abs(A\y');end
z = A*PEAKHEIGHTS;
err = norm(z-y;('
---------------------------------------------------------------------  %
function y=d1gauss(x,p,w(
 %First derivative of Gaussian (alpha test(
y=-(5.54518.*(x-p).*exp(-(2.77259.*(p-x).^2)./w^2))./w.^2;
y=y./max(y;(
---------------------------------------------------------------------  %
function coeff = fitpolynomial(t,y,order(
coeff=polyfit(t,y,order;(
 %order=order
 %coeff=coeff
---------------------------------------------------------------------  %
function y=polynomial(t,coeff(
y=polyval(coeff,t;(
---------------------------------------------------------------------  %
function err = fitsegmented(lambda,t,y(
   %Fitting functions for articulated segmented linear
  %T. C. O'Haver, 2014
global LOGPLOT
breakpoints=[t(1) lambda max(t;[(
z = segmented(t,y,breakpoints;(
 %lengthz=length(z;(
if LOGPLOT,
    err = norm(log10(z)-log10(y;('(
else
    err = norm(z-y;(
```

```
end
---------------------------------------------------------------------  %
function yi=segmented(x,y,segs(
global PEAKHEIGHTS
clear yy
for n=1:length(segs(
  yind=val2ind(x,segs(n;((
  yy(n)=y(yind(1;((
end
yi=INTERP1(segs,yy,x;(
PEAKHEIGHTS=segs;
---------------------------------------------------------------------  %
function err = fitlinslope(tau,x,y(
 %Fitting function for iterative fit to linear function
global PEAKHEIGHTS AUTOZERO BIPOLAR LOGPLOT
A = zeros(length(x),round(length(tau)/2;((
for j = 1:length(tau)/2,
    z = (x.*tau(2*j-1)+tau(2*j;'((
    A(:,j) = z./max(z;(
end
if AUTOZERO==3,A=[ones(size(y))' A];end
if BIPOLAR,PEAKHEIGHTS=A\y';else PEAKHEIGHTS=abs(A\y');end
z = A*PEAKHEIGHTS;
if LOGPLOT,
    err = norm(log10(z)-log10(y;('(
else
    err = norm(z-y;('
```

```
end
---------------------------------------------------------------------  %
function y=linslope(x,slope,intercept(
y=x.*slope+intercept;
 %y=y./max(y;(
---------------------------------------------------------------------  %
function b=iqr(a(
 %b = IQR(a)  returns the interquartile range of the values in a.  For
  %vector input, b is the difference between the 75th and 25th percentiles
  %of a.  For matrix input, b is a row vector containing the interquartile
  %range of each column of a.
  %T. C. O'Haver, 2012
mina=min(a;(
sizea=size(a;(
NumCols=sizea(2;(
for n=1:NumCols,b(:,n)=a(:,n)-mina(n);end
Sorteda=sort(b;(
lx=length(Sorteda;(
SecondQuartile=round(lx/4;(
FourthQuartile=3*round(lx/4;(
b=abs(Sorteda(FourthQuartile,:)-Sorteda(SecondQuartile;((:,
---------------------------------------------------------------------  %
function err = fitmultiple(lambda,t,y,shapesvector,m(
 %Fitting function for a multiple-shape band signal.
 %The sequence of peak shapes are defined by the vector "shape."
 %The vector "m" determines the shape of variable-shape peaks.
global PEAKHEIGHTS AUTOZERO BIPOLAR LOGPLOT coeff
numpeaks=round(length(lambda)/2;(
```

```
A = zeros(length(t),numpeaks;(
for j = 1:numpeaks,
    if shapesvector(j)==28,
        coeff=polyfit(t,y,m(j;((
        A(:,j) = polyval(coeff,t;(
    else
        A(:,j) = peakfunction(shapesvector(j),t,lambda(2*j-1),lambda(2*j),m(j;'((
    end
end
if AUTOZERO==3,A=[ones(size(y))' A];end
if BIPOLAR,PEAKHEIGHTS=A\y';else PEAKHEIGHTS=abs(A\y');end
z = A*PEAKHEIGHTS;
if LOGPLOT,
    err = norm(log10(z)-log10(y;('(
else
    err = norm(z-y;('
end
---------------------------------------------------------------------  %
function p=peakfunction(shape,x,pos,wid,m,coeff(
 %function that generates any of 20 peak types specified by number. 'shape'
 %specifies the shape type of each peak in the signal: "peakshape" = 1-20.
=١ %Gaussian 2=Lorentzian, 3=logistic, 4=Pearson, 5=exponentionally
 %broadened Gaussian; 9=exponential pulse, 10=up sigmoid,
=١٣ %Gaussian/Lorentzian blend; 14=BiGaussian, 15=Breit-Wigner-Fano (BWF, (
=١٨ %exponentionally broadened Lorentzian; 19=alpha function; 20=Voigt
 %profile; 21=triangular; 23=down sigmoid; 25=lognormal. "m" is required
 %for variable-shape peaks only.
```

```
switch shape,
    case 1
        p=gaussian(x,pos,wid;(
    case 2
        p=lorentzian(x,pos,wid;(
    case 3
        p=logistic(x,pos,wid;(
    case 4
        p=pearson(x,pos,wid,m;(
    case 5
        p=expgaussian(x,pos,wid,m;(
    case 6
        p=gaussian(x,pos,wid;(
    case 7
        p=lorentzian(x,pos,wid;(
    case 8
        p=expgaussian(x,pos,wid,m;'(
    case 9
        p=exppulse(x,pos,wid;(
    case 10
        p=upsigmoid(x,pos,wid;(
    case 11
        p=gaussian(x,pos,wid;(
    case 12
        p=lorentzian(x,pos,wid;(
    case 13
        p=GL(x,pos,wid,m;(
```

```
case 14
    p=BiGaussian(x,pos,wid,m;(
case 15
    p=BWF(x,pos,wid,m;(
case 16
    p=gaussian(x,pos,wid;(
case 17
    p=lorentzian(x,pos,wid;(
case 18
    p=explorentzian(x,pos,wid,m;'(
case 19
    p=alphafunction(x,pos,wid;(
case 20
    p=voigt(x,pos,wid,m;(
case 21
    p=triangular(x,pos,wid     ;(
case 23
    p=downsigmoid(x,pos,wid;(
case 25
    p=lognormal(x,pos,wid;(
case 26
    p=linslope(x,pos,wid;(
case 27
    p=d1gauss(x,pos,wid;(
case 28
    p=polynomial(x,coeff;(
otherwise
```

```
end % switch
```