curvefit

1.0.0

Generated by Doxygen 1.8.11

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1 Main Page

1.1 Introduction

CURVEFIT is a library for fitting functions to sets of data.

Author

Jason Christopherson

Version

1.0.0

2 Modules Index

2.1 Modules List

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3 Data Type Index

3.1 Class Hierarchy

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5 Module Documentation

5.1 curvefit_c_binding Module Reference

curvefit_c_binding

Data Types

• type c_linear_interp

A C compatible type encapsulating a linear_interp object.

• type c_lowess_smoothing

A C compatible type encapsulating a lowess_smoothing object.

• type c_nonlinear_regression

A C compatible type encapsulating a nonlinear_regression object.

• type c_polynomial_interp

A C compatible type encapsulating a polynomial_interp object.

• type c_spline_interp

A C compatible type encapsulating a spline_interp object.

• type cnonlin_reg_helper

A type for helping to interface between a C function pointer, and the nonlinear_regression type.

• interface creg_fcn

Describes a routine for finding the coefficients of a function of one variable.

Functions/Subroutines

• pure logical(c_bool) function is_monotonic_c (n, x)

Tests to see if an array is montonically increasing or decreasing.

• subroutine get_linear_interp (obj, li)

Retrieves the linear_interp object from the C compatible c_linear_interp data structure.

• subroutine lininterp_init_c (obj, n, x, y, err)

Initializes a new c_linear_interp object.

• subroutine lininterp free c (obj)

Frees resources held by a c_linear_interp object.

• subroutine lininterp_interp_c (obj, n, x, y)

Performs a linear interpolation to determine the points y that for the requested indendent variable values in x.

integer(i32) function lininterp_get_pt_count_c (obj)

Gets the number of points used by the interpolation object.

subroutine lininterp_get_pts_c (obj, n, x, y)

Gets a copy of the data points stored by the interpolation object.

subroutine get_polynomial_interp (obj, interp)

Retrieves the polynomial_interp object from the C compatible c_polynomial_interp data structure.

• subroutine polyinterp_init_c (obj, n, x, y, order, err)

Initializes a new c_polynomial_interp object.

• subroutine polyinterp_free_c (obj)

Frees resources held by a c_polynomial_interp object.

• subroutine polyinterp_interp_c (obj, n, x, y)

Performs a polynomial interpolation to determine the points y that for the requested indendent variable values in x.

• integer(i32) function polyinterp_get_pt_count_c (obj)

Gets the number of points used by the interpolation object.

• subroutine polyinterp_get_pts_c (obj, n, x, y)

Gets a copy of the data points stored by the interpolation object.

• subroutine get_spline_interp (obj, interp)

Retrieves the spline interp object from the C compatible c spline interp data structure.

• subroutine splineinterp init c (obj, n, x, y, ibcbeg, ybcbeg, ibcend, ybcend, err)

Initializes a new c_spline_interp object.

subroutine splineinterp_free_c (obj)

Frees resources held by a c_spline_interp object.

• subroutine splineinterp_interp_c (obj, n, x, y)

Performs a spline interpolation to determine the points y that for the requested indendent variable values in x.

integer(i32) function splineinterp_get_pt_count_c (obj)

Gets the number of points used by the interpolation object.

• subroutine splineinterp_get_pts_c (obj, n, x, y)

Gets a copy of the data points stored by the interpolation object.

• subroutine splineinterp_diff1_c (obj, n, x, y)

Computes the interpolated first derivative.

• subroutine splineinterp_diff2_c (obj, n, x, y)

Computes the interpolated second derivative.

• pure real(dp) function mean c (n, x)

Computes the mean of a data set.

real(dp) function median_c (n, x, srt)

Computes the median of a data set.

• pure real(dp) function variance c (n, x)

Computes the sample variance of a data set.

subroutine covariance_c (m, n, x, c, err)

Computes the covariance matrix of N data sets of M observations.

pure real(dp) function stdev_c (n, x)

Computes the corrected standard deviation of a data set.

real(dp) function conf int c (n, x, alpha, use t, err)

Computes the confidence interval based upon a standard normal distribution.

subroutine moving_average_c (n, x, npts, err)

Applies a moving average to smooth a data set.

real(dp) function linlsq_1var_c (n, x, y, err)

Employs a least squares fit to determine the coefficient A in the linear system: Y = A * X.

subroutine linlsq_nvar_c (m, n, npts, x, y, a, err)

Employs a least squares fit to determine the coefficient A in the linear system: Y = A * X.

• subroutine get_lowess_smoothing (obj, ptr)

Retrieves the lowess_smoothing object from the C compatible c_lowess_smoothing data structure.

• subroutine lowess_init_c (obj, n, x, y, srt, err)

Initializes a new c_lowess_smoothing object.

• subroutine lowess free c (obj)

Frees resources held by a c_lowess_smoothing object.

• subroutine lowess_smooth_c (obj, f, n, y, err)

Performs the actual smoothing operation.

integer(i32) function lowess get pt count c (obj)

Gets the number of points used by the lowess_smoothing object.

subroutine lowess_get_pts_c (obj, n, x, y)

Gets a copy of the data points stored by the lowess smoothing object.

subroutine lowess_get_residual_c (obj, n, x)

Gets the residuals from each data point.

• subroutine get_nonlinear_regression (obj, ptr)

Retrieves the cnonlin_reg_helper object from the C compatible c_nonlinear_regression data structure.

• subroutine nlr_init_c (obj, n, x, y, fcn, ncoeff, err)

Initializes a new c_nonlinear_regression object.

• subroutine nlr free c (obj)

Frees resources held by a c_nonlinear_regression object.

• subroutine nlr solve c (obj, n, c, ib, err)

Computes the solution to the nonlinear regression problem using the Levenberg-Marquardt method.

• integer(i32) function nlr_get_pt_count_c (obj)

Gets the number of points used by the c_nonlinear_regression object.

• subroutine nlr_get_pts_c (obj, n, x, y)

Gets a copy of the data points stored by the c_nonlinear_regression object.

• subroutine nlr_get_solver_params_c (obj, cntrl)

Gets the nonlinear regression solver solution control parameters.

subroutine nlr_set_solver_params_c (obj, cntrl)

Sets the nonlinear regression solver solution control parameters.

• subroutine crh_fcn (this, x, f)

Computes the residual between the supplied data set, and the function value given a set of coefficients.

pure logical function crh_is_fcn_defined (this)

Tests if the pointer to the function containing the equation to solve has been assigned.

• subroutine crh_set_fcn (this, fcn)

Establishes a pointer to the routine containing the equations to solve.

• subroutine seb_c (n, applied, output, fullscale, rst, err)

Computes the static error band of a data set.

real(dp) function nonlin_c (n, applied, measured)

Computes the best-fit nonlinearity of a data set.

• real(dp) function term_nonlin_c (n, applied, measured)

Computes the terminal nonlinearity of a data set.

real(dp) function hysteresis_c (n, applied, measured)

Computes the hysteresis in an ascending/descending data set.

real(dp) function rtz_c (n, applied, measured, tol)

Computes the return to zero error in an ascending/descending data set.

real(dp) function repeat_c (npts, ntests, applied, measured)

Computes the repeatability of a sequence of tests.

• subroutine xtalk_c (npts, ndof, xerr, indices, xt, err)

Computes the crosstalk errors for a multiple degree-of-freedom data set.

• subroutine split_c (n, x, na, ascend, nd, descend, nascend, ndescend, err)

Splits a data set into ascending and descending components.

5.1.1 Detailed Description

curvefit_c_binding

Purpose

Provides C bindings to the curvefit library.

5.1.2 Function/Subroutine Documentation

5.1.2.1 real(dp) function curvefit_c_binding::conf_int_c (integer(i32), intent(in), value *n*, real(dp), dimension(n), intent(in) *x*, real(dp), intent(in), value *alpha*, logical(c_bool), intent(in), value *use_t*, type(errorhandler), intent(inout) *err*)

Computes the confidence interval based upon a standard normal distribution.

Parameters

in	n	The number of data points.
in	X	An N-element array containing the data set.
in	alpha	The confidence level. This value must lie between zero and one such that: $0 < alpha < 1$.
in	use⇔	Set to true to use the t-distribution in the event of an unknown true standard deviation;
	_t	else, set to true to use a normal distribution.
in,out	err	The errorhandler object. If no error handling is desired, simply pass NULL, and errors will be dealt with by the default internal error handler. Possible errors that may be encountered are as follows.
		• CF_INVALID_INPUT_ERROR: Occurs if alpha is does not satisfy: 0 < alpha < 1.

Returns

The confidence interval as the deviation from the mean.

Remarks

The confidence interval, assuming a standard normal distribution, is as follows: mu + /- z * s / sqrt(n), where mu = the mean, and s = the standard deviation. This routine computes the z * s / sqrt(n) portion leaving the computation of the mean to the user.

Definition at line 847 of file curvefit_c_binding.f90.

5.1.2.2 subroutine curvefit_c_binding::covariance_c (integer(i32), intent(in), value *m*, integer(i32), intent(in), value *n*, real(dp), dimension(m,n), intent(in) *x*, real(dp), dimension(n,n), intent(out) *c*, type(errorhandler), intent(inout) *err*)

Computes the covariance matrix of N data sets of M observations.

Parameters

in	m	The number of observations.
in	n	The number of data sets.
in	X	The M-by-N matrix of data.
out	С	The N-by-N matrix where the resulting covariance matrix will be written.
in,out	err	The errorhandler object. If no error handling is desired, simply pass NULL, and errors will be dealt with by the default internal error handler. Possible errors that may be encountered are as follows. • CF OUT OF MEMORY ERROR: Occurs if there is insufficient memory available.
		CF_OUT_OF_MEMORY_ERROR: Occurs if there is insufficient memory available.

Definition at line 788 of file curvefit_c_binding.f90.

5.1.2.3 subroutine curvefit_c_binding::crh_fcn (class(cnonlin_reg_helper), intent(in) this, real(dp), dimension(:), intent(in) x, real(dp), dimension(:), intent(out) f)

Computes the residual between the supplied data set, and the function value given a set of coefficients.

Parameters

=	in	this	The cnonlin_reg_helper object.
-	in	Χ	An N-element array containing the N coefficients.
	out	f	An M-element array that, on output, contains the residual at each of the M data points.

Definition at line 1474 of file curvefit_c_binding.f90.

5.1.2.4 pure logical function curvefit_c_binding::crh_is_fcn_defined (class(cnonlin_reg_helper), intent(in) this)

Tests if the pointer to the function containing the equation to solve has been assigned.

Parameters

in	this	The cnonlin_reg_helper object.
----	------	--------------------------------

Returns

Returns true if the pointer has been assigned; else, false.

Definition at line 1497 of file curvefit_c_binding.f90.

5.1.2.5 subroutine curvefit_c_binding::crh_set_fcn (class(cnonlin_reg_helper), intent(inout) this, procedure(creg_fcn), intent(in), pointer fcn)

Establishes a pointer to the routine containing the equations to solve.

Parameters

in,out	this	The cnonlin_reg_helper object.
in	fcn	The function pointer.

Definition at line 1509 of file curvefit_c_binding.f90.

5.1.2.6 subroutine curvefit_c_binding::get_linear_interp (type(c_linear_interp), intent(in), target *obj*, type(linear_interp), intent(out), pointer *li*)

Retrieves the linear_interp object from the C compatible c_linear_interp data structure.

Parameters

in	obj	The C compatible c_linear_interp object.
out	li	A pointer to the resulting linear_interp object. This pointer can be NULL dependent upon the state
		of obj.

Definition at line 138 of file curvefit_c_binding.f90.

5.1.2.7 subroutine curvefit_c_binding::get_lowess_smoothing (type(c_lowess_smoothing), intent(in), target *obj,* type(lowess_smoothing), intent(out), pointer *ptr*)

Retrieves the lowess_smoothing object from the C compatible c_lowess_smoothing data structure.

Parameters

in	obj	The C compatible c_lowess_smoothing object.
out	ptr	A pointer to the resulting lowess_smoothing object. This pointer can be NULL dependent upon
		the state of obj.

Definition at line 1005 of file curvefit_c_binding.f90.

5.1.2.8 subroutine curvefit_c_binding::get_nonlinear_regression (type(c_nonlinear_regression), intent(in), target *obj,* type(cnonlin_reg_helper), intent(out), pointer *ptr*)

Retrieves the cnonlin_reg_helper object from the C compatible c_nonlinear_regression data structure.

Parameters

in	obj	The C compatible c_nonlinear_regression object.
out	ptr	A pointer to the resulting cnonlin_reg_helper object. This pointer can be NULL dependent upon
		the state of obj.

Definition at line 1221 of file curvefit_c_binding.f90.

5.1.2.9 subroutine curvefit_c_binding::get_polynomial_interp (type(c_polynomial_interp), intent(in), target *obj,* type(polynomial_interp), intent(out), pointer *interp*)

Retrieves the polynomial_interp object from the C compatible c_polynomial_interp data structure.

Parameters

in	obj	The C compatible c_polynomial_interp object.
out	interp	A pointer to the resulting polynomial_interp object. This pointer can be NULL dependent upon
		the state of obj.

Definition at line 307 of file curvefit_c_binding.f90.

5.1.2.10 subroutine curvefit_c_binding::get_spline_interp (type(c_spline_interp), intent(in), target *obj*, type(spline_interp), intent(out), pointer *interp*)

Retrieves the spline_interp object from the C compatible c_spline_interp data structure.

Parameters

in	obj	The C compatible c_spline_interp object.
out	interp	A pointer to the resulting spline_interp object. This pointer can be NULL dependent upon the
		state of obj.

Definition at line 478 of file curvefit_c_binding.f90.

5.1.2.11 real(dp) function curvefit_c_binding::hysteresis_c (integer(i32), intent(in), value *n*, real(dp), dimension(n), intent(in) applied, real(dp), dimension(n), intent(in) measured)

Computes the hysteresis in an ascending/descending data set.

Parameters

in	n	The number of data points.	
in	applied	An N-element array containing the values applied to the measurement instrument.	
in	measured	An N-element array containing the calibrated output of the instrument as a result of the values given in applied.	

Returns

The hysteresis error.

Definition at line 1610 of file curvefit_c_binding.f90.

5.1.2.12 pure logical(c_bool) function curvefit_c_binding::is_monotonic_c (integer(i32), intent(in), value *n*, real(dp), dimension(n), intent(in) *x*)

Tests to see if an array is montonically increasing or decreasing.

in	n	The number of elements in the array.
in	Х	The array to test.

Returns

Returns true if x is monotonic; else, false.

Definition at line 122 of file curvefit_c_binding.f90.

5.1.2.13 subroutine curvefit_c_binding::lininterp_free_c (type(c_linear_interp), intent(inout), target obj)

Frees resources held by a c_linear_interp object.

Parameters

in,out <i>obj</i>	The c_linear_	_interp object.
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Definition at line 200 of file curvefit c binding.f90.

5.1.2.14 integer(i32) function curvefit_c_binding::lininterp_get_pt_count_c (type(c_linear_interp), intent(in), target obj)

Gets the number of points used by the interpolation object.

Parameters

in	obj	The c	linear	_interp object.
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Returns

The number of points.

Definition at line 248 of file curvefit_c_binding.f90.

5.1.2.15 subroutine curvefit_c_binding::lininterp_get_pts_c (type(c_linear_interp), intent(in), target *obj*, integer(i32), intent(in), value *n*, real(dp), dimension(n), intent(out) *x*, real(dp), dimension(n), intent(out) *y*)

Gets a copy of the data points stored by the interpolation object.

Parameters

in	obj	The c_linear_interp object.
in	n	The size of the buffer arrays.
out	Х	An N-element array where the x-coordinate data will be written.
out	У	An N-element array where the y-coordinate data will be written.

Remarks

If n is different than the actual number of points that exist, the lesser of the two values will be utilized. The interpolation object can be queried to determine the quantity of stored points.

Definition at line 278 of file curvefit_c_binding.f90.

5.1.2.16 subroutine curvefit_c_binding::lininterp_init_c (type(c_linear_interp), intent(out) *obj,* integer(i32), intent(in), value *n,* real(dp), dimension(n), intent(in) *x,* real(dp), dimension(n), intent(in) *y,* type(errorhandler), intent(inout) *err*)

Initializes a new c_linear_interp object.

Parameters

out	obj	The c_linear_interp object to initialize.
in	n	The number of data points.
in	Х	An N-element array containing the x-components of each data point. This array must be monotonic (ascending or descending only).
in	У	An N-element array containing the y-components of each data point.
in,out	err	The errorhandler object. If no error handling is desired, simply pass NULL, and errors will be dealt with by the default internal error handler. Possible errors that may be encountered are as follows. • CF_OUT_OF_MEMORY_ERROR: Occurs if there is insufficient memory available. • CF_NONMONOTONIC_ARRAY_ERROR: Occurs if x is not monotonically increasing or decreasing.

Definition at line 173 of file curvefit_c_binding.f90.

5.1.2.17 subroutine curvefit_c_binding::lininterp_interp_c (type(c_linear_interp), intent(in), target *obj,* integer(i32), intent(in), value *n,* real(dp), dimension(n), intent(in) *x,* real(dp), dimension(n), intent(out) *y*)

Performs a linear interpolation to determine the points y that for the requested indendent variable values in x.

Parameters

in	obj	The c_linear_interp object.
in	n	The number of points to interpolate.
in	Х	An N-element array containing the values of the independent variable at which to interpolate.
out	У	An N-element array where the interpolated values can be written.

Definition at line 225 of file curvefit_c_binding.f90.

5.1.2.18 real(dp) function curvefit_c_binding::linlsq_1var_c (integer(i32), intent(in), value *n*, real(dp), dimension(n), intent(in) *x*, real(dp), dimension(n), intent(inout) *y*, type(errorhandler), intent(inout) *err*)

Employs a least squares fit to determine the coefficient A in the linear system: Y = A * X.

in	n	The number of data points.
in	х	An N-element array containing the independent variable data.
in,out	У	An N-element array containing the dependent variable data corresponding to \times . On output, the contents of this array are overwritten as it is used for storage purposes by the algorithm.

Parameters

in,out	err	The errorhandler object. If no error handling is desired, simply pass NULL, and errors will be dealt with by the default internal error handler. Possible errors that may be encountered are as follows.
		CF_OUT_OF_MEMORY_ERROR: Occurs if insufficient memory is available.
		• CF_ARRAY_SIZE_ERROR: Occurs if $\mathbf x$ and $\mathbf y$ are different sizes.

Returns

The scalar coefficient A.

Definition at line 923 of file curvefit c binding.f90.

5.1.2.19 subroutine curvefit_c_binding::linlsq_nvar_c (integer(i32), intent(in), value *m*, integer(i32), intent(in), value *n*, integer(i32), intent(in), value *npts*, real(dp), dimension(m,npts), intent(inout) *x*, real(dp), dimension(m,npts), intent(in) *y*, real(dp), dimension(m,n), intent(out) *a*, type(errorhandler), intent(inout) *err*)

Employs a least squares fit to determine the coefficient A in the linear system: Y = A * X.

Parameters

in	m	The number of dependent variables.
in	n	The number of independent variables.
in,out	Х	An N-by-NPTS matrix containing the P data points of the N independent variables.
in	У	An M-by-NPTS matrix containing the P data points of the M dependent variables.
out	а	The M-by-N matrix where the resulting coefficient matrix A will be written.
in,out	err	The errorhandler object. If no error handling is desired, simply pass NULL, and errors will be dealt with by the default internal error handler. Possible errors that may be encountered are as follows.
		CF_ARRAY_SIZE_ERROR: Occurs if any of the matrix dimensions are not compatiable. CF_OUT_OF_MEMORY_ERROR: Occurs if there is insufficient regreen, such all the compatible and the compatible are not compatible.
		 CF_OUT_OF_MEMORY_ERROR: Occurs if there is insufficient memory available.

Remarks

The algorithm attempts to compute the coefficient matrix A as follows. Y * X**T = A * X * X**T Y * X**T * INV(X * X**T) = A This does require that <math>X * X**T does not result in a singular matrix. To handle the situation where X * X**T is singular, the Moore-Penrose pseudo-inverse, computed by means of singular value decomposition, is utilized to still arrive at a solution that, at minimum, has a minimum Euclidean norm of its residual. Let: PINV(X) = X**T * INV(X * X**T), Then: A = Y * PINV(X)

Definition at line 976 of file curvefit_c_binding.f90.

5.1.2.20 subroutine curvefit_c_binding::lowess_free_c (type(c_lowess_smoothing), intent(inout), target obj)

Frees resources held by a c_lowess_smoothing object.

Parameters

in,out	obj	The c_lowess_smoothing object.
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Definition at line 1069 of file curvefit c binding.f90.

5.1.2.21 integer(i32) function curvefit_c_binding::lowess_get_pt_count_c (type(c_lowess_smoothing), intent(in) obj)

Gets the number of points used by the lowess_smoothing object.

Parameters 4 8 1

in	obj	The c	lowess	_smoothing	object.
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Returns

The number of points.

Definition at line 1138 of file curvefit_c_binding.f90.

5.1.2.22 subroutine curvefit_c_binding::lowess_get_pts_c (type(c_lowess_smoothing), intent(in) *obj,* integer(i32), intent(in), value *n,* real(dp), dimension(n), intent(out) *x,* real(dp), dimension(n), intent(out) *y*)

Gets a copy of the data points stored by the lowess_smoothing object.

Parameters

in	obj	The c_lowess_smoothing object.
in	n	The size of the buffer arrays.
out	Х	An N-element array where the x-coordinate data will be written.
out	У	An N-element array where the y-coordinate data will be written.

Remarks

If n is different than the actual number of points that exist, the lesser of the two values will be utilized. The lowess_smoothing object can be queried to determine the quantity of stored points.

Definition at line 1169 of file curvefit c binding.f90.

5.1.2.23 subroutine curvefit_c_binding::lowess_get_residual_c (type(c_lowess_smoothing), intent(in) *obj,* integer(i32), intent(in), value *n,* real(dp), dimension(n), intent(out) *x*)

Gets the residuals from each data point.

in	this	The c_lowess_smoothing object.
in	n	The number of elements available in the buffer array \mathbf{x} .
out	Х	An N-element array where the residual data should be written.

Definition at line 1197 of file curvefit_c_binding.f90.

5.1.2.24 subroutine curvefit_c_binding::lowess_init_c (type(c_lowess_smoothing), intent(out) *obj*, integer(i32), intent(in), value *n*, real(dp), dimension(n), intent(in) *x*, real(dp), dimension(n), intent(in) *y*, logical(c_bool), intent(in), value *srt*, type(errorhandler), intent(inout) *err*)

Initializes a new c_lowess_smoothing object.

Parameters

out	obj	The c_lowess_smoothing object.
in	n	The number of data points.
in	Х	An N-element array containing the x-coordinate data. Ideally, the data set should be monotonically increasing; however, if it is not, it may be sorted by the routine, dependent upon the value of srt.
in	У	An N-element array containing the y-coordinate data.
in	srt	A logical flag determining if x should be sorted.
in,out	err	The errorhandler object. If no error handling is desired, simply pass NULL, and errors will be dealt with by the default internal error handler. Possible errors that may be encountered are as follows.
		 CF_ARRAY_SIZE_ERROR: Occurs if x and y are not the same size. CF_OUT_OF_MEMORY_ERROR: Occurs if there is insufficient memory available.

Definition at line 1041 of file curvefit_c_binding.f90.

5.1.2.25 subroutine curvefit_c_binding::lowess_smooth_c (type(c_lowess_smoothing), intent(inout) *obj*, real(dp), intent(in), value *f*, integer(i32), intent(in), value *n*, real(dp), dimension(n), intent(out) *y*, type(errorhandler), intent(inout) *err*)

Performs the actual smoothing operation.

Parameters

in,out	obj	The c_lowess_smoothing object.
in	f	Specifies the amount of smoothing. More specifically, this value is the fraction of points used to compute each value. As this value increases, the output becomes smoother. Choosing a value in the range of 0.2 to 0.8 usually results in a good fit. As such, a reasonable starting point, in the absence of better information, is a value of 0.5.
in	n	The size of the buffer y. Ideally, this parameter is equal to the number of points stored in obj; however, the routine will only traverse the minimum of the this parameter or the number of points stored in obj.
out	У	An N-element array to which the smoothed data will be written.
in,out	err	The errorhandler object. If no error handling is desired, simply pass NULL, and errors will be dealt with by the default internal error handler. Possible errors that may be encountered are as follows. • CF_NO_DATA_DEFINED_ERROR: Occurs if no data has been defined. • CF_OUT_OF_MEMORY_ERROR: Occurs if there is insufficient memory available.

Definition at line 1106 of file curvefit_c_binding.f90.

5.1.2.26 pure real(dp) function curvefit_c_binding::mean_c (integer(i32), intent(in), value n, real(dp), dimension(n), intent(in) x)

Computes the mean of a data set.

Parameters

in	n	The number of data points.
in	Х	An N-element array containing the data set.

Returns

The mean of \boldsymbol{x} .

Definition at line 728 of file curvefit_c_binding.f90.

5.1.2.27 real(dp) function curvefit_c_binding::median_c (integer(i32), intent(in), value *n*, real(dp), dimension(n), intent(inout) *x*, logical(c_bool), intent(in), value *srt*)

Computes the median of a data set.

Parameters

in	n	The number of data points.
in,out	х	The data set whose median is to be found. Ideally, the data set should be monotonically increasing; however, if it is not, it may be sorted by the routine, dependent upon the value of srt. On output, the array contents are unchanged; however, they may be sorted into ascending order (dependent upon the value of srt).
in	srt	A logical flag determining if x should be sorted.

Returns

The median of \boldsymbol{x} .

Definition at line 747 of file curvefit_c_binding.f90.

5.1.2.28 subroutine curvefit_c_binding::moving_average_c (integer(i32), intent(in), value *n*, real(dp), dimension(n), intent(inout) *x*, integer(i32), intent(in), value *npts*, type(errorhandler), intent(inout) *err*)

Applies a moving average to smooth a data set.

in	n	The number of data points.
in,out	Х	On input, the signal to smooth. On output, the smoothed signal.
in	npts	The size of the averaging window. This value must be at least 2, but no more than the number of elements in \mathbf{x} .
in,out	err	The errorhandler object. If no error handling is desired, simply pass NULL, and errors will be dealt with by the default internal error handler. Possible errors that may be encountered are as follows.
		• CF_INVALID_INPUT_ERROR: Occurs if <code>npts</code> is less than 2, or greater than the length of $\mathbf{x}.$
		CF_OUT_OF_MEMORY_ERROR: Occurs if there is insufficient memory available generated by Doxygen

Definition at line 887 of file curvefit_c_binding.f90.

5.1.2.29 subroutine curvefit_c_binding::nlr_free_c (type(c_nonlinear_regression), intent(inout), target obj)

Frees resources held by a c_nonlinear_regression object.

Parameters

in,out	obj	The c_nonlinear_regression object.
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Definition at line 1293 of file curvefit c binding.f90.

5.1.2.30 integer(i32) function curvefit_c_binding::nlr_get_pt_count_c (type(c_nonlinear_regression), intent(in) obj)

Gets the number of points used by the c_nonlinear_regression object.

Parameters

in	obj	The c_nonlinear_regression object.	
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Returns

The number of points.

Definition at line 1363 of file curvefit_c_binding.f90.

5.1.2.31 subroutine curvefit_c_binding::nlr_get_pts_c (type(c_nonlinear_regression), intent(in) *obj,* integer(i32), intent(in), value *n,* real(dp), dimension(n), intent(out) *x,* real(dp), dimension(n), intent(out) *y*)

Gets a copy of the data points stored by the c_nonlinear_regression object.

Parameters

in	obj	The c_nonlinear_regression object.
in	n	The size of the buffer arrays.
out	Х	An N-element array where the x-coordinate data will be written.
out	У	An N-element array where the y-coordinate data will be written.

Remarks

If n is different than the actual number of points that exist, the lesser of the two values will be utilized. The $c_nonlinear_regression$ object can be queried to determine the quantity of stored points.

Definition at line 1394 of file curvefit_c_binding.f90.

5.1.2.32 subroutine curvefit_c_binding::nlr_get_solver_params_c (type(c_nonlinear_regression), intent(in) *obj*, type(solver_control), intent(out) *cntrl*)

Gets the nonlinear regression solver solution control parameters.

Parameters

in	obj	The c_nonlinear_regression object.
out	cntrl	The solver_control object that, on output, will contain the current solver control parameters.

Definition at line 1421 of file curvefit_c_binding.f90.

5.1.2.33 subroutine curvefit_c_binding::nlr_init_c (type(c_nonlinear_regression), intent(out) *obj*, integer(i32), intent(in), value *n*, real(dp), dimension(n), intent(in) *x*, real(dp), dimension(n), intent(in) *y*, type(c_funptr), intent(in), value *fcn*, integer(i32), intent(in), value *ncoeff*, type(errorhandler), intent(inout) *err*)

Initializes a new c_nonlinear_regression object.

Parameters

out	obj	The c_nonlinear_regression object.	
in	n	The number of data points.	
in	X	An N-element containing the independent variable values of the data set.	
in	У	An N-element array of the dependent variables corresponding to x.	
in	fcn	A pointer to the function whose coefficients are to be determined.	
in	ncoeff	The number of coefficients in the function defined in fcn.	
in,out	err	The errorhandler object. If no error handling is desired, simply pass NULL, and errors will be dealt with by the default internal error handler. Possible errors that may be encountered are as follows. • CF_OUT_OF_MEMORY_ERROR: Occurs if there is insufficient memory available. • CF_INVALID_INPUT_ERROR: Occurs if ncoeff is less than or equal to zero.	

Definition at line 1260 of file curvefit_c_binding.f90.

5.1.2.34 subroutine curvefit_c_binding::nlr_set_solver_params_c (type(c_nonlinear_regression), intent(inout) *obj,* type(solver_control), intent(in) *cntrl*)

Sets the nonlinear regression solver solution control parameters.

Parameters

in,out	obj	The c_nonlinear_regression object.
in	cntrl	The solver_control object that contains the current solver control parameters.

Definition at line 1446 of file curvefit_c_binding.f90.

5.1.2.35 subroutine curvefit_c_binding::nlr_solve_c (type(c_nonlinear_regression), intent(inout) *obj,* integer(i32), intent(in), value *n,* real(dp), dimension(n), intent(inout) *c,* type(iteration_behavior), intent(out) *ib,* type(errorhandler), intent(inout) *err*)

Computes the solution to the nonlinear regression problem using the Levenberg-Marquardt method.

Parameters

in, out	obj	The c_nonlinear_regression object.	
in	n	The number of coefficients to determine.	
in,out	С	On input, an array containing initial estimates of the coefficients. On output, the comptued	
		coefficient values.	
out	ib	An output parameter that allows the caller to obtain iteration performance statistics.	
in,out	err	The errorhandler object. If no error handling is desired, simply pass NULL, and errors will be dealt with by the default internal error handler. Possible errors that may be encountered are as follows.	
		CF_INVALID_OPERATION_ERROR: Occurs if no equations have been defined.	
		 CF_INVALID_INPUT_ERROR: Occurs if the number of equations is less than than the number of variables. 	
		CF_ARRAY_SIZE_ERROR: Occurs if any of the input arrays are not sized correctly.	
		 CF_CONVERGENCE_ERROR: Occurs if the line search cannot converge within the allowed number of iterations. 	
		CF_OUT_OF_MEMORY_ERROR: Occurs if there is insufficient memory available.	
		 CF_TOLERANCE_TOO_SMALL_ERROR: Occurs if the requested tolerance is to small to be practical for the problem at hand. 	

Definition at line 1333 of file curvefit_c_binding.f90.

5.1.2.36 real(dp) function curvefit_c_binding::nonlin_c (integer(i32), intent(in), value *n*, real(dp), dimension(n), intent(in) applied, real(dp), dimension(n), intent(in) measured)

Computes the best-fit nonlinearity of a data set.

Parameters

in	n	The number of data points.
in	applied	An N-element array containing the values applied to the measurement instrument.
in	measured	An N-element array containing the calibrated output of the instrument as a result of the values given in applied.

Returns

The nonlinearity error.

Definition at line 1568 of file curvefit_c_binding.f90.

5.1.2.37 subroutine curvefit_c_binding::polyinterp_free_c (type(c_polynomial_interp), intent(inout), target obj)

Frees resources held by a c_polynomial_interp object.

in,out	obj	The c_polynomial_	interp object.
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Definition at line 371 of file curvefit_c_binding.f90.

5.1.2.38 integer(i32) function curvefit_c_binding::polyinterp_get_pt_count_c (type(c_polynomial_interp), intent(in), target obj)

Gets the number of points used by the interpolation object.

Parameters

in	obj	The c_polynomial_interp object.	The c_polynomial_	
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Returns

The number of points.

Definition at line 419 of file curvefit_c_binding.f90.

5.1.2.39 subroutine curvefit_c_binding::polyinterp_get_pts_c (type(c_polynomial_interp), intent(in), target *obj,* integer(i32), intent(in), value *n,* real(dp), dimension(n), intent(out) *x,* real(dp), dimension(n), intent(out) *y*)

Gets a copy of the data points stored by the interpolation object.

Parameters

in	obj	The c_polynomial_interp object.
in	n	The size of the buffer arrays.
out	Х	An N-element array where the x-coordinate data will be written.
out	У	An N-element array where the y-coordinate data will be written.

Remarks

If n is different than the actual number of points that exist, the lesser of the two values will be utilized. The interpolation object can be queried to determine the quantity of stored points.

Definition at line 449 of file curvefit_c_binding.f90.

5.1.2.40 subroutine curvefit_c_binding::polyinterp_init_c (type(c_polynomial_interp), intent(out) *obj,* integer(i32), intent(in), value *n,* real(dp), dimension(n), intent(in) *x,* real(dp), dimension(n), intent(in) *y,* integer(i32), intent(in), value *order,* type(errorhandler), intent(inout) *err*)

Initializes a new c_polynomial_interp object.

out	obj	The c_polynomial_interp object to initialize.
in	n	The number of data points.
in	Х	An N-element array containing the x-components of each data point. This array must be monotonic (ascending or descending only).
in	У	An N-element array containing the y-components of each data point.
in	order	The order of the interpolating polynomial.

Parameters

in,out	err	The errorhandler object. If no error handling is desired, simply pass NULL, and errors will be dealt with by the default internal error handler. Possible errors that may be encountered are as follows.
		CF_OUT_OF_MEMORY_ERROR: Occurs if there is insufficient memory available.
		 CF_NONMONOTONIC_ARRAY_ERROR: Occurs if x is not monotonically increasing or decreasing.
		CF_INVALID_INPUT_ERROR: Occurs if order is less than 1.

Definition at line 344 of file curvefit_c_binding.f90.

5.1.2.41 subroutine curvefit_c_binding::polyinterp_interp_c (type(c_polynomial_interp), intent(in), target *obj*, integer(i32), intent(in), value *n*, real(dp), dimension(n), intent(in) *x*, real(dp), dimension(n), intent(out) *y*)

Performs a polynomial interpolation to determine the points y that for the requested indendent variable values in x.

Parameters

in	obj	The c_polynomial_interp object.
in	n	The number of points to interpolate.
in	Х	An N-element array containing the values of the independent variable at which to interpolate.
out	У	An N-element array where the interpolated values can be written.

Definition at line 396 of file curvefit_c_binding.f90.

5.1.2.42 real(dp) function curvefit_c_binding::repeat_c (integer(i32), intent(in), value *npts*, integer(i32), intent(in), value *ntests*, real(dp), dimension(npts, ntests), intent(in) *applied*, real(dp), dimension(npts, ntests), intent(in) *measured*)

Computes the repeatability of a sequence of tests.

Parameters

in	npts	The number of data points per test.
in	ntests	The number of tests.
in	applied	An NPTS-by-NTEST matrix containing at least 2 columns (tests) of NPTS values applied to
		the measurement instrument.
in	measured	An NPTS-by-NTEST matrix containing the corresponding calibrated output from the
		instrument.

Returns

The largest magnitude deviation from the initial test.

Remarks

Repeatability is considered as the largest magnitude deviation of subsequent tests from the initial test. Noting that it is very likely that consecutive test points will vary slightly, test 2 through test N are linearly interpolated such that their test points line up with those from test 1.

Definition at line 1664 of file curvefit_c_binding.f90.

5.1.2.43 real(dp) function curvefit_c_binding::rtz_c (integer(i32), intent(in), value *n*, real(dp), dimension(n), intent(in) *applied*, real(dp), dimension(n), intent(in) *measured*, real(dp), intent(in), value *tol*)

Computes the return to zero error in an ascending/descending data set.

Parameters

in	n	The number of data points.
in	applied	An N-element array containing the values applied to the measurement instrument.
in	measured	An N-element array containing the calibrated output of the instrument as a result of the values given in applied.
in	tol	An input argument that specifies the tolerance used in finding the matching zero data point.

Returns

The return to zero error.

Definition at line 1634 of file curvefit_c_binding.f90.

5.1.2.44 subroutine curvefit_c_binding::seb_c (integer(i32), intent(in), value *n*, real(dp), dimension(n), intent(in) *applied*, real(dp), dimension(n), intent(in) *output*, real(dp), intent(in), value *fullscale*, type(seb_results), intent(out) *rst*, type(errorhandler), intent(inout) *err*)

Computes the static error band of a data set.

Parameters

in	n	The number of data points.
in	applied	An N-element array containing the values applied to the measurement instrument.
in	output	An N-element array containing the values output by the instrument as a result of the values given in applied.
in	fullscale	The full scale measurement value for the instrument. The units must be consistent with those of applied.
out	rst	An seb_results object where the calculation results will be written.
in,out	err	The errorhandler object. If no error handling is desired, simply pass NULL, and errors will be dealt with by the default internal error handler. Possible errors that may be encountered are as follows.
		 CF_INVALID_INPUT_ERROR: Occurs if fullscale is sufficiently close to zero to be considered zero. Sufficiently close in this instance is considered to be the square root of machine precision.

Definition at line 1537 of file curvefit c binding.f90.

5.1.2.45 subroutine curvefit_c_binding::splineinterp_diff1_c (type(c_spline_interp), intent(in), target *obj*, integer(i32), intent(in), value *n*, real(dp), dimension(n), intent(in) *x*, real(dp), dimension(n), intent(out) *y*)

Computes the interpolated first derivative.

Parameters

in	obj	The c_spline_interp object.
in	n	The number of points to interpolate.
in	Х	An N-element array containing the values of the independent variable at which to interpolate.
out	У	An N-element array where the interpolated values can be written.

Definition at line 677 of file curvefit_c_binding.f90.

5.1.2.46 subroutine curvefit_c_binding::splineinterp_diff2_c (type(c_spline_interp), intent(in), target *obj*, integer(i32), intent(in), value *n*, real(dp), dimension(n), intent(in) *x*, real(dp), dimension(n), intent(out) *y*)

Computes the interpolated second derivative.

Parameters

in	obj	The c_spline_interp object.
in	n	The number of points to interpolate.
in	Х	An N-element array containing the values of the independent variable at which to interpolate.
out	У	An N-element array where the interpolated values can be written.

Definition at line 703 of file curvefit_c_binding.f90.

5.1.2.47 subroutine curvefit_c_binding::splineinterp_free_c (type(c_spline_interp), intent(inout), target obj)

Frees resources held by a c_spline_interp object.

Parameters

in,out	obj	The c_spline_interp object.

Definition at line 569 of file curvefit_c_binding.f90.

5.1.2.48 integer(i32) function curvefit_c_binding::splineinterp_get_pt_count_c (type(c_spline_interp), intent(in), target obj)

Gets the number of points used by the interpolation object.

Parameters

in	obj	The c_spline_	interp object.
----	-----	---------------	----------------

Returns

The number of points.

Definition at line 617 of file curvefit_c_binding.f90.

5.1.2.49 subroutine curvefit_c_binding::splineinterp_get_pts_c (type(c_spline_interp), intent(in), target *obj*, integer(i32), intent(in), value *n*, real(dp), dimension(n), intent(out) *x*, real(dp), dimension(n), intent(out) *y*)

Gets a copy of the data points stored by the interpolation object.

Parameters

in	obj	The c_spline_interp object.
in	n	The size of the buffer arrays.
out	Х	An N-element array where the x-coordinate data will be written.
out	У	An N-element array where the y-coordinate data will be written.

Remarks

If n is different than the actual number of points that exist, the lesser of the two values will be utilized. The interpolation object can be queried to determine the quantity of stored points.

Definition at line 647 of file curvefit_c_binding.f90.

5.1.2.50 subroutine curvefit_c_binding::splineinterp_init_c (type(c_spline_interp), intent(out) obj, integer(i32), intent(in), value n, real(dp), dimension(n), intent(in) x, real(dp), dimension(n), intent(in) y, integer(i32), intent(in), value ibcbeg, real(dp), intent(in), value ybcbeg, integer(i32), intent(in), value ibcend, real(dp), intent(in), value ybcend, type(errorhandler), intent(inout) err)

Initializes a new c_spline_interp object.

out	obj	The c_spline_interp object to initialize.
in	n	The number of data points.
in	х	An N-element array containing the x-components of each data point. This array must be monotonic (ascending or descending only).
in	У	An N-element array containing the y-components of each data point.
in	ibcbeg	An input that defines the nature of the boundary condition at the beginning of the spline. If an invalid parameter is used, the code defaults to SPLINE_QUADRATIC_OVER_INTERVAL.
		 SPLINE_QUADRATIC_OVER_INTERVAL: The spline is quadratic over its initial interval. No value is required for ybcbeg.
		SPLINE_KNOWN_FIRST_DERIVATIVE: The spline's first derivative at its initial point is provided in ybcbeg.
		 SPLINE_KNOWN_SECOND_DERIVATIVE: The spline's second derivative at its initial point is provided in ybcbeg.
		 SPLINE_CONTINUOUS_THIRD_DERIVATIVE: The third derivative is continuous at x(2). No value is required for ybcbeg.
in	ybcbeg	If needed, the value of the initial point boundary condition. If not needed, this parameter is ignored.

Parameters

in	ibcend	An input that defines the nature of the boundary condition at the end of the spline. If an invalid parameter is used, the code defaults to SPLINE_QUADRATIC_OVER_INTERVAL.
		 SPLINE_QUADRATIC_OVER_INTERVAL: The spline is quadratic over its final interval. No value is required for ybcend.
		 SPLINE_KNOWN_FIRST_DERIVATIVE: The spline's first derivative at its initial point is provided in ybcend.
		 SPLINE_KNOWN_SECOND_DERIVATIVE: The spline's second derivative at its initial point is provided in ybcend.
		SPLINE_CONTINUOUS_THIRD_DERIVATIVE: The third derivative is continuous at x(n-1). No value is required for ybcend.
in	ybcend	If needed, the value of the final point boundary condition. If not needed, this parameter is ignored.
in,out	err	The errorhandler object. If no error handling is desired, simply pass NULL, and errors will be dealt with by the default internal error handler. Possible errors that may be encountered are as follows.
		 CF_OUT_OF_MEMORY_ERROR: Occurs if there is insufficient memory available.
		 CF_NONMONOTONIC_ARRAY_ERROR: Occurs if x is not monotonically increasing or decreasing.

Definition at line 539 of file curvefit_c_binding.f90.

5.1.2.51 subroutine curvefit_c_binding::splineinterp_interp_c (type(c_spline_interp), intent(in), target *obj*, integer(i32), intent(in), value *n*, real(dp), dimension(n), intent(in) *x*, real(dp), dimension(n), intent(out) *y*)

Performs a spline interpolation to determine the points y that for the requested indendent variable values in x.

Parameters

in	obj	The c_spline_interp object.	
in	n	The number of points to interpolate.	
in	in x An N-element array containing the values of the independent variable at which to inter		
out	У	An N-element array where the interpolated values can be written.	

Definition at line 594 of file curvefit_c_binding.f90.

5.1.2.52 subroutine curvefit_c_binding::split_c (integer(i32), intent(in), value *n*, real(dp), dimension(n), intent(in) *x*, integer(i32), intent(in), value *na*, real(dp), dimension(na), intent(out) *ascend*, integer(i32), intent(in), value *nd*, real(dp), dimension(nd), intent(out) *descend*, integer(i32), intent(out) *nascend*, integer(i32), intent(out) *nascend*, type(errorhandler), intent(inout) *err*)

Splits a data set into ascending and descending components.

Parameters

in	n	The number of data points in \mathbf{x} .
in	X	An N-element array containing the data set to split.
in	na	The capacity of ascend.
out	ascend	An array where the ascending points will be written. Ensure this array is appropriately sized to accept all the ascending points (it can be oversized).
in	nd	The capacity of descend.
out	descend	An array where the descending points will be written. Ensure this array is appropriately sized to accept all the descending points (it can be oversized).
out	nascend	The actual number of values written into ascend.
out	ndescend	The actual number of values written into descend.
in,out	err	The errorhandler object. If no error handling is desired, simply pass NULL, and errors will be dealt with by the default internal error handler. Possible errors that may be encountered are as follows. • CF_ARRAY_SIZE_ERROR: Occurs if either ascend or descend is too small to actually accept all of the necessary data.

Remarks

The routine operates by finding the first occurrence where the data set is no longer monotonic, and then copies everything prior to that value, along with the the inflection value, into the output ascending data array. The routine then searches for either a change in direction, or a value that matches the first value in the ascending data set within some tolerance to determine the bounds on the descending data set. Once the bounds are determined, the descending data set is copied from the original array and placed in the output descending data array. This then means that any remaining data in the original data set that lies after either of the aforementioned sets is ignored.

Example

```
Х:
 0.00000000000000000
 0.38905000686645508
 0.77815997600555420
 0.97268998622894287
 1.1671400070190430
 1.5559999942779541
 1.9448399543762207
 0.97259998321533203
  -9.9999997473787516E-006
This routine splits the array into the following ascending and
descending arrays.
ASCENDING:
 0.0000000000000000
 0.38905000686645508
 0.77815997600555420
 0.97268998622894287
 1.1671400070190430
 1.5559999942779541
 1.9448399543762207
DESCENDING:
 1.9448399543762207
 0.97259998321533203
  -9.9999997473787516E-006
```

Definition at line 1782 of file curvefit_c_binding.f90.

Given the following array X,

5.1.2.53 pure real(dp) function curvefit_c_binding::stdev_c (integer(i32), intent(in), value n, real(dp), dimension(n), intent(in) x)

Computes the corrected standard deviation of a data set.

Parameters

in	n	The number of data points.
in	Χ	An N-element array containing the data set.

Returns

The standard deviation of x.

Definition at line 814 of file curvefit c binding.f90.

5.1.2.54 real(dp) function curvefit_c_binding::term_nonlin_c (integer(i32), intent(in), value *n*, real(dp), dimension(n), intent(in) applied, real(dp), dimension(n), intent(in) measured)

Computes the terminal nonlinearity of a data set.

Parameters

in	n	The number of data points.
in	applied	An N-element array containing the values applied to the measurement instrument.
in	measured	An N-element array containing the calibrated output of the instrument as a result of the values given in applied.

Returns

The nonlinearity error.

Definition at line 1589 of file curvefit_c_binding.f90.

5.1.2.55 pure real(dp) function curvefit_c_binding::variance_c (integer(i32), intent(in), value *n*, real(dp), dimension(n), intent(in) *x*)

Computes the sample variance of a data set.

Parameters

in	n	The number of data points.
in	Х	An N-element array containing the data set.

Returns

The variance of x.

Remarks

To avoid overflow-type issues, Welford's algorithm is employed. A simple illustration of this algorithm can be found here.

Definition at line 767 of file curvefit_c_binding.f90.

5.1.2.56 subroutine curvefit_c_binding::xtalk_c (integer(i32), intent(in), value *npts*, integer(i32), intent(in), value *ndof*, real(dp), dimension(npts, ndof), intent(in) *xerr*, integer(i32), dimension(2*ndof), intent(in) *indices*, real(dp), dimension(ndof, ndof), intent(out) *xt*, type(errorhandler), intent(inout) *err*)

Computes the crosstalk errors for a multiple degree-of-freedom data set.

Parameters

in	npts	The number of data points in each degree of freedom.
in	ndof	The number of degrees of freedom.
in	xerr	An NPTS-by-NDOF matrix containing the measurement error values (computed such that XERR = X MEASURED - X APPLIED).
in	indices	A 2*NDOF element array containing row indices defining the rows where each degree-of-freedom was applied in the data set xerr.
out	xt	An NDOF-by-NDOF matrix that, on output, will contain the crosstalk errors such that each loaded degree of freedom is represented by its own row, and each responding degree of freedom is represented by its own column.
in,out	err	The errorhandler object. If no error handling is desired, simply pass NULL, and errors will be dealt with by the default internal error handler. Possible errors that may be encountered are as follows. • CF_ARRAY_INDEX_ERROR: Occurs if any of the entries in indices are outside the row bounds of xerr.

Definition at line 1696 of file curvefit_c_binding.f90.

5.2 curvefit_calibration Module Reference

curvefit_calibration

Data Types

interface crosstalk

Computes the crosstalk errors for a multiple degree-of-freedom data set.

interface hysteresis

Computes the hysteresis in an ascending/descending data set.

- interface IDAMAX
- · interface nonlinearity

Computes the best-fit nonlinearity of a data set.

· interface repeatability

Computes the repeatability of a sequence of tests.

• interface return_to_zero

Computes the return to zero error in an ascending/descending data set.

· interface seb

Computes the static error band of a data set.

• type seb results

Defines a container for static error band related information.

• interface split_ascend_descend

Splits a data set into ascending and descending components.

· interface terminal_nonlinearity

Computes the terminal nonlinearity of a data set.

Functions/Subroutines

• type(seb_results) function seb_1 (applied, output, fullscale, err)

Computes the static error band of a data set.

real(dp) function bf_nonlin (applied, measured, err)

Computes the best-fit nonlinearity of a data set.

• real(dp) function term_nonlin (applied, measured, err)

Computes the terminal nonlinearity of a data set.

• real(dp) function hysteresis_1 (xascend, ascend, xdescend, descend, err)

Computes the hysteresis in an ascending/descending data set.

real(dp) function hysteresis_2 (applied, measured, err)

Computes the hysteresis in an ascending/descending data set.

• real(dp) function rtz_1 (applied, measured, tol, err)

Computes the return to zero error in an ascending/descending data set.

• real(dp) function repeat_1 (applied, measured, err)

Computes the repeatability of a sequence of tests.

• real(dp) function, dimension(size(xerr, 2), size(xerr, 2)) xtalk_1 (xerr, indices, err)

Computes the crosstalk errors for a multiple degree-of-freedom data set.

subroutine split ascend descend 1 (x, ascend, descend, nascend, ndescend, err)

Splits a data set into ascending and descending components.

5.2.1 Detailed Description

curvefit_calibration

Purpose

To provide routines for computing calibration performance metrics commonly used to assess the fitness of a calibration curve fit.

References

Wheeler, Anthony J., Ganji, Ahmad R., "Introduction to Engineering Experimentation," Third Edition, Prentice Hall.

5.2.2 Function/Subroutine Documentation

5.2.2.1 real(dp) function curvefit_calibration::bf_nonlin (real(dp), dimension(:), intent(in) applied, real(dp), dimension(:), intent(in) measured, class(errors), intent(inout), optional, target err) [private]

Computes the best-fit nonlinearity of a data set.

in	applied	An N-element array containing the values applied to the measurement instrument.
in	measured	An N-element array containing the calibrated output of the instrument as a result of the values given in applied.
out	err	An optional errors-based object that if provided can be used to retrieve information relating to any errors encountered during execution. If not provided, a default implementation of the errors class is used internally to provide error handling. Possible errors and warning messages that may be encountered are as follows.
		CF_ARRAY_SIZE_ERROR: Occurs if applied and measured are not the same size. Generated by Doxygen

Returns

The nonlinearity error.

Definition at line 211 of file curvefit calibration.f90.

5.2.2.2 real(dp) function curvefit_calibration::hysteresis_1 (real(dp), dimension(:), intent(in) xascend, real(dp), dimension(:), intent(in) ascend, real(dp), dimension(:), intent(in) ascend, real(dp), dimension(:), intent(in) descend, class(errors), intent(inout), optional, target err) [private]

Computes the hysteresis in an ascending/descending data set.

Parameters

in	xascend	An N-element array containing the ascending calibration points. This array must be monotonically increasing or decreasing.	
in	ascend	An N-element array containing the sensor output to the calibration points in xascend.	
in	xdescend	An M-element array containing the descending calibration points. This array must be monotonically increasing or decreasing.	
in	descend	An M-element array containing the sensor output to the calibration points in xdescend.	
out	err	An optional errors-based object that if provided can be used to retrieve information related any errors encountered during execution. If not provided, a default implementation of errors class is used internally to provide error handling. Possible errors and warning messages that may be encountered are as follows.	
		CF_ARRAY_SIZE_ERROR: Occurs if xascend and ascend are not the same size, or if xdescend and descend are not the same size.	
		 CF_NONMONOTONIC_ARRAY_ERROR: Occurs if the calibration data is not monotonic in nature (either ascending or descending). 	

Returns

The hysteresis error.

Remarks

In order to account for slight variations between similar ascending and descending points, the algorithm used performs a linear interpolation between data points. The resulting interpolated value is then used to compute the reported hysteresis error.

Definition at line 353 of file curvefit calibration.f90.

5.2.2.3 real(dp) function curvefit_calibration::hysteresis_2 (real(dp), dimension(:), intent(in) applied, real(dp), dimension(:), intent(in) measured, class(errors), intent(inout), optional, target err) [private]

Computes the hysteresis in an ascending/descending data set.

in	applied	An N-element array containing the values applied to the measurement instrument.	
in	measured	An N-element array containing the calibrated output of the instrument as a result of the	
		values given in applied.	

Parameters

out	err	An optional errors-based object that if provided can be used to retrieve information relating to any errors encountered during execution. If not provided, a default implementation of the errors class is used internally to provide error handling. Possible errors and warning messages that may be encountered are as follows.	
		 CF_NONMONOTONIC_ARRAY_ERROR: Occurs if the calibration data is not monotonic in nature (either ascending or descending). 	
		CF_ARRAY_SIZE_ERROR: Occurs if applied and measured are not the same size.	

Returns

The hysteresis error.

Remarks

In order to account for slight variations between similar ascending and descending points, the algorithm used performs a linear interpolation between data points. The resulting interpolated value is then used to compute the reported hysteresis error.

Definition at line 444 of file curvefit_calibration.f90.

5.2.2.4 real(dp) function curvefit_calibration::repeat_1 (real(dp), dimension(:,:), intent(in) applied, real(dp), dimension(:,:), intent(in) measured, class(errors), intent(inout), optional, target err) [private]

Computes the repeatability of a sequence of tests.

Parameters

in	applied	An NPTS-by-NTEST matrix containing at least 2 columns (tests) of NPTS values applied	
		to the measurement instrument.	
in	measured	An NPTS-by-NTEST matrix containing the corresponding calibrated output from the	
		instrument.	
out	err	An optional errors-based object that if provided can be used to retrieve information relating to any errors encountered during execution. If not provided, a default implementation of the errors class is used internally to provide error handling. Possible errors and warning messages that may be encountered are as follows.	
		CF_ARRAY_SIZE_ERROR: Occurs if applied and measured are not the same size.	

Returns

The largest magnitude deviation from the initial test.

Remarks

Repeatability is considered as the largest magnitude deviation of subsequent tests from the initial test. Noting that it is very likely that consecutive test points will vary slightly, test 2 through test N are linearly interpolated such that their test points line up with those from test 1.

Definition at line 608 of file curvefit_calibration.f90.

5.2.2.5 real(dp) function curvefit_calibration::rtz_1 (real(dp), dimension(:), intent(in) applied, real(dp), dimension(:), intent(in) measured, real(dp), intent(in), optional tol, class(errors), intent(inout), optional, target err) [private]

Computes the return to zero error in an ascending/descending data set.

Parameters

in	applied	An N-element array containing the values applied to the measurement instrument.	
in	measured	An N-element array containing the calibrated output of the instrument as a result of the	
		values given in applied.	
in	tol	An optional input that specifies the tolerance used in finding the matching data points. If no value is specified, the default value of the square root of machine precision times the	
		largest magnitude value in xcal is used.	
out	err	An optional errors-based object that if provided can be used to retrieve information relating to any errors encountered during execution. If not provided, a default implementation of the errors class is used internally to provide error handling. Possible errors and warning messages that may be encountered are as follows.	
		CF_ARRAY_SIZE_ERROR: Occurs if applied and measured are not the same size.	

Returns

The return to zero error.

Definition at line 522 of file curvefit_calibration.f90.

5.2.2.6 type(seb_results) function curvefit_calibration::seb_1 (real(dp), dimension(:), intent(in) applied, real(dp), dimension(:), intent(in) output, real(dp), intent(in) fullscale, class(errors), intent(out), optional, target err) [private]

Computes the static error band of a data set.

in	applied	An N-element array containing the values applied to the measurement instrument.	
in	output	An N-element array containing the values output by the instrument as a result of the values	
		given in applied.	
in	fullscale	The full scale measurement value for the instrument. The units must be consistent with those of applied.	
out	err	An optional errors-based object that if provided can be used to retrieve information relating to any errors encountered during execution. If not provided, a default implementation of the errors class is used internally to provide error handling. Possible errors and warning messages that may be encountered are as follows.	
		CF_ARRAY_SIZE_ERROR: Occurs if applied and output are not the same size.	
		 CF_INVALID_INPUT_ERROR: Occurs if fullscale is sufficiently close to zero to be considered zero. Sufficiently close in this instance is considered to be the square root of machine precision. 	

Returns

The static error band information.

Definition at line 126 of file curvefit calibration.f90.

5.2.2.7 subroutine curvefit_calibration::split_ascend_descend_1 (real(dp), dimension(:), intent(in) x, real(dp), dimension(:), intent(out) ascend, real(dp), dimension(:), intent(out) descend, integer(i32), intent(out) nascend, integer(i32), intent(out) nascend, class(errors), intent(inout), optional, target err) [private]

Splits a data set into ascending and descending components.

Parameters

in	X	An N-element array containing the data set to split.	
out	ascend	An array where the ascending points will be written. Ensure this array is appropriately	
		sized to accept all the ascending points (it can be oversized).	
out	descend	An array where the descending points will be written. Ensure this array is appropriately	
		sized to accept all the descending points (it can be oversized).	
out	nascend	The actual number of values written into ascend.	
out	ndescend	The actual number of values written into descend.	
out	err	An optional errors-based object that if provided can be used to retrieve information relating to any errors encountered during execution. If not provided, a default implementation of the errors class is used internally to provide error handling. Possible errors and warning messages that may be encountered are as follows. • CF_ARRAY_SIZE_ERROR: Occurs if either ascend or descend is too small to actually accept all of the necessary data.	

Remarks

The routine operates by finding the first occurrence where the data set is no longer monotonic, and then copies everything prior to that value, along with the the inflection value, into the output ascending data array. The routine then searches for either a change in direction, or a value that matches the first value in the ascending data set within some tolerance to determine the bounds on the descending data set. Once the bounds are determined, the descending data set is copied from the original array and placed in the output descending data array. This then means that any remaining data in the original data set that lies after either of the aforementioned sets is ignored.

Example

```
0.38905000686645508
0.77815997600555420
0.97268998622894287
1.1671400070190430
1.5559999942779541
1.9448399543762207
```

DESCENDING:

1.9448399543762207 0.97259998321533203 -9.9999997473787516E-006

Definition at line 1011 of file curvefit calibration.f90.

5.2.2.8 real(dp) function curvefit_calibration::term_nonlin (real(dp), dimension(:), intent(in) applied, real(dp), dimension(:), intent(in) measured, class(errors), intent(inout), optional, target err) [private]

Computes the terminal nonlinearity of a data set.

Parameters

in	applied	An N-element array containing the values applied to the measurement instrument.	
in	measured	An N-element array containing the calibrated output of the instrument as a result of the values given in applied.	
out	err	An optional errors-based object that if provided can be used to retrieve information relating to any errors encountered during execution. If not provided, a default implementation of the errors class is used internally to provide error handling. Possible errors and warning messages that may be encountered are as follows.	
		CF_ARRAY_SIZE_ERROR: Occurs if applied and measured are not the same size.	

Returns

The terminal nonlinearity error.

Definition at line 267 of file curvefit_calibration.f90.

5.2.2.9 real(dp) function, dimension(size(xerr, 2), size(xerr, 2)) curvefit_calibration::xtalk_1 (real(dp), dimension(:,:), intent(in) xerr, integer(i32), dimension(:), intent(in) indices, class(errors), intent(inout), optional, target err) [private]

Computes the crosstalk errors for a multiple degree-of-freedom data set.

in	xerr	An NPTS-by-NDOF matrix containing the measurement error values (computed such that XERR = X MEASURED - X APPLIED).
in	indices	A 2*NDOF element array containing row indices defining the rows where each degree-of-freedom was applied in the data set xerr.
out	err	An optional errors-based object that if provided can be used to retrieve information relating to any errors encountered during execution. If not provided, a default implementation of the errors class is used internally to provide error handling. Possible errors and warning messages that may be encountered are as follows.
		 CF_ARRAY_SIZE_ERROR: Occurs if indices is not 2*NDOF in size. CF_ARRAY_INDEX_ERROR: Occurs if any of the entries in indices are outside the
		row bounds of xerr.
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Returns

A NDOF-by-NDOF matrix containing the crosstalk errors such that each loaded degree of freedom is represented by its own row, and each responding degree of freedom is represented by its own column.

Usage

The following program computes the crosstalk errors for a 2 DOF system. The applied data is as follows (there are 34 data points for each DOF).

```
0
               0
3000
6000
               0
7500
               0
9000
              0
12000
              0
15000
               0
7500
              Ω
0
               0
0
-3000
              0
-6000
-7500
               0
-9000
               0
-12000
               0
-15000
-7500
               0
_____
              67.79087067
0
               135.5817413
0
0
               203.3726196
Ω
              271.1634827
0
              338.9543762
              203.3726196
0
              0
0
0
              -67.79087067
              -135.5817413
0
0
               -203.3726196
0
               -271.1634827
0
              -338.9543762
               -203.3726196
```

The data output from the instrument under test is as follows.

```
0.389050007
                  1.22E-03
0.778159976
                  2.59E-03
0.972689986
                 2.90E-03
                  3.14E-03
3.38E-03
1.167140007
1.555999994
1.944839954
                 3.56E-03
                 4.77E-03
0.972599983
-1E-05
                  -1.00E-05
                2.10E-04
-0.388886005
-0.777750015
                  5.10E-04
                 6.90E-04
-0.972150028
-1.166540027
                 8.80E-04
-1.555330038
                  1.30E-03
-1.944100022
                  1.78E-03
-0.971710026
                  5.80E-04
4.00E-05
                  3.00E-05
                0.271560013
0.543290019
-4.40E-04
-1.30E-03
-2.40E-03
                 0.815069973
-3.82E-03
                 1.086820006
-5.28E-03
                  1.358809948
```

```
0.815530002
-2.57E-03
1.50E-04
                  1.00E-05
Λ
                  Ω
1.44E-03
                  -0.271450013
                  -0.543120027
3.06E-03
4.46E-03
                  -0.814930022
5.67E-03
                   -1.086799979
6.88E-03
                  -1.35879004
4.51E-03
                  -0.815479994
-2.00E-05
                   0
```

The code to compute the crosstalk errors given the above raw data is then as follows.

```
program main
  ! Parameters
  integer(i32), parameter :: npts = 34
  integer(i32), parameter :: ndof = 2
  ! Local Variables
  integer(i32) :: indices(2*ndof)
  real(dp), dimension(npts, ndof) :: xin, xout, xerr, xmeas
  real(dp), dimension(ndof, npts) :: xint, xmeast
  real(dp), dimension(ndof, ndof) :: c, ans, xt
  ! Initialization
  -203.3726184, -271.1634912, -338.954364, -203.3726184, 0.0], &
      [npts, ndof])
         reshape([0.0, 0.38905, 0.77816, 0.97269, 1.16714, 1.556,
      1.94484, 0.9726, -1.0e-5, 0.0, -0.388886, -0.77775, -0.97215, & -1.16654, -1.55533, -1.9441, -0.97171, 4.0e-5, 0.0, -0.00044, & -0.0013, -0.0024, -0.00382, -0.00528, -0.00257, 0.00015, 0.0, & 0.00144, 0.00306, 0.00446, 0.00567, 0.00688, 0.00451, -2.0e-5, &
      0.0, 0.00122, 0.00259, 0.0029, 0.00314, 0.00338, 0.00356, 0.00477,&
      -1.0e-5, 0.0, 0.00021, 0.00051, 0.00069, 0.00088, 0.0013, 0.00178, \& 0.00058, 3.0e-5, 0.0, 0.27156, 0.54329, 0.81507, 1.08682, 1.35881, \&
      0.81553, 1.0e-5, 0.0, -0.27145, -0.54312, -0.81493, -1.0868, &
      -1.35879, -0.81548, 0.0], [npts, ndof])
  ! Compute the calibration gains
  xint = transpose(xin)
  xmeast = transpose(xout)
  c = linear_least_squares(xmeast, xint)
  xmeas = matmul(xout, transpose(c))
  xerr = xmeas - xin
  ! The indices are
  indices = [1, 17, 18, 34]
  ! Compute the crosstalk matrix
 xt = crosstalk(xerr, indices)
```

The least squares fit generates the following matrix of calibration gains.

```
7713.710427 33.5206917
-0.214743728 249.4768498
```

The resulting measured values are then as follows.

```
Ω
                  Ω
3001.05999
                  0.220815702
                 0.479040049
6002.58754
                 0.514603781
7503.146099
9003.085297
                  0.532721294
12002.64668
                  0.509090486
15002.05157
                 0.470495427
                 0.981144827
7502.514526
-0.077472309
                  -0.002492621
                0.135900968
-2999.74699
-5999.321307
                  0.294250127
-7498.860677
                 0.380902151
                0.470046784
-8998.322469
-11997.32196
                  0.658317276
```

-14996.16495	0.861552092
-7495.47032	0.353365205
0.30955403	7.48E-03
0	0
5.708846869	67.74803112
8.183633648	135.5385616
8.808803389	203.3416047
6.96458466	271.1372518
4.81985707	338.9927591
7.512893885	203.4564077
1.157391826	2.46E-03
0	0
2.008550989	-67.72080332
5.398195074	-135.4965304
7.086130239	-203.3071324
7.306450061	-271.1326527
7.522743936	-338.9881361
7.453379661	-203.4443484
-0.154274205	4.29E-06

The crosstalk error matrix is then as follows.

```
0 0.981144827
8.808803389 0
```

Definition at line 885 of file curvefit calibration.f90.

5.3 curvefit_core Module Reference

curvefit_core

Data Types

• interface is_monotonic

Tests to see if an array is montonically increasing or decreasing.

· interface reg_fcn

Describes a routine for finding the coefficients of a function of one variable.

Functions/Subroutines

• pure logical function is_monotonic_dbl (x)

Tests to see if an array is montonically increasing or decreasing.

• pure logical function is_monotonic_i32 (x)

Tests to see if an array is montonically increasing or decreasing.

Variables

• integer, parameter, public dp = real64

Defines a double-precision (64-bit) floating-point type.

• integer, parameter, public i32 = int32

Defines a 32-bit signed integer type.

• integer, parameter, public cf array size error = NL ARRAY SIZE ERROR

An error flag denoting an improperly sized array.

• integer, parameter, public cf_out_of_memory_error = NL_OUT_OF_MEMORY_ERROR

An error denoting that there is insufficient memory available.

• integer, parameter, public cf_no_data_defined_error = 300

An error denoting that no data has been defined.

- integer, parameter, public cf_invalid_input_error = NL_INVALID_INPUT_ERROR

 An error flag denoting an invalid input.
- integer, parameter, public cf_nonmonotonic_array_error = 301

An error flag denoting a non-monotonic array was given when a monotonic array was expected.

- integer, parameter, public cf_invalid_operation_error = NL_INVALID_OPERATION_ERROR

 An error resulting from an invalid operation.
- integer, parameter, public cf_convergence_error = NL_CONVERGENCE_ERROR

 An error resulting from a lack of convergence.
- integer, parameter, public cf_tolerance_too_small_error = NL_TOLERANCE_TOO_SMALL_ERROR

 An error indicating the user-requested tolerance is too small to be practical for the problem at hand.
- integer, parameter, public cf_array_index_error = 302

 An error indicating an array index was out of bounds.

5.3.1 Detailed Description

curvefit_core

Purpose

To provide core types and routines for the CURVEFIT library.

- 5.3.2 Function/Subroutine Documentation
- 5.3.2.1 pure logical function curvefit_core::is_monotonic_dbl (real(dp), dimension(:), intent(in) x)

Tests to see if an array is montonically increasing or decreasing.

Parameters

ſ	in	X	The array to test.

Returns

Returns true if x is monotonic; else, false.

Definition at line 105 of file curvefit_core.f90.

5.3.2.2 pure logical function curvefit_core::is_monotonic_i32 (integer(i32), dimension(:), intent(in) x) [private]

Tests to see if an array is montonically increasing or decreasing.

in	X	The array to test.

Returns

Returns true if x is monotonic; else, false.

Definition at line 139 of file curvefit_core.f90.

5.4 curvefit_interp Module Reference

curvefit_interp

Data Types

· type interp_manager

Describes an abstract base class allowing for interpolation of X-Y type data sets.

interface interp_xy

Defines the signature of a method used to interpolate a single value in an X-Y data set.

type linear_interp

Extends the interp_manager class allowing for linear, piecewise interpolation of a data set.

type polynomial interp

Extends the interp_manager class allowing for polynomial interpolation of a data set.

type spline_interp

Extends the interp_manager class allowing for cubic spline interpolation of a data set.

Functions/Subroutines

• subroutine im init (this, x, y, order, err)

Initializes the specified interp_manager instance.

integer function im_locate (this, pt, err)

Attempts to locate the index in the array providing a lower bounds to the specified interpolation point.

• integer(i32) function im_hunt (this, pt, err)

Attempts to locate the index in the array providing a lower bounds to the specified interpolation point. This method is typically more efficient than locate when the current index does not stray too far from the previous.

real(dp) function im perform (this, pt, err)

Interpolates to obtain the function value at the specified independent variable.

real(dp) function, dimension(size(pts)) im_perform_array (this, pts, err)

Interpolates to obtain the function value at the specified independent variables.

pure integer(i32) function im_get_num_pts (this)

Gets the number of stored data points.

• pure real(dp) function im get x (this, ind)

Gets the x component of the requested data point.

pure real(dp) function im_get_y (this, ind)

Gets the y component of the requested data point.

real(dp) function li raw interp (this, jlo, pt)

Performs the actual linear interpolation.

• subroutine pi_init (this, x, y, order, err)

Initializes the specified polynomial_interp instance.

real(dp) function pi raw interp (this, jlo, pt)

Performs the actual interpolation.

• subroutine penta_solve (a1, a2, a3, a4, a5, b, x)

Solves a pentadiagonal system of linear equations. A pentadiagonal matrix is all zeros with the exception of the diagonal, and the two immediate sub and super-diagonals. The entries of row I are stored as follows: $A(I,I-2) \rightarrow A1(I)$ $A(I,I-1) \rightarrow A2(I)$ $A(I,I) \rightarrow A3(I)$ $A(I,I+1) \rightarrow A4(I)$ $A(I,I+2) \rightarrow A5(I)$

real(dp) function si_raw_interp (this, jlo, pt)

Performs the actual interpolation.

subroutine si second deriv (this, ibcbeg, ybcbeg, ibcend, ybcend, err)

Computes the second derivative terms for the cubic-spline model.

subroutine si_init_1 (this, x, y, order, err)

Initializes the specified spline_interp instance. The end points are considered free such that the interpolant is quadratic over both the initial and final intervals.

subroutine si init 2 (this, x, y, ibcbeg, ybcbeg, ibcend, ybcend, err)

Initializes the specified spline_interp instance.

• real(dp) function si_diff1 (this, pt, err)

Interpolates to obtain the first derivative value at the specified independent variable.

real(dp) function, dimension(size(pts)) si_diff1_array (this, pts, err)

Interpolates to obtain the first derivative value at the specified independent variables.

real(dp) function si_diff2 (this, pt, err)

Interpolates to obtain the second derivative value at the specified independent variable.

• real(dp) function, dimension(size(pts)) si_diff2_array (this, pts, err)

Interpolates to obtain the second derivative value at the specified independent variables.

Variables

integer(i32), parameter, public spline_quadratic_over_interval = 1000

Indicates that the spline is quadratic over the interval under consideration (beginning or ending interval). This is equivalent to allowing a "natural" boundary condition at either the initial or final point.

integer(i32), parameter, public spline known first derivative = 1001

Indicates a known first derivative at either the beginning or ending point.

• integer(i32), parameter, public spline_known_second_derivative = 1002

Indicates a known second derivative at either the beginning or ending point.

integer(i32), parameter, public spline_continuous_third_derivative = 1003

Indicates a continuous third derivative at either the beginning or ending point.

5.4.1 Detailed Description

curvefit_interp

Purpose

To provide interpolation routines for X-Y data sets.

5.4.2 Function/Subroutine Documentation

5.4.2.1 pure integer(i32) function curvefit_interp::im_get_num_pts (class(interp_manager), intent(in) this) [private]

Gets the number of stored data points.

Parameters

iı	this	The interp	_manager object.
----	------	------------	------------------

Returns

The number of data points.

Definition at line 506 of file curvefit_interp.f90.

5.4.2.2 pure real(dp) function curvefit_interp::im_get_x (class(interp_manager), intent(in) this, integer(i32), intent(in) ind) [private]

Gets the x component of the requested data point.

Parameters

in	this	The interp_manager object.
in	ind	The one-based index of the data point to retrieve.

Returns

The x component of the requested data point.

Definition at line 520 of file curvefit_interp.f90.

5.4.2.3 pure real(dp) function curvefit_interp::im_get_y (class(interp_manager), intent(in) this, integer(i32), intent(in) ind) [private]

Gets the y component of the requested data point.

Parameters

in	this	The interp_manager object.
in	ind	The one-based index of the data point to retrieve.

Returns

The y component of the requested data point.

Definition at line 535 of file curvefit_interp.f90.

5.4.2.4 integer(i32) function curvefit_interp::im_hunt (class(interp_manager), intent(inout) this, real(dp), intent(in) pt, class(errors), intent(inout), optional, target err) [private]

Attempts to locate the index in the array providing a lower bounds to the specified interpolation point. This method is typically more efficient than locate when the current index does not stray too far from the previous.

Parameters

in,out	this	The interp_manager instance.	
in	pt	The interpolation point.	
out	err	An optional errors-based object that if provided can be used to retrieve information relating to any errors encountered during execution. If not provided, a default implementation of the errors class is used internally to provide error handling. Possible errors and warning messages that may be encountered are as follows. • CF_NO_DATA_DEFINED_ERROR: Occurs if no data has yet been defined.	

Returns

The array index below pt.

Definition at line 337 of file curvefit_interp.f90.

5.4.2.5 subroutine curvefit_interp::im_init (class(interp_manager), intent(inout) *this*, real(dp), dimension(:), intent(in) *x*, real(dp), dimension(:), intent(in) *y*, integer(i32), intent(in), optional *order*, class(errors), intent(inout), optional, target *err*)

Initializes the specified interp_manager instance.

Parameters

in,out	this	The interp_manager instance.	
in	X	An N-element array containing the independent variable data. The data in this array must be either monotonically increasing or decreasing.	
in	У	An N-element array containing the dependent variable data.	
in	order	The order of the interpolating polynomial. Notice, this parameter is optional; however, if not specified, a default of 1 is used.	
out	err	An optional errors-based object that if provided can be used to retrieve information relating to any errors encountered during execution. If not provided, a default implementation of the errors class is used internally to provide error handling. Possible errors and warning messages that may be encountered are as follows. • CF_ARRAY_SIZE_ERROR: Occurs if x and y are not the same size. • CF_OUT_OF_MEMORY_ERROR: Occurs if there is insufficient memory available. • CF_NONMONOTONIC_ARRAY_ERROR: Occurs if x is not monotonically	
		increasing or decreasing.	

Definition at line 184 of file curvefit_interp.f90.

5.4.2.6 integer function curvefit_interp::im_locate (class(interp_manager), intent(inout) this, real(dp), intent(in) pt, class(errors), intent(inout), optional, target err) [private]

Attempts to locate the index in the array providing a lower bounds to the specified interpolation point.

in,out	this	The interp_manager instance.
--------	------	------------------------------

Parameters

in	pt	The interpolation point.
out	err	An optional errors-based object that if provided can be used to retrieve information relating to any errors encountered during execution. If not provided, a default implementation of the errors class is used internally to provide error handling. Possible errors and warning messages that may be encountered are as follows. • CF_NO_DATA_DEFINED_ERROR: Occurs if no data has yet been defined.
1	1	

Returns

The array index below pt.

Definition at line 262 of file curvefit_interp.f90.

5.4.2.7 real(dp) function curvefit_interp::im_perform (class(interp_manager), intent(inout) this, real(dp), intent(in) pt, class(errors), intent(inout), optional, target err) [private]

Interpolates to obtain the function value at the specified independent variable.

Parameters

in,out	this	The interp_manager instance.
in	pt	The independent variable value to interpolate.
out	err	An optional errors-based object that if provided can be used to retrieve information relating to any errors encountered during execution. If not provided, a default implementation of the errors class is used internally to provide error handling. Possible errors and warning messages that may be encountered are as follows.
		CF_NO_DATA_DEFINED_ERROR: Occurs if no data has yet been defined.

Returns

The interpolated value.

Definition at line 445 of file curvefit_interp.f90.

5.4.2.8 real(dp) function, dimension(size(pts)) curvefit_interp::im_perform_array (class(interp_manager), intent(inout) this, real(dp), dimension(:), intent(in) pts, class(errors), intent(inout), optional, target err) [private]

Interpolates to obtain the function value at the specified independent variables.

in,out	this	The interp_manager instance.
in	pts	An M-element array containing the independent variable values to interpolate.
out	err	An optional errors-based object that if provided can be used to retrieve information relating to any errors encountered during execution. If not provided, a default implementation of the errors class is used internally to provide error handling. Possible errors and warning messages that may be encountered are as follows.
		CF_NO_DATA_DEFINED_ERROR: Occurs if no data has yet been defined.
		Generated by Doxygen

Returns

An M-element array containing the interpolated values.

Definition at line 479 of file curvefit interp.f90.

5.4.2.9 real(dp) function curvefit_interp::li_raw_interp (class(linear_interp), intent(inout) this, integer(i32), intent(in) jlo, real(dp), intent(in) pt) [private]

Performs the actual linear interpolation.

Parameters

in,out	this	The linear_interp_mgr instance.
in	jlo	The array index below which pt is found in x.
in	pt	The independent variable value to interpolate.

Returns

The interpolated value.

Definition at line 554 of file curvefit_interp.f90.

5.4.2.10 subroutine curvefit_interp::penta_solve (real(dp), dimension(:), intent(in) a1, real(dp), dimension(:), intent(inout) a2, real(dp), dimension(:), intent(inout) a3, real(dp), dimension(:), intent(inout) a4, real(dp), dimension(:), intent(in) a5, real(dp), dimension(:), intent(inout) b, real(dp), dimension(:), intent(out) x) [private]

Solves a pentadiagonal system of linear equations. A pentadiagonal matrix is all zeros with the exception of the diagonal, and the two immediate sub and super-diagonals. The entries of row I are stored as follows: A(I,I-2) -> A1(I) A(I,I-1) -> A2(I) A(I,I) -> A3(I) A(I,I+1) -> A4(I) A(I,I+2) -> A5(I)

Parameters

in	a1	An N-element array as defined above.
in,out	a2	An N-element array as defined above. This array is overwritten by this routine during the solution process.
in,out	а3	An N-element array as defined above. This array is overwritten by this routine during the solution process.
in,out	a4	An N-element array as defined above. This array is overwritten by this routine during the solution process.
in	а5	An N-element array as defined above.
in,out	b	An N-element array containing the right-hand-side. This array is overwritten by this routine during the solution process.
out	Х	An N-element array that, on output, contains the solution to the linear system.

• Spline Library

Definition at line 732 of file curvefit_interp.f90.

5.4.2.11 subroutine curvefit_interp::pi_init (class(polynomial_interp), intent(inout) this, real(dp), dimension(:), intent(in) x, real(dp), dimension(:), intent(in) y, integer(i32), intent(in), optional order, class(errors), intent(inout), optional, target err
) [private]

Initializes the specified polynomial_interp instance.

Parameters

in,out	this	The polynomial_interp instance.
in	Х	An N-element array containing the independent variable data. The data in this array must be either monotonically increasing or decreasing.
in	У	An N-element array containing the dependent variable data.
in	order	The order of the interpolating polynomial. Notice, this parameter is optional; however, if not specified, a default of 1 is used.
out	err	An optional errors-based object that if provided can be used to retrieve information relating to any errors encountered during execution. If not provided, a default implementation of the errors class is used internally to provide error handling. Possible errors and warning messages that may be encountered are as follows.
		• CF_ARRAY_SIZE_ERROR: Occurs if ${\bf x}$ and ${\bf y}$ are not the same size.
		CF_OUT_OF_MEMORY_ERROR: Occurs if there is insufficient memory available.
		CF_INVALID_INPUT_ERROR: Occurs if order is less than 1.
		 CF_NONMONOTONIC_ARRAY_ERROR: Occurs if x is not monotonically increasing or decreasing.

Definition at line 595 of file curvefit_interp.f90.

5.4.2.12 real(dp) function curvefit_interp::pi_raw_interp (class(polynomial_interp), intent(inout) this, integer(i32), intent(in) jlo, real(dp), intent(in) pt) [private]

Performs the actual interpolation.

Parameters

in,out	this	The polynomial_interp instance.
in	jlo	The array index below which pt is found in x.
in	pt	The independent variable value to interpolate.

Returns

The interpolated value.

Definition at line 649 of file curvefit_interp.f90.

5.4.2.13 real(dp) function curvefit_interp::si_diff1 (class(spline_interp), intent(inout) this, real(dp), intent(in) pt, class(errors), intent(inout), optional, target err) [private]

Interpolates to obtain the first derivative value at the specified independent variable.

Parameters

in,out	this	The interp_manager instance.
in	pt	The independent variable value to interpolate.
out	err	An optional errors-based object that if provided can be used to retrieve information relating to any errors encountered during execution. If not provided, a default implementation of the errors class is used internally to provide error handling. Possible errors and warning messages that may be encountered are as follows. • CF_NO_DATA_DEFINED_ERROR: Occurs if no data has yet been defined.

Returns

The interpolated value.

Definition at line 1135 of file curvefit_interp.f90.

5.4.2.14 real(dp) function, dimension(size(pts)) curvefit_interp::si_diff1_array (class(spline_interp), intent(inout) this, real(dp), dimension(:), intent(in) pts, class(errors), intent(inout), optional, target err) [private]

Interpolates to obtain the first derivative value at the specified independent variables.

Parameters

in,out	this	The interp_manager instance.
in	pts	An M-element array containing the independent variable values to interpolate.
out	err	An optional errors-based object that if provided can be used to retrieve information relating to any errors encountered during execution. If not provided, a default implementation of the errors class is used internally to provide error handling. Possible errors and warning messages that may be encountered are as follows.
		CF_NO_DATA_DEFINED_ERROR: Occurs if no data has yet been defined.

Returns

An M-element array containing the interpolated values.

Definition at line 1181 of file curvefit_interp.f90.

5.4.2.15 real(dp) function curvefit_interp::si_diff2 (class(spline_interp), intent(inout) this, real(dp), intent(in) pt, class(errors), intent(inout), optional, target err) [private]

Interpolates to obtain the second derivative value at the specified independent variable.

in,out	this	The interp_manager instance.
in	pt	The independent variable value to interpolate.
out	err	An optional errors-based object that if provided can be used to retrieve information relating to any errors encountered during execution. If not provided, a default implementation of the errors class is used internally to provide error handling. Possible errors and warning messages that may be encountered are as follows.
Generated by Do	xygen	CF_NO_DATA_DEFINED_ERROR: Occurs if no data has yet been defined.

Returns

The interpolated value.

Definition at line 1228 of file curvefit_interp.f90.

5.4.2.16 real(dp) function, dimension(size(pts)) curvefit_interp::si_diff2_array (class(spline_interp), intent(inout) this, real(dp), dimension(:), intent(in) pts, class(errors), intent(inout), optional, target err) [private]

Interpolates to obtain the second derivative value at the specified independent variables.

Parameters

in,out	this	The interp_manager instance.
in	pts	An M-element array containing the independent variable values to interpolate.
out	err	An optional errors-based object that if provided can be used to retrieve information relating to any errors encountered during execution. If not provided, a default implementation of the errors class is used internally to provide error handling. Possible errors and warning messages that may be encountered are as follows. • CF_NO_DATA_DEFINED_ERROR: Occurs if no data has yet been defined.

Returns

An M-element array containing the interpolated values.

Definition at line 1266 of file curvefit_interp.f90.

5.4.2.17 subroutine curvefit_interp::si_init_1 (class(spline_interp), intent(inout) this, real(dp), dimension(:), intent(in) x, real(dp), dimension(:), intent(in) y, integer(i32), intent(in), optional order, class(errors), intent(inout), optional, target err
) [private]

Initializes the specified spline_interp instance. The end points are considered free such that the interpolant is quadratic over both the initial and final intervals.

in,out	this	The spline_interp instance.
in	Х	An N-element array containing the independent variable data. The data in this array must be either monotonically increasing or decreasing.
in	У	An N-element array containing the dependent variable data.
in	order	The order of the interpolating polynomial. This parameter is ignored as the spline is a cubic approximation.
out	err	An optional errors-based object that if provided can be used to retrieve information relating to any errors encountered during execution. If not provided, a default implementation of the errors class is used internally to provide error handling. Possible errors and warning messages that may be encountered are as follows.
		• CF_ARRAY_SIZE_ERROR: Occurs if ${\bf x}$ and ${\bf y}$ are not the same size.
		CF_OUT_OF_MEMORY_ERROR: Occurs if there is insufficient memory available.
		 CF_NONMONOTONIC_ARRAY_ERROR: Occurs if x is not monotonically increasing or decreasing.

Definition at line 989 of file curvefit_interp.f90.

5.4.2.18 subroutine curvefit_interp::si_init_2 (class(spline_interp), intent(inout) this, real(dp), dimension(:), intent(in) x, real(dp), dimension(:), intent(in) y, integer(i32), intent(in), optional ibcbeg, real(dp), intent(in), optional ybcbeg, integer(i32), intent(in), optional ibcend, real(dp), intent(in), optional ybcend, class(errors), intent(inout), optional, target err) [private]

Initializes the specified spline_interp instance.

in,out	this	The spline_interp instance.	
in	Х	An N-element array containing the independent variable data. The data in this array must be either monotonically increasing or decreasing.	
in	У	An N-element array containing the dependent variable data.	
in	ibcbeg	An optional input that defines the nature of the boundary condition at the beginning of the spline. If no parameter, or an invalid parameter, is specified, the default natural condition (SPLINE_QUADRATIC_OVER_INTERVAL) is used. • SPLINE_QUADRATIC_OVER_INTERVAL: The spline is quadratic over its initial interval. No value is required for ybcbeg.	
		SPLINE_KNOWN_FIRST_DERIVATIVE: The spline's first derivative at its initial point is provided in ybobeg.	
		 SPLINE_KNOWN_SECOND_DERIVATIVE: The spline's second derivative at its initial point is provided in ybcbeg. 	
		 SPLINE_CONTINUOUS_THIRD_DERIVATIVE: The third derivative is continuous at x(2). No value is required for ybcbeg. 	
in	ybcbeg	If needed, the value of the initial point boundary condition. If needed, but not supplied, a default value of zero will be used.	
in	ibcend	An optional input that defines the nature of the boundary condition at the end of the spline. If no parameter, or an invalid parameter, is specified, the default natural condition (SPLINE_QUADRATIC_OVER_INTERVAL) is used.	
		 SPLINE_QUADRATIC_OVER_INTERVAL: The spline is quadratic over its final interval. No value is required for ybcend. 	
		 SPLINE_KNOWN_FIRST_DERIVATIVE: The spline's first derivative at its initial point is provided in ybcend. 	
		 SPLINE_KNOWN_SECOND_DERIVATIVE: The spline's second derivative at its initial point is provided in ybcend. 	
		SPLINE_CONTINUOUS_THIRD_DERIVATIVE: The third derivative is continuous at x(n-1). No value is required for ybcend.	
in	ybcend	If needed, the value of the final point boundary condition. If needed, but not supplied, a default value of zero will be used.	

Parameters

out	err	An optional errors-based object that if provided can be used to retrieve information relating to any errors encountered during execution. If not provided, a default implementation of the errors class is used internally to provide error handling. Possible errors and warning messages that may be encountered are as follows.
		• CF_ARRAY_SIZE_ERROR: Occurs if ${\bf x}$ and ${\bf y}$ are not the same size.
		 CF_OUT_OF_MEMORY_ERROR: Occurs if there is insufficient memory available.
		CF_INVALID_INPUT_ERROR: Occurs if order is less than 1.
		• CF_NONMONOTONIC_ARRAY_ERROR: Occurs if $\mathbf x$ is not monotonically increasing or decreasing.

Definition at line 1070 of file curvefit_interp.f90.

5.4.2.19 real(dp) function curvefit_interp::si_raw_interp (class(spline_interp), intent(inout) *this*, integer(i32), intent(in) *jlo*, real(dp), intent(in) *pt*) [private]

Performs the actual interpolation.

Parameters

in,out	this	The spline_interp instance.
in	jlo	The array index below which pt is found in x.
in	pt	The independent variable value to interpolate.

Returns

The interpolated value.

Definition at line 774 of file curvefit_interp.f90.

5.4.2.20 subroutine curvefit_interp::si_second_deriv (class(spline_interp), intent(inout) this, integer(i32), intent(in) ibcbeg, real(dp), intent(in) ybcbeg, integer(i32), intent(in) ibcend, real(dp), intent(in) ybcend, class(errors), intent(inout), optional, target err) [private]

Computes the second derivative terms for the cubic-spline model.

in,out	this	The spline_interp_mgr instance.
in	ibcbeg	Defines the nature of the boundary condition at the beginning of the spline.
		SPLINE_QUADRATIC_OVER_INTERVAL: The spline is quadratic over its initial interval.
		SPLINE_KNOWN_FIRST_DERIVATIVE: The spline's first derivative at its initial point is provided in ybcbeg.
		SPLINE_KNOWN_SECOND_DERIVATIVE: The spline's second derivative at its initial point is provided in ybcbeg.
		SPLINE_CONTINUOUS_THIRD_DERIVATIVE: The third derivative is continuous at x(2). Generated by Doxygen

Parameters

in	ybcbeg	If needed, the value of the initial point boundary condition.	
in	ibcend	Defines the nature of the boundary condition at the end of the spline.	
		 SPLINE_QUADRATIC_OVER_INTERVAL: The spline is quadratic over its final interval. 	
		 SPLINE_KNOWN_FIRST_DERIVATIVE: The spline's first derivative at its initial point is provided in ybcend. 	
		 SPLINE_KNOWN_SECOND_DERIVATIVE: The spline's second derivative at its initial point is provided in ybcend. 	
		 SPLINE_CONTINUOUS_THIRD_DERIVATIVE: The third derivative is continuous at x(n-1). 	
in	ybcend	If needed, the value of the final point boundary condition.	
out	err	An optional errors-based object that if provided can be used to retrieve information relating to any errors encountered during execution. If not provided, a default implementation of the errors class is used internally to provide error handling. Possible errors and warning messages that may be encountered are as follows. • CF_OUT_OF_MEMORY_ERROR: Occurs if there is insufficient memory available.	

Remarks

This code is a slight modification of the SPLINE_CUBIC_SET routine from the SPLINE library.

Definition at line 842 of file curvefit_interp.f90.

5.5 curvefit_regression Module Reference

curvefit_regression

Data Types

• interface linear_least_squares

Employs a least squares fit to determine the coefficient A in the linear system: Y = A * X, where A can either be a scalar, or a matrix.

• type lowess_smoothing

Defines a type for computing a smoothing of an X-Y data set using a robust locally weighted scatterplot smoothing (LOWESS) algorithm.

• interface moving_average

Applies a moving average to smooth a data set.

• type nonlinear_regression

A type for supporting nonlinear regression calculations.

Functions/Subroutines

• subroutine moving_average_1 (x, npts, err)

Applies a moving average to smooth a data set.

• subroutine lowest (x, y, xs, ys, nleft, nright, w, userw, rw, ok)

A support routine for the LOWESS library used to compute the smoothing of a desired value from a data set.

• subroutine lowess (x, y, f, nsteps, delta, ys, rw, res)

Computes a smoothing of an X-Y data set using a robust locally weighted scatterplot smoothing (LOWESS) algorithm. Fitted values are computed at each of the supplied x values.

subroutine Is_init (this, x, y, srt, err)

Initializes the lowess_smoothing object.

real(dp) function, dimension(:), allocatable ls_smooth (this, f, err)

Performs the actual smoothing operation.

pure integer(i32) function ls_get_num_pts (this)

Gets the number of stored data points.

pure real(dp) function ls_get_x (this, ind)

Gets the x component of the requested data point.

pure real(dp) function ls_get_y (this, ind)

Gets the y component of the requested data point.

• subroutine ls_get_residual (this, x)

Gets the residuals from each data point.

• subroutine nr_init (this, x, y, fcn, ncoeff, err)

Initializes the nonlinear_regression object.

• subroutine nr fcn (this, x, f)

Computes the residual between the supplied data set, and the function value given a set of coefficients.

• pure logical function nr_is_fcn_defined (this)

Determines if the function has been defined.

pure integer(i32) function nr_get_eqn_count (this)

Gets the number of equations required to solve the regression problem.

pure integer(i32) function nr_get_var_count (this)

Gets the number of variables (coefficients).

subroutine nr_solve (this, c, res, ib, err)

Computes the solution to the nonlinear regression problem using the Levenberg-Marquardt method.

pure integer(i32) function nr_get_max_eval (this)

Gets the maximum number of function evaluations allowed during a single solve.

subroutine nr_set_max_eval (this, n)

Sets the maximum number of function evaluations allowed during a single solve.

• pure real(dp) function nr_get_fcn_tol (this)

Gets the convergence on function value tolerance.

• subroutine nr_set_fcn_tol (this, x)

Sets the convergence on function value tolerance.

• pure real(dp) function nr_get_var_tol (this)

Gets the convergence on change in variable tolerance.

• subroutine nr_set_var_tol (this, x)

Sets the convergence on change in variable tolerance.

pure real(dp) function nr_get_grad_tol (this)

Gets the convergence on slope of the gradient vector tolerance.

subroutine nr_set_grad_tol (this, x)

Sets the convergence on slope of the gradient vector tolerance.

• pure logical function nr_get_print_status (this)

Gets a logical value determining if iteration status should be printed.

subroutine nr_set_print_status (this, x)

Sets a logical value determining if iteration status should be printed.

• pure integer(i32) function nr_get_num_pts (this)

Gets the number of stored data points.

pure real(dp) function nr_get_x (this, ind)

Gets the x component of the requested data point.

pure real(dp) function nr_get_y (this, ind)

Gets the y component of the requested data point.

real(dp) function linear_least_squares_1var (x, y, err)

Employs a least squares fit to determine the coefficient A in the linear system: Y = A * X.

real(dp) function, dimension(size(y, 1), size(x, 1)) linear_least_squares_nvar (x, y, thrsh, err)
 Employs a least squares fit to determine the coefficient A in the linear system: Y = A * X.

5.5.1 Detailed Description

curvefit_regression

Purpose

To provide routines for perforing regression operations, and other data smoothing operations on sets of numerical data.

5.5.2 Function/Subroutine Documentation

5.5.2.1 real(dp) function curvefit_regression::linear_least_squares_1var (real(dp), dimension(:), intent(in) x, real(dp), dimension(:), intent(inout) y, class(errors), intent(inout), optional, target err) [private]

Employs a least squares fit to determine the coefficient A in the linear system: Y = A * X.

Parameters

in	X	An N-element array containing the independent variable data.
in,out	У	An N-element array containing the dependent variable data corresponding to x. On output, the contents of this array are overwritten as it is used for storage purposes by the algorithm.
out	err	An optional errors-based object that if provided can be used to retrieve information relating to any errors encountered during execution. If not provided, a default implementation of the errors class is used internally to provide error handling. Possible errors and warning messages that may be encountered are as follows.
		 CF_OUT_OF_MEMORY_ERROR: Occurs if insufficient memory is available. CF_ARRAY_SIZE_ERROR: Occurs if x and y are different sizes.

Returns

The scalar coefficient A.

Definition at line 1081 of file curvefit_regression.f90.

5.5.2.2 real(dp) function, dimension(size(y,1), size(x,1)) curvefit_regression::linear_least_squares_nvar (real(dp), dimension(:,:), intent(inout) x, real(dp), dimension(:,:), intent(in) y, real(dp), intent(in), optional thrsh, class(errors), intent(inout), optional, target err) [private]

Employs a least squares fit to determine the coefficient A in the linear system: Y = A * X.

Parameters

in,out	X	An M-by-P matrix containing the P data points of the M independent variables.
in	У	An N-by-P matrix containing the P data points of the N dependent variables.
in	thrsh	An optional threshold value that defines a lower cutoff for singular values. Any singular values falling below this value will have their reciprocal replaced with zero.
out	err	An optional errors-based object that if provided can be used to retrieve information relating to any errors encountered during execution. If not provided, a default implementation of the errors class is used internally to provide error handling. Possible errors and warning messages that may be encountered are as follows.
		 CF_ARRAY_SIZE_ERROR: Occurs if any of the matrix dimensions are not compatiable. CF_OUT_OF_MEMORY_ERROR: Occurs if there is insufficient memory available.

Returns

An N-by-M matrix relating Y to X such that: Y = A * X.

Remarks

The algorithm attempts to compute the coefficient matrix A as follows. Y * X * * T = A * X * X * * T Y * X * * T * INV(X * X * * T) = A This does require that <math>X * X * * T does not result in a singular matrix. To handle the situation where X * X * * T is singular, the Moore-Penrose pseudo-inverse, computed by means of singular value decomposition, is utilized to still arrive at a solution that, at minimum, has a minimum Euclidean norm of its residual. Let: PINV(X) = X * * T * INV(X * X * * T), Then: A = Y * PINV(X)

Definition at line 1150 of file curvefit regression.f90.

5.5.2.3 subroutine curvefit_regression::lowess (real(dp), dimension(:), intent(in) x, real(dp), dimension(:), intent(in) y, real(dp), intent(in) f, integer(i32), intent(in) nsteps, real(dp), intent(in) delta, real(dp), dimension(:), intent(out) ys, real(dp), dimension(:), intent(out) res) [private]

Computes a smoothing of an X-Y data set using a robust locally weighted scatterplot smoothing (LOWESS) algorithm. Fitted values are computed at each of the supplied x values.

in	X	An N-element containing the independent variable values of the data set. This array must be in a monotonically increasing order.
in	У	An N-element array of the dependent variables corresponding to \boldsymbol{x} .
in	f	Specifies the amount of smoothing. More specifically, this value is the fraction of points used to compute each value. As this value increases, the output becomes smoother. Choosing a value in the range of 0.2 to 0.8 usually results in a good fit. As such, a reasonable starting point, in the absence of better information, is a value of 0.5.
in	nsteps	The number of iterations in the robust fit. If set to zero, a nonrobust fit is returned. Seeting this parameter equal to 2 should serve most purposes.

Parameters

in	delta	A nonnegative parameter which may be used to save computations. If N is less than 100, set delta equal to 0.0. If N is larger than 100, set delta = $\operatorname{range}(x) / k$, where k determines the interpolation window used by the linear weighted regression computations.
out	ys	An N-element array that, on output, contains the fitted values.
out	rw	An N-element array that, on output, contains the robustness weights given to each data point.
out	rs	An N-element array that, on output, contains the residual y - ys.

Remarks

This routines is an implementation of the LOWESS routine from the LOWESS library. A link to this library, along with a basic description of the algorithm is available here. For a detailed understanding of the algorithm, see the paper by William Cleveland.

Definition at line 362 of file curvefit regression.f90.

5.5.2.4 subroutine curvefit_regression::lowest (real(dp), dimension(:), intent(in) x, real(dp), dimension(:), intent(in) y, real(dp), intent(in) xs, real(dp), intent(out) ys, integer(i32), intent(in) nleft, integer(i32), intent(in) nright, real(dp), dimension(:), intent(out) w, logical, intent(in) userw, real(dp), dimension(:), intent(in) rw, logical, intent(out) ok) [private]

A support routine for the LOWESS library used to compute the smoothing of a desired value from a data set.

Parameters

in	Х	An N-element containing the independent variable values of the data set. This array must be in a monotonically increasing order.
in	У	An N-element array of the dependent variables corresponding to x.
in	xs	The value of the independent variable at which the smoothing is computed.
out	ys	The fitted value.
in	nleft	The index of the first point which should be considered in computing the fit.
in	nright	The index of the last point which should be considered in computing the fit.
out	W	An N-element array that, on output, contains the weights for y in the expression for ys.
in	userw	If true, a robust fit is carried out using the weights in rw. If false, the values in rw are not used.
in	rw	An N-element array containing the robustness weights.
out	ok	Returns true if the calculations were performed; however, returns false if the weights are all zero-valued.

Remarks

This routines is an implementation of the LOWEST routine from the LOWESS library. A link to this library, along with a basic description of the algorithm is available here. For a detailed understanding of the algorithm, see the paper by William Cleveland.

Definition at line 250 of file curvefit_regression.f90.

5.5.2.5 pure integer(i32) function curvefit_regression::ls_get_num_pts (class(lowess_smoothing), intent(in) this) [private]

Gets the number of stored data points.

Parameters

|--|

Returns

The number of data points.

Definition at line 613 of file curvefit_regression.f90.

5.5.2.6 subroutine curvefit_regression::ls_get_residual (class(lowess_smoothing), intent(in) *this*, real(dp), dimension(:), intent(out) x) [private]

Gets the residuals from each data point.

Parameters

in	this	The lowess_smoothing object.
out	Χ	An N-element array where the residual data should be written.

Definition at line 665 of file curvefit_regression.f90.

5.5.2.7 pure real(dp) function curvefit_regression::ls_get_x (class(lowess_smoothing), intent(in) *this*, integer(i32), intent(in) *ind*) [private]

Gets the x component of the requested data point.

Parameters

in	this	The lowess_smoothing object.
in	ind	The one-based index of the data point to retrieve.

Returns

The x component of the requested data point.

Definition at line 630 of file curvefit_regression.f90.

5.5.2.8 pure real(dp) function curvefit_regression::ls_get_y (class(lowess_smoothing), intent(in) *this*, integer(i32), intent(in) *ind*) [private]

Gets the y component of the requested data point.

in	this	The lowess_smoothing object.
in	ind	The one-based index of the data point to retrieve.

Returns

The y component of the requested data point.

Definition at line 648 of file curvefit_regression.f90.

5.5.2.9 subroutine curvefit_regression::ls_init (class(lowess_smoothing), intent(inout) this, real(dp), dimension(:), intent(in) x, real(dp), dimension(:), intent(in) y, logical, intent(in), optional srt, class(errors), intent(inout), optional, target err) [private]

Initializes the lowess_smoothing object.

Parameters

in,out	this	The lowess_smoothing object.
in	Х	An N-element containing the independent variable values of the data set. This array must be in a monotonically increasing order. The routine is capable of sorting the array into ascending order, dependent upon the value of \mathtt{srt} . If sorting is performed, this routine will also shuffle y to match.
in	У	An N-element array of the dependent variables corresponding to x.
in	srt	An optional flag determining if \mathbf{x} should be sorted. The default is to sort (true).
out	err	An optional errors-based object that if provided can be used to retrieve information relating to any errors encountered during execution. If not provided, a default implementation of the errors class is used internally to provide error handling. Possible errors and warning messages that may be encountered are as follows.
		 CF_ARRAY_SIZE_ERROR: Occurs if x and y are not the same size. CF_OUT_OF_MEMORY_ERROR: Occurs if there is insufficient memory available.

Definition at line 477 of file curvefit_regression.f90.

5.5.2.10 real(dp) function, dimension(:), allocatable curvefit_regression::ls_smooth (class(lowess_smoothing), intent(inout) this, real(dp), intent(in) f, class(errors), intent(inout), optional, target err) [private]

Performs the actual smoothing operation.

in,out	this	The lowess_smoothing object.
in	f	Specifies the amount of smoothing. More specifically, this value is the fraction of points used to compute each value. As this value increases, the output becomes smoother. Choosing a value in the range of 0.2 to 0.8 usually results in a good fit. As such, a reasonable starting point, in the absence of better information, is a value of 0.5.
out	err	An optional errors-based object that if provided can be used to retrieve information relating to any errors encountered during execution. If not provided, a default implementation of the errors class is used internally to provide error handling. Possible errors and warning messages that may be encountered are as follows.
		 CF_NO_DATA_DEFINED_ERROR: Occurs if no data has been defined. CF_OUT_OF_MEMORY_ERROR: Occurs if there is insufficient memory available.

Returns

The smoothed data points.

Definition at line 569 of file curvefit_regression.f90.

5.5.2.11 subroutine curvefit_regression::moving_average_1 (real(dp), dimension(:), intent(inout) x, integer(i32), intent(in) npts, class(errors), intent(inout), optional, target err) [private]

Applies a moving average to smooth a data set.

Parameters

in,out	Х	On input, the signal to smooth. On output, the smoothed signal.
in	npts	The size of the averaging window. This value must be at least 2, but no more than the number of elements in \mathbf{x} .
out	err	An optional errors-based object that if provided can be used to retrieve information relating to any errors encountered during execution. If not provided, a default implementation of the errors class is used internally to provide error handling. Possible errors and warning messages that may be encountered are as follows.
		 CF_INVALID_INPUT_ERROR: Occurs if npts is less than 2, or greater than the length of x. CF_OUT_OF_MEMORY_ERROR: Occurs if there is insufficient memory available.

Definition at line 164 of file curvefit_regression.f90.

5.5.2.12 subroutine curvefit_regression::nr_fcn (class(nonlinear_regression), intent(in) *this*, real(dp), dimension(:), intent(in) *x*, real(dp), dimension(:), intent(out) *f*) [private]

Computes the residual between the supplied data set, and the function value given a set of coefficients.

Parameters

in	this	The nonlinear_regression object.
in	Х	An N-element array containing the N coefficients.
out	f	An M-element array that, on output, contains the residual at each of the M data points.

Definition at line 766 of file curvefit_regression.f90.

5.5.2.13 pure integer(i32) function curvefit_regression::nr_get_eqn_count (class(nonlinear_regression), intent(in) this) [private]

Gets the number of equations required to solve the regression problem.

in	this	The nonlinear_regression object.
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Returns

The number of equations.

Definition at line 801 of file curvefit_regression.f90.

5.5.2.14 pure real(dp) function curvefit_regression::nr_get_fcn_tol (class(nonlinear_regression), intent(in) this)

[private]

Gets the convergence on function value tolerance.

Parameters

in	this	The nonlinear_regression object.	ne nonlinear_regression object.
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Returns

The tolerance value.

Definition at line 925 of file curvefit regression.f90.

5.5.2.15 pure real(dp) function curvefit_regression::nr_get_grad_tol (class(nonlinear_regression), intent(in) this)
[private]

Gets the convergence on slope of the gradient vector tolerance.

Parameters

ir	l	this	The nonlinear_	regression object.
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Returns

The tolerance value.

Definition at line 969 of file curvefit_regression.f90.

5.5.2.16 pure integer(i32) function curvefit_regression::nr_get_max_eval (class(nonlinear_regression), intent(in) this) [private]

Gets the maximum number of function evaluations allowed during a single solve.

Parameters

in	this	The nonlinear_	regression object.

Returns

The maximum number of function evaluations.

Definition at line 902 of file curvefit_regression.f90.

5.5.2.17 pure integer(i32) function curvefit_regression::nr_get_num_pts (class(nonlinear_regression), intent(in) this)

[private]

Gets the number of stored data points.

Parameters

in	this	The nonlinear_regression object.
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Returns

The number of data points.

Definition at line 1016 of file curvefit_regression.f90.

5.5.2.18 pure logical function curvefit_regression::nr_get_print_status (class(nonlinear_regression), intent(in) this) [private]

Gets a logical value determining if iteration status should be printed.

Parameters

in	this	The nonlinear	regression object.
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Returns

True if the iteration status should be printed; else, false.

Definition at line 992 of file curvefit_regression.f90.

5.5.2.19 pure integer(i32) function curvefit_regression::nr_get_var_count (class(nonlinear_regression), intent(in) this) [private]

Gets the number of variables (coefficients).

Parameters

-				
	in	this	The nonlinear_	regression object.

Returns

The number of variables.

Definition at line 817 of file curvefit_regression.f90.

5.5.2.20 pure real(dp) function curvefit_regression::nr_get_var_tol (class(nonlinear_regression), intent(in) this) [private]

Gets the convergence on change in variable tolerance.

Parameters

|--|

Returns

The tolerance value.

Definition at line 947 of file curvefit_regression.f90.

5.5.2.21 pure real(dp) function curvefit_regression::nr_get_x (class(nonlinear_regression), intent(in) *this*, integer(i32), intent(in) *ind*) [private]

Gets the x component of the requested data point.

Parameters

in	this	The nonlinear_regression object.
in	ind	The one-based index of the data point to retrieve.

Returns

The x component of the requested data point.

Definition at line 1033 of file curvefit_regression.f90.

5.5.2.22 pure real(dp) function curvefit_regression::nr_get_y (class(nonlinear_regression), intent(in) this, integer(i32), intent(in) ind) [private]

Gets the y component of the requested data point.

Parameters

in	this	The nonlinear_regression object.
in	ind	The one-based index of the data point to retrieve.

Returns

The y component of the requested data point.

Definition at line 1051 of file curvefit_regression.f90.

5.5.2.23 subroutine curvefit_regression::nr_init (class(nonlinear_regression), intent(inout) this, real(dp), dimension(:), intent(in) x, real(dp), dimension(:), intent(in) y, procedure(reg_fcn), intent(in), pointer fcn, integer(i32), intent(in) fncoeff, class(errors), intent(inout), optional, target fncoeff, class(errors), intent(inout), optional, i

Initializes the nonlinear_regression object.

Parameters

in,out	this	The nonlinear_regression object.
in	X	An N-element containing the independent variable values of the data set.
in	У	An N-element array of the dependent variables corresponding to x.
in	fcn	A pointer to the function whose coefficients are to be determined.
in	ncoeff	The number of coefficients in the function defined in fcn.
out	err	An optional errors-based object that if provided can be used to retrieve information relating to any errors encountered during execution. If not provided, a default implementation of the errors class is used internally to provide error handling. Possible errors and warning messages that may be encountered are as follows. • CF_ARRAY_SIZE_ERROR: Occurs if x and y are not the same size. • CF_OUT_OF_MEMORY_ERROR: Occurs if there is insufficient memory available. • CF_INVALID_INPUT_ERROR: Occurs if ncoeff is less than or equal to zero.

Definition at line 702 of file curvefit_regression.f90.

5.5.2.24 pure logical function curvefit_regression::nr_is_fcn_defined (class(nonlinear_regression), intent(in) this) [private]

Determines if the function has been defined.

Parameters

in	this	The nonlinear_	regression object.
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Returns

Returns true if the function has been defined; else, false.

Definition at line 788 of file curvefit_regression.f90.

5.5.2.25 subroutine curvefit_regression::nr_set_fcn_tol (class(nonlinear_regression), intent(inout) this, real(dp), intent(in) x) [private]

Sets the convergence on function value tolerance.

Parameters

in,out	this	The nonlinear_regression object.
in	Χ	The tolerance value.

Definition at line 936 of file curvefit_regression.f90.

5.5.2.26 subroutine curvefit_regression::nr_set_grad_tol (class(nonlinear_regression), intent(inout) this, real(dp), intent(in) x) [private]

Sets the convergence on slope of the gradient vector tolerance.

Parameters

in	this	The nonlinear_	regression object.	1
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Returns

The tolerance value.

Definition at line 980 of file curvefit_regression.f90.

5.5.2.27 subroutine curvefit_regression::nr_set_max_eval (class(nonlinear_regression), intent(inout) this, integer(i32), intent(in) n) [private]

Sets the maximum number of function evaluations allowed during a single solve.

Parameters

in,out	this	The nonlinear_regression object.	
in	n	The maximum number of function evaluations.	

Definition at line 914 of file curvefit_regression.f90.

5.5.2.28 subroutine curvefit_regression::nr_set_print_status (class(nonlinear_regression), intent(inout) this, logical, intent(in) x) [private]

Sets a logical value determining if iteration status should be printed.

Parameters

in,out	this	The nonlinear_regression object.	
in	X	True if the iteration status should be printed; else, false.	

Definition at line 1004 of file curvefit_regression.f90.

5.5.2.29 subroutine curvefit_regression::nr_set_var_tol (class(nonlinear_regression), intent(inout) this, real(dp), intent(in) x) [private]

Sets the convergence on change in variable tolerance.

Parameters

in,out	this	The nonlinear_regression object.
in	X	The tolerance value.

Definition at line 958 of file curvefit_regression.f90.

5.5.2.30 subroutine curvefit_regression::nr_solve (class(nonlinear_regression), intent(inout) *this,* real(dp), dimension(:), intent(inout) *c,* real(dp), dimension(:), intent(out), optional, target *res,* type(iteration_behavior), intent(out), optional *ib,* class(errors), intent(inout), optional, target *err*) [private]

Computes the solution to the nonlinear regression problem using the Levenberg-Marquardt method.

Parameters

in	this	The nonlinear_regression object.
in,out	С	On input, an array containing initial estimates of the coefficients. On output, the comptued coefficient values.
out	res	An optional output array, whose size corresponds to the number of data points, that can be used to retrieve the residual error at each data point.
out	ib	An optional output, that if provided, allows the caller to obtain iteration performance statistics.
out	err	An optional errors-based object that if provided can be used to retrieve information relating to any errors encountered during execution. If not provided, a default implementation of the errors class is used internally to provide error handling. Possible errors and warning messages that may be encountered are as follows.
		CF_INVALID_OPERATION_ERROR: Occurs if no equations have been defined.
		 CF_INVALID_INPUT_ERROR: Occurs if the number of equations is less than than the number of variables.
		CF_ARRAY_SIZE_ERROR: Occurs if any of the input arrays are not sized correctly.
		 CF_CONVERGENCE_ERROR: Occurs if the line search cannot converge within the allowed number of iterations.
		CF_OUT_OF_MEMORY_ERROR: Occurs if there is insufficient memory available.
		 CF_TOLERANCE_TOO_SMALL_ERROR: Occurs if the requested tolerance is to small to be practical for the problem at hand.

Definition at line 851 of file curvefit_regression.f90.

5.6 curvefit_statistics Module Reference

curvefit_statistics

Data Types

• interface confidence_interval

Computes the confidence interval based upon a standard normal distribution.

• interface covariance

Computes the covariance matrix of two data sets.

• interface incomplete_beta

Computes the incomplete beta function: I(a,b) = 1 / B(a,b) * integrate(t**(a - 1) * (1 - t)**(b - 1), t, 0, x)

• interface incomplete_gamma

Computes the incomplete gamma function: P(a,x) = 1 / gamma(a) * integrate(exp(-t) * t**(a - 1), t, 0, x).

· interface incomplete gamma comp

Computes the complement of the incomplete gamma function: Q(a,x) = 1 - P(a,x), where P(a,x) = 1 / gamma(a) * integrate(exp(-t) * t**(a - 1), t, 0, x).

· interface mean

Computes the mean of a data set.

interface median

Computes the median of a data set.

· interface standard deviation

Computes the corrected standard deviation of a data set.

interface t value

Computes the t-value (t-score) given a percentage of the area under the standard normal distribution curve.

interface variance

Computes the sample variance of a data set.

interface z value

Computes the z-value (z-score) given a percentage of the area under the standard normal distribution curve.

Functions/Subroutines

pure real(dp) function mean dbl (x)

Computes the mean of a data set.

real(dp) function median dbl (x, srt)

Computes the median of a data set.

• pure real(dp) function variance_dbl (x)

Computes the sample variance of a data set.

• real(dp) function, dimension(2, 2) covariance 2sets (x, y, err)

Computes the covariance matrix of two data sets.

real(dp) function, dimension(size(x, 2), size(x, 2)) covariance_mtx (x, err)

Computes the covariance matrix of N data sets of M observations.

pure real(dp) function stdev_dbl (x)

Computes the corrected standard deviation of a data set.

real(dp) function conf_int (x, alpha, use_t, err)

Computes the confidence interval based upon a standard normal distribution.

real(dp) function std_norm_dist_z_score (alpha, err)

Computes the z-value (z-score) given a percentage of the area under the standard normal distribution curve.

real(dp) function t_dist_score (alpha, n, err)

Computes the t-value (t-score) given a percentage of the area under the standard normal distribution curve.

real(dp) function incomplete_gamma_scalar (a, x, err)

Computes the incomplete gamma function: $P(a,x) = 1 / \text{gamma}(a) * \text{integrate}(\exp(-t) * t * * (a - 1), t, 0, x).$

real(dp) function, dimension(size(x)) incomplete_gamma_array (a, x, err)

Computes the incomplete gamma function: P(a,x) = 1 / gamma(a) * integrate(exp(-t) * t**(a - 1), t, 0, x).

real(dp) function incomplete_gamma_comp_scalar (a, x, err)

Computes the complement of the incomplete gamma function: Q(a,x) = 1 - P(a,x), where P(a,x) = 1 / gamma(a) * integrate(exp(-t) * t**(a - 1), t, 0, x).

real(dp) function, dimension(size(x)) incomplete_gamma_comp_array (a, x, err)

Computes the complement of the incomplete gamma function: Q(a,x) = 1 - P(a,x), where P(a,x) = 1 / gamma(a) * integrate(exp(-t) * t**(a - 1), t, 0, x).

pure real(dp) function inc_gamma_series (a, x)

Computes the incomplete gamma function: P(a,x) = 1 / gamma(a) * integrate(exp(-t) * t**(a - 1), t, 0, x) is computed by its series representation.

• pure real(dp) function inc gamma cf (a, x)

Computes the incomplete gamma function: Q(a,x) = 1 - P(a,x), where P(a,x) = 1 / gamma(a) * integrate(exp(-t) * t**(a - 1), t, 0, x) is computed by Lentz's continued fraction approach.

• real(dp) function inc_beta_scalar (a, b, x, err)

Computes the incomplete beta function: I(a,b) = 1 / B(a,b) * integrate(t**(a - 1) * (1 - t)**(b - 1), t, 0, x)

• real(dp) function, dimension(size(x)) inc_beta_array (a, b, x, err)

Computes the incomplete beta function: I(a,b) = 1 / B(a,b) * integrate(t**(a - 1) * (1 - t)**(b - 1), t, 0, x)

• real(dp) function inc_beta_cf (a, b, x)

Evaluates the incomplete beta function as a continued fraction.

5.6.1 Detailed Description

curvefit_statistics

Purpose

To provide a set of statistical routines for exploring curve fits of sets of numeric data.

5.6.2 Function/Subroutine Documentation

5.6.2.1 real(dp) function curvefit_statistics::conf_int (real(dp), dimension(:), intent(in) x, real(dp), intent(in) alpha, logical, intent(in), optional use_t, class(errors), intent(inout), optional, target err) [private]

Computes the confidence interval based upon a standard normal distribution.

Parameters

in	Х	The data set.
in	alpha	The confidence level. This value must lie between zero and one such that: $0 < alpha < 1$.
in	use↔ _t	Set to true to use the t-distribution in the event of an unknown true standard deviation; else, set to true to use a normal distribution. The default is false, such that a normal distribution is used by a default.
out	err	An optional errors-based object that if provided can be used to retrieve information relating to any errors encountered during execution. If not provided, a default implementation of the errors class is used internally to provide error handling. Possible errors and warning messages that may be encountered are as follows. • CF_INVALID_INPUT_ERROR: Occurs if alpha is does not satisfy: 0 < alpha < 1.

Returns

The confidence interval as the deviation from the mean.

Remarks

The confidence interval, assuming a standard normal distribution, is as follows: mu +/- z * s / sqrt(n), where mu = the mean, and s = the standard deviation. This routine computes the z * s / sqrt(n) portion leaving the computation of the mean to the user.

Definition at line 401 of file curvefit statistics.f90.

5.6.2.2 real(dp) function, dimension(2,2) curvefit_statistics::covariance_2sets (real(dp), dimension(:), intent(in) x, real(dp), dimension(:), intent(in) y, class(errors), intent(inout), optional, target err) [private]

Computes the covariance matrix of two data sets.

in	Х	An N-element array containing the first data set.
in	У	An N-element array containing the second data set.
out	err	An optional errors-based object that if provided can be used to retrieve information relating to any errors encountered during execution. If not provided, a default implementation of the errors class is used internally to provide error handling. Possible errors and warning messages that may be
		encountered are as follows. • CF_ARRAY_SIZE_ERROR: Occurs if x and y are not the same size.

Returns

The 2-by-2 covariance matrix.

Definition at line 244 of file curvefit_statistics.f90.

5.6.2.3 real(dp) function, dimension(size(x, 2), size(x, 2)) curvefit_statistics::covariance_mtx (real(dp), dimension(:,:), intent(in) x, class(errors), intent(inout), optional, target err) [private]

Computes the covariance matrix of N data sets of M observations.

Parameters

in	Х	The M-by-N matrix.
out	err	An optional errors-based object that if provided can be used to retrieve information relating to any errors encountered during execution. If not provided, a default implementation of the errors class is used internally to provide error handling. Possible errors and warning messages that may be encountered are as follows.
		CF_OUT_OF_MEMORY_ERROR: Occurs if there is insufficient memory available.

Returns

The N-by-N covariance matrix.

Definition at line 308 of file curvefit_statistics.f90.

5.6.2.4 real(dp) function, dimension(size(x)) curvefit_statistics::inc_beta_array (real(dp), intent(in) a, real(dp), intent(in) b, real(dp), dimension(:), intent(in) x, class(errors), intent(inout), optional, target err) [private]

Computes the incomplete beta function: I(a,b) = 1 / B(a,b) * integrate(t**(a - 1) * (1 - t)**(b - 1), t, 0, x)

Parameters

in	а	The parameter a.
in	b	The parameter b.
in	Х	The parameter x. This parameter must lie in the interval: [0, 1].
out	err	An optional errors-based object that if provided can be used to retrieve information relating to any errors encountered during execution. If not provided, a default implementation of the errors class is used internally to provide error handling. Possible errors and warning messages that may be encountered are as follows.
		• CF_INVALID_INPUT_ERROR: Occurs if $\mathbf x$ is not within its allowed range.

Definition at line 1054 of file curvefit_statistics.f90.

5.6.2.5 real(dp) function curvefit_statistics::inc_beta_cf (real(dp), intent(in) a, real(dp), intent(in) b, real(dp), intent(in) x)

[private]

Evaluates the incomplete beta function as a continued fraction.

Parameters

in	а	The parameter a.	
in	b	The parameter b.	
in	X	The independent variable.	

Returns

The result.

Definition at line 1120 of file curvefit statistics.f90.

5.6.2.6 real(dp) function curvefit_statistics::inc_beta_scalar (real(dp), intent(in) a, real(dp), intent(in) b, real(dp), intent(in) x, class(errors), intent(inout), optional, target err) [private]

Computes the incomplete beta function: I(a,b) = 1 / B(a,b) * integrate(t**(a - 1) * (1 - t)**(b - 1), t, 0, x)

Parameters

in	а	The parameter a.
in	b	The parameter b.
in	Х	The parameter x. This parameter must lie in the interval: [0, 1].
out	err	An optional errors-based object that if provided can be used to retrieve information relating to any errors encountered during execution. If not provided, a default implementation of the errors class is used internally to provide error handling. Possible errors and warning messages that may be encountered are as follows.
		 CF_INVALID_INPUT_ERROR: Occurs if x is not within its allowed range.

Definition at line 994 of file curvefit_statistics.f90.

5.6.2.7 pure real(dp) function curvefit_statistics::inc_gamma_cf (real(dp), intent(in) a, real(dp), intent(in) x) [private]

Computes the incomplete gamma function: Q(a,x) = 1 - P(a,x), where P(a,x) = 1 / gamma(a) * integrate(exp(-t) * t**(a - 1), t, 0, x) is computed by Lentz's continued fraction approach.

Parameters

in	а	The parameter a.
in	X	The parameter x. This parameter must be greater than 0.

Returns

The incomplete gamma function.

Remarks

This implementation is based upon the Numerical Recipes implementation found in section 6.2 of the text (routine: gcf).

Definition at line 934 of file curvefit_statistics.f90.

5.6.2.8 pure real(dp) function curvefit_statistics::inc_gamma_series (real(dp), intent(in) a, real(dp), intent(in) x)

[private]

Computes the incomplete gamma function: P(a,x) = 1 / gamma(a) * integrate(exp(-t) * t**(a - 1), t, 0, x) is computed by its series representation.

Parameters

in	а	The parameter a.
in	X	The parameter x. This parameter must be greater than 0.

Returns

The incomplete gamma function.

Remarks

This implementation is based upon the Numerical Recipes implementation found in section 6.2 of the text (routine: gser).

Definition at line 886 of file curvefit_statistics.f90.

5.6.2.9 real(dp) function, dimension(size(x)) curvefit_statistics::incomplete_gamma_array (real(dp), intent(in) a, real(dp), dimension(:), intent(in) x, class(errors), intent(inout), optional, target err) [private]

Computes the incomplete gamma function: $P(a,x) = 1 / \text{gamma}(a) * \text{integrate}(\exp(-t) * t * *(a - 1), t, 0, x).$

Parameters

in	а	The coefficient. This parameter must be positive-valued.
in	х	An N-element array of independent variables. All values must be greater than or equal to zero.
out	err	An optional errors-based object that if provided can be used to retrieve information relating to any errors encountered during execution. If not provided, a default implementation of the errors class is used internally to provide error handling. Possible errors and warning messages that may be encountered are as follows. • CF_INVALID_INPUT_ERROR: Occurs if x is negative, or if a is not positive.
	return	The values of the function at x.

Remarks

This implementation is based upon the Numerical Recipes implementation found in section 6.2 of the text (routine: gammp).

Definition at line 679 of file curvefit statistics.f90.

5.6.2.10 real(dp) function, dimension(size(x)) curvefit_statistics::incomplete_gamma_comp_array (real(dp), intent(in) a, real(dp), dimension(:), intent(in) x, class(errors), intent(inout), optional, target err) [private]

Computes the complement of the incomplete gamma function: Q(a,x) = 1 - P(a,x), where P(a,x) = 1 / gamma(a) * integrate(exp(-t) * t**(a - 1), t, 0, x).

Parameters

in	а	The coefficient. This parameter must be positive-valued.
in	х	An N-element array of independent variables. All values must be greater than or equal to zero.
out	err	An optional errors-based object that if provided can be used to retrieve information relating to any errors encountered during execution. If not provided, a default implementation of the errors class is used internally to provide error handling. Possible errors and warning messages that may be encountered are as follows. • CF_INVALID_INPUT_ERROR: Occurs if x is negative, or if a is not positive.
	return	The values of the function at x.

Remarks

This implementation is based upon the Numerical Recipes implementation found in section 6.2 of the text (routine: gammq).

Definition at line 818 of file curvefit_statistics.f90.

5.6.2.11 real(dp) function curvefit_statistics::incomplete_gamma_comp_scalar (real(dp), intent(in) a, real(dp), intent(in) x, class(errors), intent(inout), optional, target err) [private]

Computes the complement of the incomplete gamma function: Q(a,x) = 1 - P(a,x), where P(a,x) = 1 / gamma(a) * integrate(exp(-t) * t**(a - 1), t, 0, x).

Parameters

in	а	The coefficient. This parameter must be positive-valued.
in	х	The independent variable. This parameter must be greater than or equal to zero.
out	err	An optional errors-based object that if provided can be used to retrieve information relating to any errors encountered during execution. If not provided, a default implementation of the errors class is used internally to provide error handling. Possible errors and warning messages that may be encountered are as follows. • CF_INVALID_INPUT_ERROR: Occurs if x is negative, or if a is not positive.
	return	The value of the function at x.

Remarks

This implementation is based upon the Numerical Recipes implementation found in section 6.2 of the text (routine: gammq).

Definition at line 755 of file curvefit_statistics.f90.

5.6.2.12 real(dp) function curvefit_statistics::incomplete_gamma_scalar (real(dp), intent(in) a, real(dp), intent(in) x, class(errors), intent(inout), optional, target err) [private]

Computes the incomplete gamma function: P(a,x) = 1 / gamma(a) * integrate(exp(-t) * t * *(a - 1), t, 0, x).

Parameters

in	а	The coefficient. This parameter must be positive-valued.
in	х	The independent variable. This parameter must be greater than or equal to zero.
out	err	An optional errors-based object that if provided can be used to retrieve information relating to any errors encountered during execution. If not provided, a default implementation of the errors class is used internally to provide error handling. Possible errors and warning messages that may be encountered are as follows. • CF_INVALID_INPUT_ERROR: Occurs if x is negative, or if a is not positive.
	return	The value of the function at x .

Remarks

This implementation is based upon the Numerical Recipes implementation found in section 6.2 of the text (routine: gammp).

Definition at line 617 of file curvefit_statistics.f90.

5.6.2.13 pure real(dp) function curvefit_statistics::mean_dbl (real(dp), dimension(:), intent(in) x) [private]

Computes the mean of a data set.

Parameters

in x	The data set.
------	---------------

Returns

The mean of x.

Definition at line 117 of file curvefit_statistics.f90.

5.6.2.14 real(dp) function curvefit_statistics::median_dbl (real(dp), dimension(:), intent(inout) x, logical, intent(in), optional srt
) [private]

Computes the median of a data set.

Parameters

in,out	X	The data set whose median is to be found. Ideally, the data set should be monotonically increasing; however, if it is not, it may be sorted by the routine, dependent upon the value of srt. On output, the array contents are unchanged; however, they may be sorted into ascending order (dependent upon the value of srt).
in	srt	An optional flag determining if \boldsymbol{x} should be sorted. The default is to sort (true).

Returns

The median of x.

Definition at line 152 of file curvefit_statistics.f90.

5.6.2.15 real(dp) function curvefit_statistics::std_norm_dist_z_score (real(dp), intent(in) alpha, class(errors), intent(inout), optional, target err) [private]

Computes the z-value (z-score) given a percentage of the area under the standard normal distribution curve.

Parameters

in	alpha	The percentage of the area under the curve. This value must be between 0 and 1 such that: $0 < alpha < 1$.
out	err	An optional errors-based object that if provided can be used to retrieve information relating to any errors encountered during execution. If not provided, a default implementation of the errors class is used internally to provide error handling. Possible errors and warning messages that may be encountered are as follows.
		CF_INVALID_INPUT_ERROR: Occurs if alpha is does not satisfy: 0 < alpha < 1.

Returns

The z-score or z-value by solving for z where: alpha = ERF(z / sqrt(2)), where ERF is the error function.

Definition at line 467 of file curvefit_statistics.f90.

5.6.2.16 pure real(dp) function curvefit_statistics::stdev_dbl (real(dp), dimension(:), intent(in) x) [private]

Computes the corrected standard deviation of a data set.

Parameters

in	X	The data set.

Returns

The standard deviation of x.

Definition at line 366 of file curvefit_statistics.f90.

5.6.2.17 real(dp) function curvefit_statistics::t_dist_score (real(dp), intent(in) alpha, integer(i32), intent(in) n, class(errors), intent(inout), optional, target err) [private]

Computes the t-value (t-score) given a percentage of the area under the standard normal distribution curve.

Parameters

in	alpha	The percentage of the area under the curve. This value must be between 0 and 1 such that: 0 < alpha < 1.
out	err	An optional errors-based object that if provided can be used to retrieve information relating to any errors encountered during execution. If not provided, a default implementation of the errors class is used internally to provide error handling. Possible errors and warning messages that may be encountered are as follows.
		CF_INVALID_INPUT_ERROR: Occurs if alpha is does not satisfy: 0 < alpha < 1.

Returns

The t-socre or t-value.

Definition at line 538 of file curvefit_statistics.f90.

5.6.2.18 pure real(dp) function curvefit_statistics::variance_dbl (real(dp), dimension(:), intent(in) x) [private]

Computes the sample variance of a data set.

Parameters

in $ $ x $ $ The data set.

Returns

The variance of x.

Remarks

To avoid overflow-type issues, Welford's algorithm is employed. A simple illustration of this algorithm can be found here.

Definition at line 202 of file curvefit_statistics.f90.

6 Data Type Documentation

6.1 curvefit_c_binding::c_linear_interp Type Reference

A C compatible type encapsulating a linear_interp object.

Public Attributes

type(c_ptr) ptr

A pointer to the linear_interp object.

integer(i32) n

The size of the linear_interp object, in bytes.

6.1.1 Detailed Description

A C compatible type encapsulating a linear_interp object.

Definition at line 45 of file curvefit_c_binding.f90.

The documentation for this type was generated from the following file:

/home/jason/Documents/Code/curvefit/src/curvefit_c_binding.f90

6.2 curvefit_c_binding::c_lowess_smoothing Type Reference

A C compatible type encapsulating a lowess_smoothing object.

Public Attributes

• type(c_ptr) ptr

A pointer to the lowess_smoothing object.

• integer(i32) n

The size of the lowess_smoothing object, in bytes.

6.2.1 Detailed Description

A C compatible type encapsulating a lowess_smoothing object.

Definition at line 72 of file curvefit_c_binding.f90.

The documentation for this type was generated from the following file:

• /home/jason/Documents/Code/curvefit/src/curvefit_c_binding.f90

6.3 curvefit_c_binding::c_nonlinear_regression Type Reference

A C compatible type encapsulating a nonlinear_regression object.

Public Attributes

type(c_ptr) ptr

A pointer to the nonlinear_regression object.

• integer(i32) n

The size of the nonlinear_regression object, in bytes.

6.3.1 Detailed Description

A C compatible type encapsulating a nonlinear_regression object.

Definition at line 81 of file curvefit_c_binding.f90.

The documentation for this type was generated from the following file:

• /home/jason/Documents/Code/curvefit/src/curvefit c binding.f90

6.4 curvefit_c_binding::c_polynomial_interp Type Reference

A C compatible type encapsulating a polynomial_interp object.

Public Attributes

• type(c_ptr) ptr

A pointer to the polynomial_interp object.

• integer(i32) n

The size of the polynomial_interp object, in bytes.

6.4.1 Detailed Description

A C compatible type encapsulating a polynomial_interp object.

Definition at line 54 of file curvefit c binding.f90.

The documentation for this type was generated from the following file:

• /home/jason/Documents/Code/curvefit/src/curvefit_c_binding.f90

6.5 curvefit_c_binding::c_spline_interp Type Reference

A C compatible type encapsulating a spline_interp object.

Public Attributes

type(c_ptr) ptr

A pointer to the spline_interp object.

• integer(i32) n

The size of the spline_interp object, in bytes.

6.5.1 Detailed Description

A C compatible type encapsulating a spline_interp object.

Definition at line 63 of file curvefit_c_binding.f90.

The documentation for this type was generated from the following file:

• /home/jason/Documents/Code/curvefit/src/curvefit_c_binding.f90

6.6 curvefit_c_binding::cnonlin_reg_helper Type Reference

A type for helping to interface between a C function pointer, and the nonlinear_regression type.

Inheritance diagram for curvefit_c_binding::cnonlin_reg_helper:

6.7 curvefit_statistics::confidence_interval Interface Reference

Computes the confidence interval based upon a standard normal distribution.

Private Member Functions

real(dp) function conf_int (x, alpha, use_t, err)
 Computes the confidence interval based upon a standard normal distribution.

6.7.1 Detailed Description

Computes the confidence interval based upon a standard normal distribution.

Definition at line 63 of file curvefit statistics.f90.

6.7.2 Member Function/Subroutine Documentation

6.7.2.1 real(dp) function curvefit_statistics::confidence_interval::conf_int (real(dp), dimension(:), intent(in) x, real(dp), intent(in) alpha, logical, intent(in), optional use_t, class(errors), intent(inout), optional, target err) [private]

Computes the confidence interval based upon a standard normal distribution.

Parameters

in	X	The data set.
in	alpha	The confidence level. This value must lie between zero and one such that: $0 < alpha < 1$.
in	use↔ _t	Set to true to use the t-distribution in the event of an unknown true standard deviation; else, set to true to use a normal distribution. The default is false, such that a normal distribution is used by a default.
out	err	An optional errors-based object that if provided can be used to retrieve information relating to any errors encountered during execution. If not provided, a default implementation of the errors class is used internally to provide error handling. Possible errors and warning messages that may be encountered are as follows. • CF_INVALID_INPUT_ERROR: Occurs if alpha is does not satisfy: 0 < alpha < 1.

Returns

The confidence interval as the deviation from the mean.

Remarks

The confidence interval, assuming a standard normal distribution, is as follows: mu +/- z * s / sqrt(n), where mu = the mean, and s = the standard deviation. This routine computes the z * s / sqrt(n) portion leaving the computation of the mean to the user.

Definition at line 401 of file curvefit_statistics.f90.

The documentation for this interface was generated from the following file:

/home/jason/Documents/Code/curvefit/src/curvefit_statistics.f90

6.8 curvefit_statistics::covariance Interface Reference

Computes the covariance matrix of two data sets.

Private Member Functions

- real(dp) function, dimension(2, 2) covariance_2sets (x, y, err)

 Computes the covariance matrix of two data sets.
- real(dp) function, dimension(size(x, 2), size(x, 2)) covariance_mtx (x, err)

 Computes the covariance matrix of N data sets of M observations.

6.8.1 Detailed Description

Computes the covariance matrix of two data sets.

Definition at line 49 of file curvefit statistics.f90.

6.8.2 Member Function/Subroutine Documentation

6.8.2.1 real(dp) function, dimension(2,2) curvefit_statistics::covariance::covariance_2sets (real(dp), dimension(:), intent(in) x, real(dp), dimension(:), intent(in) y, class(errors), intent(inout), optional, target err) [private]

Computes the covariance matrix of two data sets.

Parameters

in	Х	An N-element array containing the first data set.
in	У	An N-element array containing the second data set.
out	err	An optional errors-based object that if provided can be used to retrieve information relating to any errors encountered during execution. If not provided, a default implementation of the errors class is used internally to provide error handling. Possible errors and warning messages that may be encountered are as follows.
		• CF_ARRAY_SIZE_ERROR: Occurs if ${\bf x}$ and ${\bf y}$ are not the same size.

Returns

The 2-by-2 covariance matrix.

Definition at line 244 of file curvefit_statistics.f90.

6.8.2.2 real(dp) function, dimension(size(x, 2), size(x, 2)) curvefit_statistics::covariance::covariance_mtx (real(dp), dimension(:,:), intent(in) x, class(errors), intent(inout), optional, target err) [private]

Computes the covariance matrix of N data sets of M observations.

Parameters

in	Х	The M-by-N matrix.
out	err	An optional errors-based object that if provided can be used to retrieve information relating to any errors encountered during execution. If not provided, a default implementation of the errors class is used internally to provide error handling. Possible errors and warning messages that may be encountered are as follows.
		CF_OUT_OF_MEMORY_ERROR: Occurs if there is insufficient memory available.

Returns

The N-by-N covariance matrix.

Definition at line 308 of file curvefit_statistics.f90.

The documentation for this interface was generated from the following file:

/home/jason/Documents/Code/curvefit/src/curvefit_statistics.f90

6.9 curvefit_c_binding::creg_fcn Interface Reference

Describes a routine for finding the coefficients of a function of one variable.

Public Member Functions

• real(dp) function **creg_fcn** (x, n, c)

6.9.1 Detailed Description

Describes a routine for finding the coefficients of a function of one variable.

Parameters

in	X	The independent variable.
in	n	The number of coefficients in c.
in	С	An array of function coefficients.

Returns

The value of the function at \mathbf{x} .

Definition at line 32 of file curvefit_c_binding.f90.

The documentation for this interface was generated from the following file:

• /home/jason/Documents/Code/curvefit/src/curvefit_c_binding.f90

6.10 curvefit_calibration::crosstalk Interface Reference

Computes the crosstalk errors for a multiple degree-of-freedom data set.

Private Member Functions

• real(dp) function, dimension(size(xerr, 2), size(xerr, 2)) xtalk_1 (xerr, indices, err)

Computes the crosstalk errors for a multiple degree-of-freedom data set.

6.10.1 Detailed Description

Computes the crosstalk errors for a multiple degree-of-freedom data set.

Definition at line 93 of file curvefit_calibration.f90.

6.10.2 Member Function/Subroutine Documentation

6.10.2.1 real(dp) function, dimension(size(xerr, 2), size(xerr, 2)) curvefit_calibration::crosstalk::xtalk_1 (real(dp), dimension(:,:), intent(in) xerr, integer(i32), dimension(:), intent(in) indices, class(errors), intent(inout), optional, target err)

[private]

Computes the crosstalk errors for a multiple degree-of-freedom data set.

Parameters

in	xerr	An NPTS-by-NDOF matrix containing the measurement error values (computed such that XERR = X MEASURED - X APPLIED).
in	indices	A 2*NDOF element array containing row indices defining the rows where each degree-of-freedom was applied in the data set xerr.
out	err	An optional errors-based object that if provided can be used to retrieve information relating to any errors encountered during execution. If not provided, a default implementation of the errors class is used internally to provide error handling. Possible errors and warning messages that may be encountered are as follows.
		CF_ARRAY_SIZE_ERROR: Occurs if indices is not 2*NDOF in size.
		CF_ARRAY_INDEX_ERROR: Occurs if any of the entries in indices are outside the row bounds of xerr.

Returns

A NDOF-by-NDOF matrix containing the crosstalk errors such that each loaded degree of freedom is represented by its own row, and each responding degree of freedom is represented by its own column.

Usage

The following program computes the crosstalk errors for a 2 DOF system. The applied data is as follows (there are 34 data points for each DOF).

0 0 3000 0

```
6000
               0
7500
               0
9000
               Ω
12000
15000
              0
7500
              0
0
               0
Ω
              Ω
-3000
-6000
               0
-7500
              Ω
-9000
-12000
               0
-15000
               0
-7500
0
               Ω
0
             0
               67.79087067
0
               135.5817413
               203.3726196
0
0
              271.1634827
               338.9543762
0
              203.3726196
Ω
0
              0
0
              0
               -67.79087067
0
               -135.5817413
0
               -203.3726196
0
               -271.1634827
               -338.9543762
0
               -203.3726196
Ω
```

The data output from the instrument under test is as follows.

```
1.22E-03
2.59E-03
0.389050007
0.778159976
0.972689986
                 2.90E-03
                 3.14E-03
1.167140007
1.555999994
                  3.38E-03
1.944839954
                  3.56E-03
0.972599983
                 4.77E-03
-1E-05
                  -1.00E-05
-0.388886005
                2.10E-04
                 5.10E-04
-0.777750015
                  6.90E-04
-0.972150028
-1.166540027
                 8.80E-04
                 1.30E-03
1.78E-03
-1.555330038
-1.944100022
-0.971710026
                 5.80E-04
4.00E-05
                  3.00E-05
                 0
-4.40E-04
                0.271560013
0.543290019
-1.30E-03
                 0.815069973
-2.40E-03
-3.82E-03
                 1.086820006
-5.28E-03
                  1.358809948
                 0.815530002
-2.57E-03
1.50E-04
                  1.00E-05
1.44E-03
                  -0.271450013
3.06E-03
                  -0.543120027
4.46E-03
                  -0.814930022
                  -1.086799979
5.67E-03
6.88E-03
                  -1.35879004
4.51E-03
                  -0.815479994
-2.00E-05
```

The code to compute the crosstalk errors given the above raw data is then as follows.

program main

```
! Parameters
  integer(i32), parameter :: npts = 34
  integer(i32), parameter :: ndof = 2
  ! Local Variables
  integer(i32) :: indices(2*ndof)
  real(dp), dimension(npts, ndof) :: xin, xout, xerr, xmeas
  real(dp), dimension(ndof, npts) :: xint, xmeast
  real(dp), dimension(ndof, ndof) :: c, ans, xt
  ! Initialization
  [npts, ndof])
  xout = reshape([0.0, 0.38905, 0.77816, 0.97269, 1.16714, 1.556, &
1.94484, 0.9726, -1.0e-5, 0.0, -0.388886, -0.77775, -0.97215, &
-1.16654, -1.55533, -1.9441, -0.97171, 4.0e-5, 0.0, -0.00044, &
-0.0013, -0.0024, -0.00382, -0.00528, -0.00257, 0.00015, 0.0, &
0.00144, 0.00306, 0.00446, 0.00567, 0.00688, 0.00451, -2.0e-5,
      0.0, 0.00122, 0.00259, 0.0029, 0.00314, 0.00338, 0.00356, 0.00477,&
      -1.0e-5, 0.0, 0.00021, 0.00051, 0.00069, 0.00088, 0.0013, 0.00178,&
      0.00058, 3.0e-5, 0.0, 0.27156, 0.54329, 0.81507, 1.08682, 1.35881,&
      0.81553, 1.0e-5, 0.0, -0.27145, -0.54312, -0.81493, -1.0868, &
      -1.35879, -0.81548, 0.0], [npts, ndof])
  ! Compute the calibration gains
  xint = transpose(xin)
  xmeast = transpose(xout)
  c = linear_least_squares(xmeast, xint)
  xmeas = matmul(xout, transpose(c))
  xerr = xmeas - xin
  ! The indices are
  indices = [1, 17, 18, 34]
  ! Compute the crosstalk matrix
  xt = crosstalk(xerr, indices)
end program
```

The least squares fit generates the following matrix of calibration gains.

```
7713.710427 33.5206917
-0.214743728 249.4768498
```

The resulting measured values are then as follows.

```
Ω
3001.05999
                0.220815702
6002.58754
                 0.479040049
                 0.514603781
7503.146099
9003.085297
                0.532721294
12002.64668
                 0.509090486
15002.05157
                 0.470495427
7502.514526
                0.981144827
-0.077472309
                 -0.002492621
-2999.74699
                0.135900968
                0.294250127
-5999.321307
-7498.860677
                 0.380902151
                0.470046784
-8998.322469
-11997.32196
                0.658317276
-14996.16495
                 0.861552092
-7495.47032
                 0.353365205
0.30955403
                 7.48E-03
Ω
                Ο
5.708846869
                67.74803112
                 135.5385616
8.183633648
                203.3416047
8.808803389
6.96458466
                 271.1372518
4.81985707
                 338.9927591
7.512893885
                 203.4564077
1.157391826
                 2.46E-03
                0
Ω
2.008550989
                  -67.72080332
```

```
      5.398195074
      -135.4965304

      7.086130239
      -203.3071324

      7.306450061
      -271.1326527

      7.522743936
      -338.9881361

      7.453379661
      -203.4443484

      -0.154274205
      4.29E-06
```

The crosstalk error matrix is then as follows.

```
0 0.981144827
8.808803389 0
```

Definition at line 885 of file curvefit calibration.f90.

The documentation for this interface was generated from the following file:

/home/jason/Documents/Code/curvefit/src/curvefit_calibration.f90

6.11 curvefit_calibration::hysteresis Interface Reference

Computes the hysteresis in an ascending/descending data set.

Private Member Functions

- real(dp) function hysteresis_1 (xascend, ascend, xdescend, descend, err)
 Computes the hysteresis in an ascending/descending data set.
- real(dp) function hysteresis_2 (applied, measured, err)
 Computes the hysteresis in an ascending/descending data set.

6.11.1 Detailed Description

Computes the hysteresis in an ascending/descending data set.

Definition at line 72 of file curvefit_calibration.f90.

6.11.2 Member Function/Subroutine Documentation

6.11.2.1 real(dp) function curvefit_calibration::hysteresis::hysteresis_1 (real(dp), dimension(:), intent(in) xascend, real(dp), dimension(:), intent(in) ascend, real(dp), dimension(:), intent(in) xdescend, real(dp), dimension(:), intent(in) descend, class(errors), intent(inout), optional, target err) [private]

Computes the hysteresis in an ascending/descending data set.

Parameters

in	xascend	An N-element array containing the ascending calibration points. This array must be monotonically increasing or decreasing.
in	ascend	An N-element array containing the sensor output to the calibration points in xascend.
in	xdescend	An M-element array containing the descending calibration points. This array must be monotonically increasing or decreasing.
in	descend	An M-element array containing the sensor output to the calibration points in xdescend.
out	err	An optional errors-based object that if provided can be used to retrieve information relating to any errors encountered during execution. If not provided, a default imple free matricly of the errors class is used internally to provide error handling. Possible errors and warning messages that may be encountered are as follows.

Returns

The hysteresis error.

Remarks

In order to account for slight variations between similar ascending and descending points, the algorithm used performs a linear interpolation between data points. The resulting interpolated value is then used to compute the reported hysteresis error.

Definition at line 353 of file curvefit_calibration.f90.

6.11.2.2 real(dp) function curvefit_calibration::hysteresis::hysteresis_2 (real(dp), dimension(:), intent(in) applied, real(dp), dimension(:), intent(in) measured, class(errors), intent(inout), optional, target err) [private]

Computes the hysteresis in an ascending/descending data set.

Parameters

in	applied	An N-element array containing the values applied to the measurement instrument.
in	measured	An N-element array containing the calibrated output of the instrument as a result of the values given in applied.
out	err	An optional errors-based object that if provided can be used to retrieve information relating to any errors encountered during execution. If not provided, a default implementation of the errors class is used internally to provide error handling. Possible errors and warning messages that may be encountered are as follows.
		 CF_NONMONOTONIC_ARRAY_ERROR: Occurs if the calibration data is not monotonic in nature (either ascending or descending).
		CF_ARRAY_SIZE_ERROR: Occurs if applied and measured are not the same size.

Returns

The hysteresis error.

Remarks

In order to account for slight variations between similar ascending and descending points, the algorithm used performs a linear interpolation between data points. The resulting interpolated value is then used to compute the reported hysteresis error.

Definition at line 444 of file curvefit_calibration.f90.

The documentation for this interface was generated from the following file:

/home/jason/Documents/Code/curvefit/src/curvefit_calibration.f90

6.12 curvefit_calibration::IDAMAX Interface Reference

Private Member Functions

• function idamax (n, dx, incx)

6.12.1 Detailed Description

Definition at line 45 of file curvefit calibration.f90.

The documentation for this interface was generated from the following file:

/home/jason/Documents/Code/curvefit/src/curvefit_calibration.f90

6.13 curvefit_statistics::incomplete_beta Interface Reference

Computes the incomplete beta function: I(a,b) = 1 / B(a,b) * integrate(t**(a - 1) * (1 - t)**(b - 1), t, 0, x)

Private Member Functions

- real(dp) function inc_beta_scalar (a, b, x, err)

 Computes the incomplete beta function: I(a,b) = 1 / B(a,b) * integrate(t**(a 1) * (1 t)**(b 1), t, 0, x)
- real(dp) function, dimension(size(x)) inc_beta_array (a, b, x, err)

 Computes the incomplete beta function: I(a,b) = 1 / B(a,b) * integrate(t**(a 1) * (1 t)**(b 1), t, 0, x)

6.13.1 Detailed Description

Computes the incomplete beta function: I(a,b) = 1 / B(a,b) * integrate(t**(a - 1) * (1 - t)**(b - 1), t, 0, x)

Definition at line 101 of file curvefit_statistics.f90.

6.13.2 Member Function/Subroutine Documentation

6.13.2.1 real(dp) function, dimension(size(x)) curvefit_statistics::incomplete_beta::inc_beta_array (real(dp), intent(in) a, real(dp), intent(in) b, real(dp), dimension(:), intent(in) x, class(errors), intent(inout), optional, target err)

[private]

Computes the incomplete beta function: I(a,b) = 1 / B(a,b) * integrate(t**(a - 1) * (1 - t)**(b - 1), t, 0, x)

Parameters

in	а	The parameter a.
in	b	The parameter b.
in	Х	The parameter x. This parameter must lie in the interval: [0, 1].
out	err	An optional errors-based object that if provided can be used to retrieve information relating to any errors encountered during execution. If not provided, a default implementation of the errors class is used internally to provide error handling. Possible errors and warning messages that may be encountered are as follows.
		• CF_INVALID_INPUT_ERROR: Occurs if $\mathbf x$ is not within its allowed range.

Definition at line 1054 of file curvefit_statistics.f90.

6.13.2.2 real(dp) function curvefit_statistics::incomplete_beta::inc_beta_scalar (real(dp), intent(in) a, real(dp), intent(in) b, real(dp), intent(in) x, class(errors), intent(inout), optional, target err) [private]

Computes the incomplete beta function: I(a,b) = 1 / B(a,b) * integrate(t**(a - 1) * (1 - t)**(b - 1), t, 0, x)

Parameters

in	а	The parameter a.	
in	b	The parameter b.	
in	Х	The parameter x. This parameter must lie in the interval: [0, 1].	
out	err	An optional errors-based object that if provided can be used to retrieve information relating to any errors encountered during execution. If not provided, a default implementation of the errors class is used internally to provide error handling. Possible errors and warning messages that may be encountered are as follows.	
		CF_INVALID_INPUT_ERROR: Occurs if x is not within its allowed range.	

Definition at line 994 of file curvefit_statistics.f90.

The documentation for this interface was generated from the following file:

/home/jason/Documents/Code/curvefit/src/curvefit_statistics.f90

6.14 curvefit_statistics::incomplete_gamma Interface Reference

Computes the incomplete gamma function: P(a,x) = 1 / gamma(a) * integrate(exp(-t) * t**(a - 1), t, 0, x).

Private Member Functions

- real(dp) function incomplete_gamma_scalar (a, x, err)
 Computes the incomplete gamma function: P(a,x) = 1 / gamma(a) * integrate(exp(-t) * t**(a 1), t, 0, x).
- real(dp) function, dimension(size(x)) incomplete_gamma_array (a, x, err)

 Computes the incomplete gamma function: P(a,x) = 1 / gamma(a) * integrate(exp(-t) * t**(a 1), t, 0, x).

6.14.1 Detailed Description

Computes the incomplete gamma function: P(a,x) = 1 / gamma(a) * integrate(exp(-t) * t**(a - 1), t, 0, x).

Definition at line 84 of file curvefit statistics.f90.

6.14.2 Member Function/Subroutine Documentation

6.14.2.1 real(dp) function, dimension(size(x)) curvefit_statistics::incomplete_gamma::incomplete_gamma_array (real(dp), intent(in) a, real(dp), dimension(:), intent(in) x, class(errors), intent(inout), optional, target err) [private]

Computes the incomplete gamma function: P(a,x) = 1 / gamma(a) * integrate(exp(-t) * t * * (a - 1), t, 0, x).

Parameters

in	а	The coefficient. This parameter must be positive-valued.	
in x An N-element array of independent variables. All values must be gre		An N-element array of independent variables. All values must be greater than or equal to zero.	
out	err	An optional errors-based object that if provided can be used to retrieve information relating to any errors encountered during execution. If not provided, a default implementation of the errors class is used internally to provide error handling. Possible errors and warning messages that may be encountered are as follows. • CF_INVALID_INPUT_ERROR: Occurs if x is negative, or if a is not positive.	
return The values of the function at x.		The values of the function at x.	

Remarks

This implementation is based upon the Numerical Recipes implementation found in section 6.2 of the text (routine: gammp).

Definition at line 679 of file curvefit_statistics.f90.

6.14.2.2 real(dp) function curvefit_statistics::incomplete_gamma::incomplete_gamma_scalar (real(dp), intent(in) a, real(dp), intent(in) x, class(errors), intent(inout), optional, target err) [private]

Computes the incomplete gamma function: P(a,x) = 1 / gamma(a) * integrate(exp(-t) * t * * (a - 1), t, 0, x).

Parameters

in	а	The coefficient. This parameter must be positive-valued.
in	n x The independent variable. This parameter must be greater than or equal to zero.	
out	err	An optional errors-based object that if provided can be used to retrieve information relating to any errors encountered during execution. If not provided, a default implementation of the errors class is used internally to provide error handling. Possible errors and warning messages that may be encountered are as follows. • CF_INVALID_INPUT_ERROR: Occurs if x is negative, or if a is not positive.
	return	The value of the function at x.

Remarks

This implementation is based upon the Numerical Recipes implementation found in section 6.2 of the text (routine: gammp).

Definition at line 617 of file curvefit_statistics.f90.

The documentation for this interface was generated from the following file:

/home/jason/Documents/Code/curvefit/src/curvefit_statistics.f90

6.15 curvefit_statistics::incomplete_gamma_comp Interface Reference

Computes the complement of the incomplete gamma function: Q(a,x) = 1 - P(a,x), where P(a,x) = 1 / gamma(a) * integrate(exp(-t) * t**(a - 1), t, 0, x).

Private Member Functions

- real(dp) function incomplete_gamma_comp_scalar (a, x, err)
 Computes the complement of the incomplete gamma function: Q(a,x) = 1 P(a,x), where P(a,x) = 1 / gamma(a) * integrate(exp(-t) * t**(a 1), t, 0, x).
- real(dp) function, dimension(size(x)) incomplete_gamma_comp_array (a, x, err)
 Computes the complement of the incomplete gamma function: Q(a,x) = 1 P(a,x), where P(a,x) = 1 / gamma(a) * integrate(exp(-t) * t**(a 1), t, 0, x).

6.15.1 Detailed Description

Computes the complement of the incomplete gamma function: Q(a,x) = 1 - P(a,x), where P(a,x) = 1 / gamma(a) * integrate(exp(-t) * t**(a - 1), t, 0, x).

Definition at line 93 of file curvefit_statistics.f90.

- 6.15.2 Member Function/Subroutine Documentation
- 6.15.2.1 real(dp) function, dimension(size(x)) curvefit_statistics::incomplete_gamma_comp::incomplete_gamma_comp_array (real(dp), intent(in) a, real(dp), dimension(:), intent(in) x, class(errors), intent(inout), optional, target err)

 [private]

Computes the complement of the incomplete gamma function: Q(a,x) = 1 - P(a,x), where P(a,x) = 1 / gamma(a) * integrate(exp(-t) * t**(a - 1), t, 0, x).

Parameters

in	а	The coefficient. This parameter must be positive-valued.
in	in x An N-element array of independent variables. All values must be greater than or e	
out	err	An optional errors-based object that if provided can be used to retrieve information relating to any errors encountered during execution. If not provided, a default implementation of the errors class is used internally to provide error handling. Possible errors and warning messages that may be encountered are as follows. • CF_INVALID_INPUT_ERROR: Occurs if x is negative, or if a is not positive.
	return	The values of the function at x.

Remarks

This implementation is based upon the Numerical Recipes implementation found in section 6.2 of the text (routine: gammq).

Definition at line 818 of file curvefit_statistics.f90.

6.15.2.2 real(dp) function curvefit_statistics::incomplete_gamma_comp::incomplete_gamma_comp_scalar (real(dp), intent(in) a, real(dp), intent(in) x, class(errors), intent(inout), optional, target err) [private]

Computes the complement of the incomplete gamma function: Q(a,x) = 1 - P(a,x), where P(a,x) = 1 / gamma(a) * integrate(exp(-t) * t**(a - 1), t, 0, x).

Parameters

in	а	The coefficient. This parameter must be positive-valued.
in x The independent variable. This parameter must be greater than or equal to zero.		The independent variable. This parameter must be greater than or equal to zero.
out	err	An optional errors-based object that if provided can be used to retrieve information relating to any errors encountered during execution. If not provided, a default implementation of the errors class is used internally to provide error handling. Possible errors and warning messages that may be encountered are as follows. • CF_INVALID_INPUT_ERROR: Occurs if x is negative, or if a is not positive.
	return	The value of the function at x.

Remarks

This implementation is based upon the Numerical Recipes implementation found in section 6.2 of the text (routine: gammq).

Definition at line 755 of file curvefit statistics.f90.

The documentation for this interface was generated from the following file:

/home/jason/Documents/Code/curvefit/src/curvefit statistics.f90

6.16 curvefit_interp::interp_manager Type Reference

Describes an abstract base class allowing for interpolation of X-Y type data sets.

Inheritance diagram for curvefit_interp::interp_manager:

Public Member Functions

- procedure, public initialize => im_init
 Initializes the interp_manager instance.
- procedure, non_overridable, public locate => im_locate

Attempts to locate the index in the array providing a lower bounds to the specified interpolation point.

• procedure, non_overridable, public hunt => im_hunt

Attempts to locate the index in the array providing a lower bounds to the specified interpolation point.

• generic, public interpolate => im_perform, im_perform_array

Interpolates to obtain the function value at the specified independent variable.

• procedure, public get_count => im_get_num_pts

Gets the number of stored data points.

procedure, public get_x => im_get_x

Gets the x component of the requested data point.

procedure, public get_y => im_get_y

Gets the y component of the requested data point.

Private Member Functions

- procedure(interp_xy), deferred raw_interp
 - Performs the actual interpolation.
- procedure, non_overridable im_perform
- procedure, non_overridable im_perform_array

Private Attributes

- integer(i32) m_order
- integer(i32) m_savedindex
- integer(i32) m_indexcheck
- logical m correlated
- real(dp), dimension(:), allocatable m_x
- real(dp), dimension(:), allocatable m_y

6.16.1 Detailed Description

Describes an abstract base class allowing for interpolation of X-Y type data sets.

Notes

This interpolation object is conceptually based upon the interpolation scheme utilized by the Numerical Recipes in C++ text.

Definition at line 48 of file curvefit_interp.f90.

The documentation for this type was generated from the following file:

/home/jason/Documents/Code/curvefit/src/curvefit_interp.f90

6.17 curvefit_interp::interp_xy Interface Reference

Defines the signature of a method used to interpolate a single value in an X-Y data set.

Private Member Functions

• real(dp) function interp_xy (this, jlo, pt)

6.17.1 Detailed Description

Defines the signature of a method used to interpolate a single value in an X-Y data set.

Parameters

in,out	this	The interp_manager based instance.
in	jlo	The array index below which pt is found in x.
in	pt	The independent variable value to interpolate.

Returns

The interpolated value.

Definition at line 148 of file curvefit interp.f90.

The documentation for this interface was generated from the following file:

/home/jason/Documents/Code/curvefit/src/curvefit interp.f90

6.18 curvefit_core::is_monotonic Interface Reference

Tests to see if an array is montonically increasing or decreasing.

Private Member Functions

- pure logical function is_monotonic_dbl (x)
 Tests to see if an array is monotonically increasing or decreasing.
- pure logical function is_monotonic_i32 (x)

Tests to see if an array is montonically increasing or decreasing.

6.18.1 Detailed Description

Tests to see if an array is montonically increasing or decreasing.

Definition at line 74 of file curvefit_core.f90.

6.18.2 Member Function/Subroutine Documentation

```
6.18.2.1 pure logical function curvefit_core::is_monotonic::is_monotonic_dbl ( real(dp), dimension(:), intent(in) x )

[private]
```

Tests to see if an array is montonically increasing or decreasing.

Parameters

$\int $ in $\int x$ The array to te

Returns

Returns true if x is monotonic; else, false.

Definition at line 105 of file curvefit_core.f90.

6.18.2.2 pure logical function curvefit_core::is_monotonic::is_monotonic_i32 (integer(i32), dimension(:), intent(in) x) [private]

Tests to see if an array is montonically increasing or decreasing.

Parameters

in X	The array to test.
------	--------------------

Returns

Returns true if x is monotonic; else, false.

Definition at line 139 of file curvefit_core.f90.

The documentation for this interface was generated from the following file:

/home/jason/Documents/Code/curvefit/src/curvefit_core.f90

6.19 curvefit_interp::linear_interp Type Reference

Extends the interp_manager class allowing for linear, piecewise interpolation of a data set.

Inheritance diagram for curvefit_interp::linear_interp:

Collaboration diagram for curvefit_interp::linear_interp:

Private Member Functions

procedure raw_interp => li_raw_interp
 Performs the actual interpolation.

Additional Inherited Members

6.19.1 Detailed Description

Extends the interp_manager class allowing for linear, piecewise interpolation of a data set.

Definition at line 84 of file curvefit_interp.f90.

The documentation for this type was generated from the following file:

/home/jason/Documents/Code/curvefit/src/curvefit_interp.f90

6.20 curvefit_regression::linear_least_squares Interface Reference

Employs a least squares fit to determine the coefficient A in the linear system: Y = A * X, where A can either be a scalar, or a matrix.

Private Member Functions

real(dp) function linear_least_squares_1var (x, y, err)

Employs a least squares fit to determine the coefficient A in the linear system: Y = A * X.

• real(dp) function, dimension(size(y, 1), size(x, 1)) linear_least_squares_nvar (x, y, thrsh, err)

Employs a least squares fit to determine the coefficient A in the linear system: Y = A * X.

6.20.1 Detailed Description

Employs a least squares fit to determine the coefficient A in the linear system: Y = A * X, where A can either be a scalar, or a matrix.

Definition at line 36 of file curvefit_regression.f90.

- 6.20.2 Member Function/Subroutine Documentation
- 6.20.2.1 real(dp) function curvefit_regression::linear_least_squares::linear_least_squares_1var (real(dp), dimension(:), intent(in) x, real(dp), dimension(:), intent(inout) y, class(errors), intent(inout), optional, target err) [private]

Employs a least squares fit to determine the coefficient A in the linear system: Y = A * X.

Parameters

in	х	An N-element array containing the independent variable data.
in, out	У	An N-element array containing the dependent variable data corresponding to x. On output,
		the contents of this array are overwritten as it is used for storage purposes by the algorithm.
out	err	An optional errors-based object that if provided can be used to retrieve information relating to any errors encountered during execution. If not provided, a default implementation of the errors class is used internally to provide error handling. Possible errors and warning messages that may be encountered are as follows.
		 CF_OUT_OF_MEMORY_ERROR: Occurs if insufficient memory is available. CF_ARRAY_SIZE_ERROR: Occurs if x and y are different sizes.
1	1	

Returns

The scalar coefficient A.

Definition at line 1081 of file curvefit_regression.f90.

6.20.2.2 real(dp) function, dimension(size(y,1), size(x,1)) curvefit_regression::linear_least_squares::linear_least_squares_nvar (real(dp), dimension(:,:), intent(inout) x, real(dp), dimension(:,:), intent(in) y, real(dp), intent(in), optional thrsh, class(errors), intent(inout), optional, target err) [private]

Employs a least squares fit to determine the coefficient A in the linear system: Y = A * X.

Parameters

in,out	X	An M-by-P matrix containing the P data points of the M independent variables.
--------	---	---

Parameters

in	У	An N-by-P matrix containing the P data points of the N dependent variables.
in	thrsh	An optional threshold value that defines a lower cutoff for singular values. Any singular values falling below this value will have their reciprocal replaced with zero.
out	err	An optional errors-based object that if provided can be used to retrieve information relating to any errors encountered during execution. If not provided, a default implementation of the errors class is used internally to provide error handling. Possible errors and warning messages that may be encountered are as follows.
		CF_ARRAY_SIZE_ERROR: Occurs if any of the matrix dimensions are not compatiable.
		CF_OUT_OF_MEMORY_ERROR: Occurs if there is insufficient memory available.

Returns

An N-by-M matrix relating Y to X such that: Y = A * X.

Remarks

The algorithm attempts to compute the coefficient matrix A as follows. Y * X**T = A * X * X**T Y * X**T * INV(X * X**T) = A This does require that <math>X * X**T does not result in a singular matrix. To handle the situation where X * X**T is singular, the Moore-Penrose pseudo-inverse, computed by means of singular value decomposition, is utilized to still arrive at a solution that, at minimum, has a minimum Euclidean norm of its residual. Let: PINV(X) = X**T * INV(X * X**T), Then: A = Y * PINV(X)

Definition at line 1150 of file curvefit_regression.f90.

The documentation for this interface was generated from the following file:

 $\bullet \ \ / home/jason/Documents/Code/curve fit/src/curve fit_regression.f90$

6.21 curvefit_regression::lowess_smoothing Type Reference

Defines a type for computing a smoothing of an X-Y data set using a robust locally weighted scatterplot smoothing (LOWESS) algorithm.

Public Member Functions

- procedure, public initialize => ls_init
 - Initializes the lowess_smoothing object.
- procedure, public smooth => ls_smooth
 - Performs the actual smoothing operation.
- procedure, public get_count => ls_get_num_pts
 - Gets the number of stored data points.
- procedure, public get_x => ls_get_x
 - Gets the x component of the requested data point.
- procedure, public get_y => ls_get_y
 - Gets the y component of the requested data point.
- procedure, public get_residuals => ls_get_residual

Gets the residuals from each data point.

Private Attributes

• real(dp), dimension(:), allocatable m_x

N-element array of x data points - sorted into ascending order.

• real(dp), dimension(:), allocatable m_y

N-element array of y data points.

real(dp), dimension(:), allocatable m_weights

N-element array containing the robustness weights for each data point.

• real(dp), dimension(:), allocatable m_residuals

N-element array containing the residuals (Y - YS)

• real(dp) m_delta

Scaling parameter used to define the nature of the linear interpolations used by the algorithm.

logical m_init = .false.

Tracks whether or not Is_init has been called.

6.21.1 Detailed Description

Defines a type for computing a smoothing of an X-Y data set using a robust locally weighted scatterplot smoothing (LOWESS) algorithm.

Definition at line 46 of file curvefit_regression.f90.

The documentation for this type was generated from the following file:

/home/jason/Documents/Code/curvefit/src/curvefit_regression.f90

6.22 curvefit_statistics::mean Interface Reference

Computes the mean of a data set.

Private Member Functions

pure real(dp) function mean_dbl (x)
 Computes the mean of a data set.

6.22.1 Detailed Description

Computes the mean of a data set.

Definition at line 31 of file curvefit statistics.f90.

6.22.2 Member Function/Subroutine Documentation

6.22.2.1 pure real(dp) function curvefit_statistics::mean::mean_dbl (real(dp), dimension(:), intent(in) x) [private]

Computes the mean of a data set.

Parameters

Returns

The mean of \boldsymbol{x} .

Definition at line 117 of file curvefit_statistics.f90.

The documentation for this interface was generated from the following file:

/home/jason/Documents/Code/curvefit/src/curvefit_statistics.f90

6.23 curvefit_statistics::median Interface Reference

Computes the median of a data set.

Private Member Functions

real(dp) function median_dbl (x, srt)
 Computes the median of a data set.

6.23.1 Detailed Description

Computes the median of a data set.

Definition at line 37 of file curvefit_statistics.f90.

6.23.2 Member Function/Subroutine Documentation

6.23.2.1 real(dp) function curvefit_statistics::median::median_dbl (real(dp), dimension(:), intent(inout) x, logical, intent(in), optional srt) [private]

Computes the median of a data set.

Parameters

in,out	X	The data set whose median is to be found. Ideally, the data set should be monotonically increasing; however, if it is not, it may be sorted by the routine, dependent upon the value of srt. On output, the array contents are unchanged; however, they may be sorted into ascending order (dependent upon the value of srt).
in	srt	An optional flag determining if \boldsymbol{x} should be sorted. The default is to sort (true).

Returns

The median of x.

Definition at line 152 of file curvefit_statistics.f90.

The documentation for this interface was generated from the following file:

• /home/jason/Documents/Code/curvefit/src/curvefit_statistics.f90

6.24 curvefit_regression::moving_average Interface Reference

Applies a moving average to smooth a data set.

Private Member Functions

subroutine moving_average_1 (x, npts, err)
 Applies a moving average to smooth a data set.

6.24.1 Detailed Description

Applies a moving average to smooth a data set.

Definition at line 29 of file curvefit_regression.f90.

6.24.2 Member Function/Subroutine Documentation

6.24.2.1 subroutine curvefit_regression::moving_average::moving_average_1 (real(dp), dimension(:), intent(inout) x, integer(i32), intent(in) npts, class(errors), intent(inout), optional, target err) [private]

Applies a moving average to smooth a data set.

Parameters

in,out	Х	On input, the signal to smooth. On output, the smoothed signal.
in	npts	The size of the averaging window. This value must be at least 2, but no more than the number of elements in \times .
out	err	An optional errors-based object that if provided can be used to retrieve information relating to any errors encountered during execution. If not provided, a default implementation of the errors class is used internally to provide error handling. Possible errors and warning messages that may be encountered are as follows.
		 CF_INVALID_INPUT_ERROR: Occurs if npts is less than 2, or greater than the length of x. CF_OUT_OF_MEMORY_ERROR: Occurs if there is insufficient memory available.
		of _oof_of_wellion file to the file of the

Definition at line 164 of file curvefit_regression.f90.

The documentation for this interface was generated from the following file:

/home/jason/Documents/Code/curvefit/src/curvefit regression.f90

6.25 curvefit_regression::nonlinear_regression Type Reference

A type for supporting nonlinear regression calculations.

Inheritance diagram for curvefit_regression::nonlinear_regression:

Collaboration diagram for curvefit_regression::nonlinear_regression:

Public Member Functions

• procedure, public initialize => nr_init

Initializes the nonlinear regression object.

• procedure, public fcn => nr fcn

Computes the residual between the supplied data set, and the function value given a set of coefficients.

procedure, public is_fcn_defined => nr_is_fcn_defined

Determines if the function has been defined.

procedure, public get_equation_count => nr_get_eqn_count

Gets the number of equations required to solve the regression problem.

procedure, public get_variable_count => nr_get_var_count

Gets the number of variables (coefficients).

procedure, public solve => nr solve

Computes the solution to the nonlinear regression problem using the Levenberg-Marquardt method.

procedure, public get_max_fcn_evals => nr_get_max_eval

Gets the maximum number of function evaluations allowed during a single solve.

procedure, public set_max_fcn_evals => nr_set_max_eval

Sets the maximum number of function evaluations allowed during a single solve.

procedure, public get_fcn_tolerance => nr_get_fcn_tol

Gets the convergence on function value tolerance.

• procedure, public set fcn tolerance => nr set fcn tol

Sets the convergence on function value tolerance.

procedure, public get_var_tolerance => nr_get_var_tol

Gets the convergence on change in variable tolerance.

procedure, public set_var_tolerance => nr_set_var_tol

Sets the convergence on change in variable tolerance.

procedure, public get_gradient_tolerance => nr_get_grad_tol

Gets the convergence on slope of the gradient vector tolerance.

procedure, public set gradient tolerance => nr set grad tol

Sets the convergence on slope of the gradient vector tolerance.

procedure, public get_print_status => nr_get_print_status

Gets a logical value determining if iteration status should be printed.

procedure, public set_print_status => nr_set_print_status

Sets a logical value determining if iteration status should be printed.

procedure, public get_count => nr_get_num_pts

Gets the number of stored data points.

• procedure, public get_x => nr_get_x

Gets the x component of the requested data point.

procedure, public get_y => nr_get_y

Gets the y component of the requested data point.

Private Attributes

procedure(reg_fcn), pointer, nopass m_rfcn => null()

A pointer to the routine containing the function of interest.

• real(dp), dimension(:), allocatable m_x

The x data points.

real(dp), dimension(:), allocatable m_y

The y data points.

integer(i32) m_ncoeff = 0

The number of coefficients in the function of interest.

• logical m_init = .false.

Tracks whether or not nr_init has been called.

type(least_squares_solver) m_solver

The Levenberg-Marquardt solver.

6.25.1 Detailed Description

A type for supporting nonlinear regression calculations.

Definition at line 79 of file curvefit regression.f90.

The documentation for this type was generated from the following file:

• /home/jason/Documents/Code/curvefit/src/curvefit_regression.f90

6.26 curvefit_calibration::nonlinearity Interface Reference

Computes the best-fit nonlinearity of a data set.

Private Member Functions

real(dp) function bf_nonlin (applied, measured, err)
 Computes the best-fit nonlinearity of a data set.

6.26.1 Detailed Description

Computes the best-fit nonlinearity of a data set.

Definition at line 60 of file curvefit_calibration.f90.

6.26.2 Member Function/Subroutine Documentation

6.26.2.1 real(dp) function curvefit_calibration::nonlinearity::bf_nonlin (real(dp), dimension(:), intent(in) applied, real(dp), dimension(:), intent(in) measured, class(errors), intent(inout), optional, target err) [private]

Computes the best-fit nonlinearity of a data set.

Parameters

in	applied	An N-element array containing the values applied to the measurement instrument.
in	measured	An N-element array containing the calibrated output of the instrument as a result of the values given in applied.
out	err	An optional errors-based object that if provided can be used to retrieve information relating to any errors encountered during execution. If not provided, a default implementation of the errors class is used internally to provide error handling. Possible errors and warning messages that may be encountered are as follows. • CF_ARRAY_SIZE_ERROR: Occurs if applied and measured are not the same size.

Returns

The nonlinearity error.

Definition at line 211 of file curvefit_calibration.f90.

The documentation for this interface was generated from the following file:

/home/jason/Documents/Code/curvefit/src/curvefit_calibration.f90

6.27 curvefit_interp::polynomial_interp Type Reference

Extends the interp_manager class allowing for polynomial interpolation of a data set.

Inheritance diagram for curvefit_interp::polynomial_interp:

Collaboration diagram for curvefit_interp::polynomial_interp:

Public Member Functions

procedure, public initialize => pi_init
 Initializes the polynomial_interp instance.

Private Member Functions

procedure raw_interp => pi_raw_interp
 Performs the actual interpolation.

Private Attributes

- real(dp), dimension(:), allocatable m_c
- real(dp), dimension(:), allocatable m_d
- real(dp) m_dy

6.27.1 Detailed Description

Extends the interp_manager class allowing for polynomial interpolation of a data set.

Definition at line 93 of file curvefit_interp.f90.

The documentation for this type was generated from the following file:

• /home/jason/Documents/Code/curvefit/src/curvefit_interp.f90

6.28 curvefit_core::reg_fcn Interface Reference

Describes a routine for finding the coefficients of a function of one variable.

Private Member Functions

real(real64) function reg_fcn (x, c)

6.28.1 Detailed Description

Describes a routine for finding the coefficients of a function of one variable.

Parameters

in	X	The independent variable.
in	С	An array of function coefficients.

Returns

The value of the function at x.

Definition at line 88 of file curvefit_core.f90.

The documentation for this interface was generated from the following file:

/home/jason/Documents/Code/curvefit/src/curvefit_core.f90

6.29 curvefit_calibration::repeatability Interface Reference

Computes the repeatability of a sequence of tests.

Private Member Functions

real(dp) function repeat_1 (applied, measured, err)
 Computes the repeatability of a sequence of tests.

6.29.1 Detailed Description

Computes the repeatability of a sequence of tests.

Definition at line 86 of file curvefit calibration.f90.

6.29.2 Member Function/Subroutine Documentation

6.29.2.1 real(dp) function curvefit_calibration::repeatability::repeat_1 (real(dp), dimension(:,:), intent(in) applied, real(dp), dimension(:,:), intent(in) measured, class(errors), intent(inout), optional, target err) [private]

Computes the repeatability of a sequence of tests.

Parameters

in	applied	An NPTS-by-NTEST matrix containing at least 2 columns (tests) of NPTS values applied
		to the measurement instrument.
in	measured	An NPTS-by-NTEST matrix containing the corresponding calibrated output from the
		instrument.
out	err	An optional errors-based object that if provided can be used to retrieve information relating to any errors encountered during execution. If not provided, a default implementation of the errors class is used internally to provide error handling. Possible errors and warning messages that may be encountered are as follows.
		CF_ARRAY_SIZE_ERROR: Occurs if applied and measured are not the same size.

Returns

The largest magnitude deviation from the initial test.

Remarks

Repeatability is considered as the largest magnitude deviation of subsequent tests from the initial test. Noting that it is very likely that consecutive test points will vary slightly, test 2 through test N are linearly interpolated such that their test points line up with those from test 1.

Definition at line 608 of file curvefit_calibration.f90.

The documentation for this interface was generated from the following file:

/home/jason/Documents/Code/curvefit/src/curvefit_calibration.f90

6.30 curvefit_calibration::return_to_zero Interface Reference

Computes the return to zero error in an ascending/descending data set.

Private Member Functions

real(dp) function rtz_1 (applied, measured, tol, err)
 Computes the return to zero error in an ascending/descending data set.

6.30.1 Detailed Description

Computes the return to zero error in an ascending/descending data set.

Definition at line 80 of file curvefit_calibration.f90.

6.30.2 Member Function/Subroutine Documentation

6.30.2.1 real(dp) function curvefit_calibration::return_to_zero::rtz_1 (real(dp), dimension(:), intent(in) applied, real(dp), dimension(:), intent(in) measured, real(dp), intent(in), optional tol, class(errors), intent(inout), optional, target err)

[private]

Computes the return to zero error in an ascending/descending data set.

Parameters

in	applied	An N-element array containing the values applied to the measurement instrument.
in	measured	An N-element array containing the calibrated output of the instrument as a result of the values given in applied.
in	tol	An optional input that specifies the tolerance used in finding the matching data points. If no value is specified, the default value of the square root of machine precision times the largest magnitude value in xcal is used.
out	err	An optional errors-based object that if provided can be used to retrieve information relating to any errors encountered during execution. If not provided, a default implementation of the errors class is used internally to provide error handling. Possible errors and warning messages that may be encountered are as follows.
		CF_ARRAY_SIZE_ERROR: Occurs if applied and measured are not the same size.

Returns

The return to zero error.

Definition at line 522 of file curvefit_calibration.f90.

The documentation for this interface was generated from the following file:

• /home/jason/Documents/Code/curvefit/src/curvefit_calibration.f90

6.31 curvefit_calibration::seb Interface Reference

Computes the static error band of a data set.

Private Member Functions

type(seb_results) function seb_1 (applied, output, fullscale, err)
 Computes the static error band of a data set.

6.31.1 Detailed Description

Computes the static error band of a data set.

Definition at line 54 of file curvefit_calibration.f90.

6.31.2 Member Function/Subroutine Documentation

6.31.2.1 type(seb_results) function curvefit_calibration::seb::seb_1 (real(dp), dimension(:), intent(in) applied, real(dp), dimension(:), intent(in) output, real(dp), intent(in) fullscale, class(errors), intent(out), optional, target err)

[private]

Computes the static error band of a data set.

Parameters

in	applied	An N-element array containing the values applied to the measurement instrument.
in	output	An N-element array containing the values output by the instrument as a result of the values
		given in applied.
in	fullscale	The full scale measurement value for the instrument. The units must be consistent with
		those of applied.
out	err	An optional errors-based object that if provided can be used to retrieve information relating to any errors encountered during execution. If not provided, a default implementation of the errors class is used internally to provide error handling. Possible errors and warning messages that may be encountered are as follows.
		CF_ARRAY_SIZE_ERROR: Occurs if applied and output are not the same size.
		 CF_INVALID_INPUT_ERROR: Occurs if fullscale is sufficiently close to zero to be considered zero. Sufficiently close in this instance is considered to be the square root of machine precision.

Returns

The static error band information.

Definition at line 126 of file curvefit_calibration.f90.

The documentation for this interface was generated from the following file:

• /home/jason/Documents/Code/curvefit/src/curvefit_calibration.f90

6.32 curvefit_calibration::seb_results Type Reference

Defines a container for static error band related information.

Private Attributes

• real(dp) seb

The static error band.

real(dp) output

The static error band output, at full scale load.

• real(dp) slope

The slope of the static error band fit.

6.32.1 Detailed Description

Defines a container for static error band related information.

Definition at line 32 of file curvefit_calibration.f90.

The documentation for this type was generated from the following file:

/home/jason/Documents/Code/curvefit/src/curvefit calibration.f90

6.33 curvefit_interp::spline_interp Type Reference

Extends the interp_manager class allowing for cubic spline interpolation of a data set.

Inheritance diagram for curvefit_interp::spline_interp:

Collaboration diagram for curvefit_interp::spline_interp:

Public Member Functions

• procedure, public initialize => si_init_1

Initializes the spline_interp instance.

procedure, public initialize_spline => si_init_2

Initializes the spline_interp instance while allowing definition of boundary conditions.

• generic, public first_derivative => si_diff1, si_diff1_array

Interpolates to obtain the first derivative value at the specified independent variable.

• generic, public second_derivative => si_diff2, si_diff2_array

Interpolates to obtain the second derivative value at the specified independent variable.

Private Member Functions

• procedure raw_interp => si_raw_interp

Performs the actual interpolation.

• procedure compute_diff2 => si_second_deriv

Computes the second derivative terms for the cubic-spline model.

- procedure si_diff1
- procedure si_diff1_array
- · procedure si diff2
- procedure si_diff2_array

Private Attributes

• real(dp), dimension(:), allocatable m_ypp

6.33.1 Detailed Description

Extends the interp_manager class allowing for cubic spline interpolation of a data set.

Definition at line 108 of file curvefit_interp.f90.

The documentation for this type was generated from the following file:

/home/jason/Documents/Code/curvefit/src/curvefit_interp.f90

6.34 curvefit_calibration::split_ascend_descend Interface Reference

Splits a data set into ascending and descending components.

Private Member Functions

• subroutine split_ascend_descend_1 (x, ascend, descend, nascend, ndescend, err)

Splits a data set into ascending and descending components.

6.34.1 Detailed Description

Splits a data set into ascending and descending components.

Definition at line 99 of file curvefit_calibration.f90.

6.34.2 Member Function/Subroutine Documentation

6.34.2.1 subroutine curvefit_calibration::split_ascend_descend::split_ascend_descend_1 (real(dp), dimension(:), intent(in) x, real(dp), dimension(:), intent(out) ascend, real(dp), dimension(:), intent(out) descend, integer(i32), intent(out) nascend, integer(i32), intent(out) ndescend, class(errors), intent(inout), optional, target err) [private]

Splits a data set into ascending and descending components.

Parameters

in	X	An N-element array containing the data set to split.
out	ascend	An array where the ascending points will be written. Ensure this array is appropriately
		sized to accept all the ascending points (it can be oversized).
out	descend	An array where the descending points will be written. Ensure this array is appropriately
		sized to accept all the descending points (it can be oversized).
out	nascend	The actual number of values written into ascend.
out	ndescend	The actual number of values written into descend.
out	err	An optional errors-based object that if provided can be used to retrieve information relating
		to any errors encountered during execution. If not provided, a default implementation of the
Generated by Doxygen		errors class is used internally to provide error handling. Possible errors and warning
Generated	by boxygen	messages that may be encountered are as follows.
		CF ARRAY SIZE ERROR: Occurs if either ascend or descend is too small to
		actually accept all of the necessary data.

Remarks

The routine operates by finding the first occurrence where the data set is no longer monotonic, and then copies everything prior to that value, along with the the inflection value, into the output ascending data array. The routine then searches for either a change in direction, or a value that matches the first value in the ascending data set within some tolerance to determine the bounds on the descending data set. Once the bounds are determined, the descending data set is copied from the original array and placed in the output descending data array. This then means that any remaining data in the original data set that lies after either of the aforementioned sets is ignored.

Example

```
Given the following array X,
  0.0000000000000000
 0.38905000686645508
 0.77815997600555420
 0.97268998622894287
 1.1671400070190430
 1.5559999942779541
  1.9448399543762207
 0.97259998321533203
  -9.9999997473787516E-006
This routine splits the array into the following ascending and
descending arrays.
ASCENDING:
 0.0000000000000000
  0.38905000686645508
 0.77815997600555420
 0.97268998622894287
 1.1671400070190430
 1.5559999942779541
 1.9448399543762207
DESCENDING:
  1.9448399543762207
  0.97259998321533203
  -9.9999997473787516E-006
```

Definition at line 1011 of file curvefit_calibration.f90.

The documentation for this interface was generated from the following file:

• /home/jason/Documents/Code/curvefit/src/curvefit calibration.f90

6.35 curvefit_statistics::standard_deviation Interface Reference

Computes the corrected standard deviation of a data set.

Private Member Functions

pure real(dp) function stdev_dbl (x)
 Computes the corrected standard deviation of a data set.

6.35.1 Detailed Description

Computes the corrected standard deviation of a data set.

Definition at line 56 of file curvefit_statistics.f90.

6.35.2 Member Function/Subroutine Documentation

6.35.2.1 pure real(dp) function curvefit_statistics::standard_deviation::stdev_dbl (real(dp), dimension(:), intent(in) x) [private]

Computes the corrected standard deviation of a data set.

Parameters

Returns

The standard deviation of x.

Definition at line 366 of file curvefit_statistics.f90.

The documentation for this interface was generated from the following file:

/home/jason/Documents/Code/curvefit/src/curvefit_statistics.f90

6.36 curvefit_statistics::t_value Interface Reference

Computes the t-value (t-score) given a percentage of the area under the standard normal distribution curve.

Private Member Functions

• real(dp) function t_dist_score (alpha, n, err)

Computes the t-value (t-score) given a percentage of the area under the standard normal distribution curve.

6.36.1 Detailed Description

Computes the t-value (t-score) given a percentage of the area under the standard normal distribution curve.

Definition at line 77 of file curvefit_statistics.f90.

6.36.2 Member Function/Subroutine Documentation

6.36.2.1 real(dp) function curvefit_statistics::t_value::t_dist_score (real(dp), intent(in) alpha, integer(i32), intent(in) n, class(errors), intent(inout), optional, target err) [private]

Computes the t-value (t-score) given a percentage of the area under the standard normal distribution curve.

Parameters

in	alpha	The percentage of the area under the curve. This value must be between 0 and 1 such that: 0
		< alpha $<$ 1.
out	err	An optional errors-based object that if provided can be used to retrieve information relating to
Generated	by Doxyge	n any errors encountered during execution. If not provided, a default implementation of the errors class is used internally to provide error handling. Possible errors and warning messages that may be encountered are as follows.
		OF INVALID INDUT EDDOD O 1/2 3 3 1 1 1 1 1/4 0 4 1 1 4

Returns

The t-socre or t-value.

Definition at line 538 of file curvefit_statistics.f90.

The documentation for this interface was generated from the following file:

• /home/jason/Documents/Code/curvefit/src/curvefit_statistics.f90

6.37 curvefit_calibration::terminal_nonlinearity Interface Reference

Computes the terminal nonlinearity of a data set.

Private Member Functions

real(dp) function term_nonlin (applied, measured, err)
 Computes the terminal nonlinearity of a data set.

6.37.1 Detailed Description

Computes the terminal nonlinearity of a data set.

Definition at line 66 of file curvefit_calibration.f90.

6.37.2 Member Function/Subroutine Documentation

6.37.2.1 real(dp) function curvefit_calibration::terminal_nonlinearity::term_nonlin (real(dp), dimension(:), intent(in) applied, real(dp), dimension(:), intent(in) measured, class(errors), intent(inout), optional, target err) [private]

Computes the terminal nonlinearity of a data set.

Parameters

in	applied	An N-element array containing the values applied to the measurement instrument.
in	measured	An N-element array containing the calibrated output of the instrument as a result of the values given in applied.
out	err	An optional errors-based object that if provided can be used to retrieve information relating to any errors encountered during execution. If not provided, a default implementation of the errors class is used internally to provide error handling. Possible errors and warning messages that may be encountered are as follows.
		CF_ARRAY_SIZE_ERROR: Occurs if applied and measured are not the same size.

Returns

The terminal nonlinearity error.

Definition at line 267 of file curvefit calibration.f90.

The documentation for this interface was generated from the following file:

/home/jason/Documents/Code/curvefit/src/curvefit calibration.f90

6.38 curvefit_statistics::variance Interface Reference

Computes the sample variance of a data set.

Private Member Functions

pure real(dp) function variance_dbl (x)
 Computes the sample variance of a data set.

6.38.1 Detailed Description

Computes the sample variance of a data set.

Definition at line 43 of file curvefit statistics.f90.

6.38.2 Member Function/Subroutine Documentation

6.38.2.1 pure real(dp) function curvefit_statistics::variance::variance_dbl(real(dp), dimension(:), intent(in) x) [private]

Computes the sample variance of a data set.

Parameters

in	X	The data set.

Returns

The variance of x.

Remarks

To avoid overflow-type issues, Welford's algorithm is employed. A simple illustration of this algorithm can be found here.

Definition at line 202 of file curvefit_statistics.f90.

The documentation for this interface was generated from the following file:

/home/jason/Documents/Code/curvefit/src/curvefit_statistics.f90

6.39 curvefit_statistics::z_value Interface Reference

Computes the z-value (z-score) given a percentage of the area under the standard normal distribution curve.

Private Member Functions

real(dp) function std_norm_dist_z_score (alpha, err)
 Computes the z-value (z-score) given a percentage of the area under the standard normal distribution curve.

6.39.1 Detailed Description

Computes the z-value (z-score) given a percentage of the area under the standard normal distribution curve.

Definition at line 70 of file curvefit_statistics.f90.

6.39.2 Member Function/Subroutine Documentation

6.39.2.1 real(dp) function curvefit_statistics::z_value::std_norm_dist_z_score (real(dp), intent(in) alpha, class(errors), intent(inout), optional, target err) [private]

Computes the z-value (z-score) given a percentage of the area under the standard normal distribution curve.

Parameters

in	alpha	The percentage of the area under the curve. This value must be between 0 and 1 such that: $0 < alpha < 1$.
out	err	An optional errors-based object that if provided can be used to retrieve information relating to any errors encountered during execution. If not provided, a default implementation of the errors class is used internally to provide error handling. Possible errors and warning messages that may be encountered are as follows.
		CF_INVALID_INPUT_ERROR: Occurs if alpha is does not satisfy: 0 < alpha < 1.

Returns

The z-score or z-value by solving for z where: alpha = ERF(z / sqrt(2)), where ERF is the error function.

Definition at line 467 of file curvefit_statistics.f90.

The documentation for this interface was generated from the following file:

• /home/jason/Documents/Code/curvefit/src/curvefit_statistics.f90

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