

nonlin

1.1.5

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Contents

1	Main Page	2
1.1	Introduction	2
2	Modules Index	2
2.1	Modules List	2
3	Data Type Index	2
3.1	Class Hierarchy	2
4	Data Type Index	4
4.1	Data Types List	4
5	Module Documentation	6
5.1	nonlin_c_binding Module Reference	6
5.1.1	Detailed Description	8
5.1.2	Function/Subroutine Documentation	8
5.2	nonlin_least_squares Module Reference	22
5.2.1	Detailed Description	22
5.2.2	Function/Subroutine Documentation	22
5.3	nonlin_linesearch Module Reference	27
5.3.1	Detailed Description	28
5.3.2	Function/Subroutine Documentation	28
5.4	nonlin_optimize Module Reference	32
5.4.1	Detailed Description	33
5.4.2	Function/Subroutine Documentation	33
5.5	nonlin_polynomials Module Reference	40
5.5.1	Detailed Description	41
5.5.2	Function/Subroutine Documentation	41
5.6	nonlin_solve Module Reference	49
5.6.1	Detailed Description	50
5.6.2	Function/Subroutine Documentation	50
5.7	nonlin_types Module Reference	57
5.7.1	Detailed Description	60
5.7.2	Function/Subroutine Documentation	60

6 Data Type Documentation	73
6.1 <code>nonlin_polynomials::assignment(=)</code> Interface Reference	73
6.1.1 Detailed Description	73
6.1.2 Member Function/Subroutine Documentation	73
6.2 <code>nonlin_optimize::bfgs</code> Type Reference	74
6.2.1 Detailed Description	74
6.3 <code>nonlin_solve::brent_solver</code> Type Reference	74
6.3.1 Detailed Description	74
6.4 <code>nonlin_c_binding::c_polynomial</code> Type Reference	75
6.4.1 Detailed Description	75
6.5 <code>nonlin_c_binding::cfcn1var</code> Interface Reference	75
6.5.1 Detailed Description	75
6.6 <code>nonlin_c_binding::cfcn1var_helper</code> Type Reference	76
6.7 <code>nonlin_c_binding::cfcnnvar</code> Interface Reference	76
6.7.1 Detailed Description	76
6.8 <code>nonlin_c_binding::cfcnnvar_helper</code> Type Reference	76
6.8.1 Detailed Description	77
6.9 <code>nonlin_c_binding::cggradientfcn</code> Interface Reference	77
6.9.1 Detailed Description	77
6.10 <code>nonlin_c_binding::cjacobianfcn</code> Interface Reference	78
6.10.1 Detailed Description	78
6.11 <code>nonlin_c_binding::cvecfcn</code> Interface Reference	78
6.11.1 Detailed Description	78
6.12 <code>nonlin_c_binding::cvecfcn_helper</code> Type Reference	79
6.12.1 Detailed Description	79
6.13 <code>nonlin_types::equation_optimizer</code> Type Reference	80
6.13.1 Detailed Description	80
6.14 <code>nonlin_types::equation_solver</code> Type Reference	80
6.14.1 Detailed Description	81
6.15 <code>nonlin_types::equation_solver_1var</code> Type Reference	82

6.15.1 Detailed Description	82
6.16 <code>nonlin_types::fcn1var</code> Interface Reference	83
6.16.1 Detailed Description	83
6.17 <code>nonlin_types::fcn1var_helper</code> Type Reference	83
6.17.1 Detailed Description	84
6.18 <code>nonlin_types::fcnnvar</code> Interface Reference	84
6.18.1 Detailed Description	84
6.19 <code>nonlin_types::fcnnvar_helper</code> Type Reference	84
6.19.1 Detailed Description	85
6.20 <code>nonlin_types::gradientfcn</code> Interface Reference	85
6.20.1 Detailed Description	85
6.21 <code>nonlin_types::iteration_behavior</code> Type Reference	86
6.21.1 Detailed Description	86
6.22 <code>nonlin_types::jacobianfcn</code> Interface Reference	86
6.22.1 Detailed Description	86
6.23 <code>nonlin_least_squares::least_squares_solver</code> Type Reference	87
6.23.1 Detailed Description	87
6.24 <code>nonlin_linesearch::line_search</code> Type Reference	87
6.24.1 Detailed Description	88
6.25 <code>nonlin_c_binding::line_search_control</code> Type Reference	89
6.25.1 Detailed Description	89
6.26 <code>nonlin_optimize::line_search_optimizer</code> Type Reference	89
6.26.1 Detailed Description	90
6.27 <code>nonlin_solve::line_search_solver</code> Type Reference	90
6.27.1 Detailed Description	91
6.28 <code>nonlin_optimize::nelder_mead</code> Type Reference	91
6.28.1 Detailed Description	92
6.29 <code>nonlin_solve::newton_solver</code> Type Reference	92
6.29.1 Detailed Description	92
6.30 <code>nonlin_types::nonlin_optimize</code> Interface Reference	92

6.30.1 Detailed Description	92
6.31 <code>nonlin_types::nonlin_solver</code> Interface Reference	93
6.31.1 Detailed Description	93
6.32 <code>nonlin_types::nonlin_solver_1var</code> Interface Reference	94
6.32.1 Detailed Description	94
6.33 <code>nonlin_polynomials::operator(*)</code> Interface Reference	94
6.33.1 Detailed Description	95
6.33.2 Member Function/Subroutine Documentation	95
6.34 <code>nonlin_polynomials::operator(+)</code> Interface Reference	96
6.34.1 Detailed Description	96
6.34.2 Member Function/Subroutine Documentation	96
6.35 <code>nonlin_polynomials::operator(-)</code> Interface Reference	97
6.35.1 Detailed Description	97
6.35.2 Member Function/Subroutine Documentation	97
6.36 <code>nonlin_polynomials::polynomial</code> Type Reference	97
6.36.1 Detailed Description	98
6.37 <code>nonlin_solve::quasi_newton_solver</code> Type Reference	98
6.37.1 Detailed Description	99
6.38 <code>nonlin_c_binding::solver_control</code> Type Reference	99
6.38.1 Detailed Description	99
6.39 <code>nonlin_types::value_pair</code> Type Reference	100
6.39.1 Detailed Description	100
6.40 <code>nonlin_types::vecfcn</code> Interface Reference	100
6.40.1 Detailed Description	100
6.41 <code>nonlin_types::vecfcn_helper</code> Type Reference	101
6.41.1 Detailed Description	101

1 Main Page

1.1 Introduction

NONLIN is a library that provides routines to compute the solutions to systems of nonlinear equations.

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Version

1.1.5

2 Modules Index

2.1 Modules List

Here is a list of all documented modules with brief descriptions:

nonlin_c_binding	
nonlin_c_binding	6
nonlin_least_squares	
nonlin_least_squares	22
nonlin_linesearch	
nonlin_linesearch	27
nonlin_optimize	
nonlin_optimize	32
nonlin_polynomials	
polynomials	40
nonlin_solve	
nonlin_solve	49
nonlin_types	
nonlin_types	57

3 Data Type Index

3.1 Class Hierarchy

This inheritance list is sorted roughly, but not completely, alphabetically:

nonlin_polynomials::assignment(=)	73
nonlin_c_binding::c_polynomial	75

nonlin_c_binding::cfcn1var	75
nonlin_c_binding::cfcnnvar	76
nonlin_c_binding::cgradientfcn	77
nonlin_c_binding::cjacobianfcn	78
nonlin_c_binding::cvecfcn	78
nonlin_types::equation_optimizer	80
nonlin_optimize::line_search_optimizer	89
nonlin_optimize::bfgs	74
nonlin_optimize::nelder_mead	91
nonlin_types::equation_solver	80
nonlin_least_squares::least_squares_solver	87
nonlin_solve::line_search_solver	90
nonlin_solve::newton_solver	92
nonlin_solve::quasi_newton_solver	98
nonlin_types::equation_solver_1var	82
nonlin_solve::brent_solver	74
nonlin_types::fcn1var	83
nonlin_types::fcn1var_helper	83
nonlin_c_binding::cfcn1var_helper	76
nonlin_types::fcnnvar	84
nonlin_types::fcnnvar_helper	84
nonlin_c_binding::cfcnnvar_helper	76
nonlin_types::gradientfcn	85
nonlin_types::iteration_behavior	86
nonlin_types::jacobianfcn	86
nonlin_linesearch::line_search	87
nonlin_c_binding::line_search_control	89
nonlin_types::nonlin_optimize	92
nonlin_types::nonlin_solver	93
nonlin_types::nonlin_solver_1var	94
nonlin_polynomials::operator(*)	94
nonlin_polynomials::operator(+)	96

<code>nonlin_polynomials::operator(-)</code>	97
<code>nonlin_polynomials::polynomial</code>	97
<code>nonlin_c_binding::solver_control</code>	99
<code>nonlin_types::value_pair</code>	100
<code>nonlin_types::vecfcn</code>	100
<code>nonlin_types::vecfcn_helper</code>	101
<code>nonlin_c_binding::cvecfcn_helper</code>	79

4 Data Type Index

4.1 Data Types List

Here are the data types with brief descriptions:

<code>nonlin_polynomials::assignment(=)</code> Defines polynomial assignment	73
<code>nonlin_optimize::bfgs</code> Defines a Broyden–Fletcher–Goldfarb–Shanno (BFGS) solver for minimization of functions of multiple variables	74
<code>nonlin_solve::brent_solver</code> Defines a solver based upon Brent's method for solving an equation of one variable without using derivatives	74
<code>nonlin_c_binding::c_polynomial</code> A C compatible type encapsulating a polynomial object	75
<code>nonlin_c_binding::cfcn1var</code> The C-friendly interface to <code>fcn1var</code>	75
<code>nonlin_c_binding::cfcn1var_helper</code> A type allowing the use of <code>cfcn1var</code> in the solver codes	76
<code>nonlin_c_binding::cfcnnvar</code> The C-friendly interface to <code>fcnnvar</code>	76
<code>nonlin_c_binding::cfcnnvar_helper</code> A type allowing the use of <code>cfcnnvar</code> in the solver codes	76
<code>nonlin_c_binding::cgradientfcn</code> A C-friendly interface to <code>gradientfcn</code>	77
<code>nonlin_c_binding::cjacobianfcn</code> The C-friendly interface to <code>jacobianfcn</code>	78
<code>nonlin_c_binding::cvecfcn</code> The C-friendly interface to <code>vecfcn</code>	78
<code>nonlin_c_binding::cvecfcn_helper</code> A type allowing the use of <code>cvecfcn</code> in the solver codes	79

<code>nonlin_types::equation_optimizer</code>	
A base class for optimization of an equation of multiple variables	80
<code>nonlin_types::equation_solver</code>	
A base class for various solvers of nonlinear systems of equations	80
<code>nonlin_types::equation_solver_1var</code>	
A base class for various solvers of equations of one variable	82
<code>nonlin_types::fcn1var</code>	
Describes a function of one variable	83
<code>nonlin_types::fcn1var_helper</code>	
Defines a type capable of encapsulating an equation of one variable of the form: $f(x) = 0$	83
<code>nonlin_types::fcnnvar</code>	
Describes a function of N variables	84
<code>nonlin_types::fcnnvar_helper</code>	
Defines a type capable of encapsulating an equation of N variables	84
<code>nonlin_types::gradientfcn</code>	
Describes a routine capable of computing the gradient vector of an equation of N variables	85
<code>nonlin_types::iteration_behavior</code>	
Defines a set of parameters that describe the behavior of the iteration process	86
<code>nonlin_types::jacobianfcn</code>	
Describes a routine capable of computing the Jacobian matrix of M functions of N unknowns	86
<code>nonlin_least_squares::least_squares_solver</code>	
Defines a Levenberg-Marquardt based solver for unconstrained least-squares problems	87
<code>nonlin_linesearch::line_search</code>	
Defines a type capable of performing an inexact, backtracking line search to find a point as far along the specified direction vector that is usable for unconstrained minimization problems	87
<code>nonlin_c_binding::line_search_control</code>	
Defines a set of line search controls	89
<code>nonlin_optimize::line_search_optimizer</code>	
A class describing equation optimizers that use a line search algorithm to improve convergence behavior	89
<code>nonlin_solve::line_search_solver</code>	
A class describing nonlinear solvers that use a line search algorithm to improve convergence behavior	90
<code>nonlin_optimize::nelder_mead</code>	
Defines a solver based upon Nelder and Mead's simplex algorithm for minimization of functions of multiple variables	91
<code>nonlin_solve::newton_solver</code>	
Defines a Newton solver	92
<code>nonlin_types::nonlin_optimize</code>	
Describes the interface of a routine for optimizing an equation of N variables	92
<code>nonlin_types::nonlin_solver</code>	
Describes the interface of a nonlinear equation solver	93

nonlin_types::nonlin_solver_1var	
Describes the interface of a solver for an equation of one variable	94
nonlin_polynomials::operator(*)	
Defines polynomial multiplication	94
nonlin_polynomials::operator(+)	
Defines polynomial addition	96
nonlin_polynomials::operator(-)	
Defines polynomial subtraction	97
nonlin_polynomials::polynomial	
Defines a polynomial, and associated routines for performing polynomial operations	97
nonlin_solve::quasi_newton_solver	
Defines a quasi-Newton type solver based upon Broyden's method	98
nonlin_c_binding::solver_control	
Defines a set of solver control information	99
nonlin_types::value_pair	
Defines a pair of numeric values	100
nonlin_types::vecfcn	
Describes an M-element vector-valued function of N-variables	100
nonlin_types::vecfcn_helper	
Defines a type capable of encapsulating a system of nonlinear equations of the form: $F(X) = 0$	101

5 Module Documentation

5.1 nonlin_c_binding Module Reference

[nonlin_c_binding](#)

Data Types

- type [c_polynomial](#)
A C compatible type encapsulating a polynomial object.
- interface [cfcn1var](#)
The C-friendly interface to fcn1var.
- type [cfcn1var_helper](#)
A type allowing the use of cfcn1var in the solver codes.
- interface [cfcnnvar](#)
The C-friendly interface to fcnnvar.
- type [cfcnnvar_helper](#)
A type allowing the use of cfcnnvar in the solver codes.
- interface [cgradientfcn](#)
A C-friendly interface to gradientfcn.
- interface [cjacobianfcn](#)
The C-friendly interface to jacobianfcn.
- interface [cvecfcn](#)

The C-friendly interface to `vecfcn`.

- type `cvecfcn_helper`
A type allowing the use of `cvecfcn` in the solver codes.
- type `line_search_control`
Defines a set of line search controls.
- type `solver_control`
Defines a set of solver control information.

Functions/Subroutines

- real(dp) function `cf1h_fcn` (this, x)
Executes the routine containing the function to evaluate.
- pure logical function `cf1h_is_fcn_defined` (this)
Tests if the pointer to the function containing the equation to solve has been assigned.
- subroutine `cf1h_set_fcn` (this, fcn)
Establishes a pointer to the routine containing the equations to solve.
- subroutine `cvfh_set_fcn` (this, fcn, nfcn, nvar)
Establishes a pointer to the routine containing the system of equations to solve.
- pure logical function `cvfh_is_fcn_defined` (this)
Tests if the pointer to the procedure containing the system of equations to solve has been assigned.
- subroutine `cvfh_fcn` (this, x, f)
Executes the routine containing the system of equations to solve. No action is taken if the pointer to the subroutine has not been defined.
- subroutine `cvfh_set_jac` (this, jac)
Establishes a pointer to the routine for computing the Jacobian matrix of the system of equations. If no routine is defined, the Jacobian matrix will be computed numerically (this is the default state).
- pure logical function `cvfh_is_jac_defined` (this)
Tests if the pointer to the subroutine containing the system of equations to solve has been assigned.
- subroutine `cfnh_set_fcn` (this, fcn, nvar)
Establishes a pointer to the routine containing the equation to solve.
- pure logical function `cfnh_is_fcn_defined` (this)
Tests if the pointer to the procedure containing the system of equations to solve has been assigned.
- real(dp) function `cfnh_fcn` (this, x)
Executes the routine containing the function to evaluate.
- subroutine `cfnh_set_grad` (this, fcn)
Establishes a pointer to the routine containing the gradient vector of the function.
- pure logical function `cfnh_is_grad_defined` (this)
Tests if the pointer to the routine containing the gradient has been assigned.
- subroutine `brent_solver_c` (fcn, lim, x, f, tol, ib, err)
Solves an equation of one variable using Brent's method.
- subroutine `quasi_newton_c` (fcn, jac, n, x, fvec, tol, lsearch, ib, err)
Applies the quasi-Newton's method developed by Broyden in conjunction with a backtracking type line search to solve N equations of N unknowns.
- subroutine `newton_c` (fcn, jac, n, x, fvec, tol, lsearch, ib, err)
Applies Newton's method in conjunction with a backtracking type line search to solve N equations of N unknowns.
- subroutine `levmarq_c` (fcn, jac, neqn, nvar, x, fvec, tol, ib, err)
Applies the Levenberg-Marquardt method to solve the nonlinear least-squares problem.
- subroutine `set_nonlin_defaults` (tol)
Sets defaults for the `solver_control` type.
- subroutine `set_nonlin_ls_defaults` (ls)
Sets defaults for the `line_search_control` type.

- subroutine [nelder_mead_c](#) (fcn, nvar, x, f, smplx, tol, ib, err)
Utilizes the Nelder-Mead simplex method for finding a minimum value of the specified function.
- subroutine [bfgs_c](#) (fcn, grad, nvar, x, f, tol, lsearch, ib, err)
Utilizes the Broyden-Fletcher-Goldfarb-Shanno (BFGS) algorithm for finding a minimum value of the specified function.
- subroutine [alloc_polynomial](#) (obj, order)
Initializes a new polynomial object.
- subroutine [free_polynomial](#) (obj)
Frees resources held by a [c_polynomial](#) object.
- subroutine [get_polynomial](#) (obj, poly)
Retrieves the polynomial object from the C compatible [c_polynomial](#) data structure.
- integer(i32) function [get_polynomial_order_c](#) (poly)
Gets the order of the polynomial.
- subroutine [fit_polynomial](#) (poly, n, x, y, order, err)
Fits a polynomial of the specified order to a data set.
- subroutine [fit_polynomial_thru_zero](#) (poly, n, x, y, order, err)
Fits a polynomial of the specified order that passes through zero to a data set.
- subroutine [evaluate_polynomial](#) (poly, n, x, y)
Evaluates a polynomial at the specified points.
- subroutine [evaluate_polynomial_cmplx](#) (poly, n, x, y)
Evaluates a polynomial at the specified points.
- subroutine [polynomial_roots_c](#) (poly, n, rts, err)
Computes all the roots of a polynomial by computing the eigenvalues of the polynomial companion matrix.
- real(dp) function [get_polynomial_coefficient](#) (poly, ind, err)
*Gets the requested polynomial coefficient by index. The coefficient index is established as follows: $c(1) + c(2) * x + c(3) * x**2 + \dots c(n) * x**n-1$.*
- subroutine [set_polynomial_set_coefficient](#) (poly, ind, x, err)
*Sets the requested polynomial coefficient by index. The coefficient index is established as follows: $c(1) + c(2) * x + c(3) * x**2 + \dots c(n) * x**n-1$.*
- subroutine [polynomial_add](#) (p1, p2, rst)
Adds two polynomials.
- subroutine [polynomial_subtract](#) (p1, p2, rst)
Subtracts two polynomials.
- subroutine [polynomial_multiply](#) (p1, p2, rst)
Multiplies two polynomials.
- subroutine [polynomial_copy](#) (src, dst)
Copies the contents of one polynomial object to another.

5.1.1 Detailed Description

[nonlin_c_binding](#)

Purpose

Provides C bindings to the nonlin library.

5.1.2 Function/Subroutine Documentation

5.1.2.1 subroutine [nonlin_c_binding::alloc_polynomial](#) (type([c_polynomial](#)), intent(out) *obj*, integer(i32), intent(in), value *order*)

Initializes a new polynomial object.

Parameters

out	<i>obj</i>	The c_polynomial object to initialize.
in	<i>order</i>	The order of the polynomial. This value must be > 0 .

Definition at line 922 of file `nonlin_c_binding.f90`.

5.1.2.2 `subroutine nonlin_c_binding::bfgs_c (type(c_funptr), intent(in), value fcn, type(c_funptr), intent(in), value grad, integer(i32), intent(in), value nvar, real(dp), dimension(nvar), intent(inout) x, real(dp), intent(out) f, type(solver_control), intent(in) tol, type(c_ptr), intent(in), value lsearch, type(iteration_behavior), intent(out) ib, type(errorhandler), intent(inout) err)`

Utilizes the Broyden-Fletcher-Goldfarb-Shanno (BFGS) algorithm for finding a minimum value of the specified function.

Parameters

in	<i>fcn</i>	A pointer to the routine containing the function on which to operate.
in	<i>grad</i>	An optional pointer to a routine capable of computing the gradient of the function contained within <i>fcn</i> . If no routine is supplied (NULL), the solver will numerically estimate the gradient.
in	<i>nvar</i>	The dimension of the problem (number of variables).
in, out	<i>x</i>	On input, the initial guess at the optimal point. On output, the updated optimal point estimate.
out	<i>f</i>	An optional output, that if provided, returns the value of the function at <i>x</i> .
in	<i>tol</i>	A solver_control object defining the solver control parameters.
out	<i>ib</i>	On output, an <code>iteration_behavior</code> object containing the iteration performance statistics.
in	<i>err</i>	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. <ul style="list-style-type: none"> NL_INVALID_OPERATION_ERROR: Occurs if no equations have been defined. NL_INVALID_INPUT_ERROR: Occurs if <i>x</i> is not appropriately sized for the problem as defined in <i>fcn</i>. NL_OUT_OF_MEMORY_ERROR: Occurs if there is insufficient memory available. NL_CONVERGENCE_ERROR: Occurs if the algorithm cannot converge within the allowed number of iterations.

Definition at line 856 of file `nonlin_c_binding.f90`.

5.1.2.3 `subroutine nonlin_c_binding::brent_solver_c (type(c_funptr), intent(in), value fcn, type(value_pair), intent(in), value lim, real(dp), intent(out) x, real(dp), intent(out) f, type(solver_control), intent(in) tol, type(iteration_behavior), intent(out) ib, type(errorhandler), intent(inout) err)`

Solves an equation of one variable using Brent's method.

Parameters

in	<i>fcn</i>	A pointer to the routine containing the function to solve.
in	<i>lim</i>	A <code>value_pair</code> object defining the search limits.

Parameters

out	<i>x</i>	On output, the solution.
out	<i>f</i>	On output, the residual as computed at <i>x</i> .
in	<i>tol</i>	A solver_control object defining the solver control parameters.
out	<i>ib</i>	On output, an <code>iteration_behavior</code> object containing the iteration performance statistics.
in	<i>err</i>	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. <ul style="list-style-type: none"> • <code>NL_INVALID_OPERATION_ERROR</code>: Occurs if no equations have been defined. • <code>NL_INVALID_INPUT_ERROR</code>: Occurs if the number of equations is different than the number of variables. • <code>NL_CONVERGENCE_ERROR</code>: Occurs if the algorithm cannot converge within the allowed number of iterations.

Definition at line 424 of file `nonlin_c_binding.f90`.

5.1.2.4 `real(dp) function nonlin_c_binding::cf1h_fcn (class(cfcn1var_helper), intent(in) this, real(dp), intent(in) x)`

Executes the routine containing the function to evaluate.

Parameters

in	<i>this</i>	The cfcn1var_helper object.
in	<i>x</i>	The value of the independent variable at which the function should be evaluated.

Returns

The value of the function at *x*.

Definition at line 218 of file `nonlin_c_binding.f90`.

5.1.2.5 `pure logical function nonlin_c_binding::cf1h_is_fcn_defined (class(cfcn1var_helper), intent(in) this)`

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

Parameters

in	<i>this</i>	The cfcn1var_helper object.
----	-------------	---

Returns

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

Definition at line 233 of file `nonlin_c_binding.f90`.

5.1.2.6 `subroutine nonlin_c_binding::cf1h_set_fcn (class(cfcn1var_helper), intent(inout) this, procedure(cfcn1var), intent(in), pointer fcn)`

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

Parameters

<code>in, out</code>	<code>this</code>	The <code>cfcn1var_helper</code> object.
<code>in</code>	<code>fcn</code>	The function pointer.

Definition at line 245 of file `nonlin_c_binding.f90`.

5.1.2.7 `real(dp) function nonlin_c_binding::cfnh_fcn (class(cfcnnvar_helper), intent(in) this, real(dp), dimension(:), intent(in) x)`

Executes the routine containing the function to evaluate.

Parameters

<code>in</code>	<code>this</code>	The <code>cfcnnvar_helper</code> object.
<code>in</code>	<code>x</code>	The value of the independent variable at which the function should be evaluated.

Returns

The value of the function at `x`.

Definition at line 366 of file `nonlin_c_binding.f90`.

5.1.2.8 `pure logical function nonlin_c_binding::cfnh_is_fcn_defined (class(cfcnnvar_helper), intent(in) this)`

Tests if the pointer to the procedure containing the system of equations to solve has been assigned.

Parameters

<code>in</code>	<code>this</code>	The <code>cfcnnvar_helper</code> object.
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Returns

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

Definition at line 353 of file `nonlin_c_binding.f90`.

5.1.2.9 `pure logical function nonlin_c_binding::cfnh_is_grad_defined (class(cfcnnvar_helper), intent(in) this)`

Tests if the pointer to the routine containing the gradient has been assigned.

Parameters

<code>in</code>	<code>this</code>	The <code>cfcnnvar_helper</code> object.
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Returns

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

Definition at line 395 of file `nonlin_c_binding.f90`.

5.1.2.10 `subroutine nonlin_c_binding::cfnh_set_fcn (class(cfcnnvar_helper), intent(inout) this, procedure(cfcnnvar), intent(in), pointer fcn, integer(i32), intent(in) nvar)`

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

Parameters

<code>in, out</code>	<code>this</code>	The <code>cfcnnvar_helper</code> object.
<code>in</code>	<code>fcn</code>	The function pointer.
<code>in</code>	<code>nvar</code>	The number of variables.

Definition at line 337 of file `nonlin_c_binding.f90`.

5.1.2.11 `subroutine nonlin_c_binding::cfnh_set_grad (class(cfcnnvar_helper), intent(inout) this, procedure(cgradientfcn), intent(in), pointer fcn)`

Establishes a pointer to the routine containing the gradient vector of the function.

Parameters

<code>in, out</code>	<code>this</code>	The <code>cfcnnvar_helper</code> object.
<code>in</code>	<code>fcn</code>	The pointer to the gradient routine.

Definition at line 383 of file `nonlin_c_binding.f90`.

5.1.2.12 `subroutine nonlin_c_binding::cvfh_fcn (class(cvecfcn_helper), intent(in) this, real(dp), dimension(:), intent(in) x, real(dp), dimension(:), intent(out) f)`

Executes the routine containing the system of equations to solve. No action is taken if the pointer to the subroutine has not been defined.

Parameters

<code>in</code>	<code>this</code>	The <code>cvecfcn_helper</code> object.
<code>in</code>	<code>x</code>	An N-element array containing the independent variables.
<code>out</code>	<code>f</code>	An M-element array that, on output, contains the values of the M functions.

Definition at line 291 of file `nonlin_c_binding.f90`.

5.1.2.13 `pure logical function nonlin_c_binding::cvfh_is_fcn_defined (class(cvecfcn_helper), intent(in) this)`

Tests if the pointer to the procedure containing the system of equations to solve has been assigned.

Parameters

<code>in</code>	<code>this</code>	The <code>cvecfcn_helper</code> object.
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Returns

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

Definition at line 277 of file `nonlin_c_binding.f90`.

5.1.2.14 pure logical function `nonlin_c_binding::cvfh_is_jac_defined` (`class(cvecfcn_helper)`, `intent(in) this`)

Tests if the pointer to the subroutine containing the system of equations to solve has been assigned.

Parameters

<code>in</code>	<code>this</code>	The <code>cvecfcn_helper</code> object.
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Returns

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

Definition at line 322 of file `nonlin_c_binding.f90`.

5.1.2.15 subroutine `nonlin_c_binding::cvfh_set_fcn` (`class(cvecfcn_helper)`, `intent(inout) this`, `procedure(cvecfcn)`, `intent(in)`, `pointer fcn`, `integer(i32)`, `intent(in) nfcn`, `integer(i32)`, `intent(in) nvar`)

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

Parameters

<code>in, out</code>	<code>this</code>	The <code>cvecfcn_helper</code> object.
<code>in</code>	<code>fcn</code>	The function pointer.
<code>in</code>	<code>nfcn</code>	The number of functions.
<code>in</code>	<code>nvar</code>	The number of variables.

Definition at line 261 of file `nonlin_c_binding.f90`.

5.1.2.16 subroutine `nonlin_c_binding::cvfh_set_jac` (`class(cvecfcn_helper)`, `intent(inout) this`, `procedure(cjacobianfcn)`, `intent(in)`, `pointer jac`)

Establishes a pointer to the routine for computing the Jacobian matrix of the system of equations. If no routine is defined, the Jacobian matrix will be computed numerically (this is the default state).

Parameters

<code>in, out</code>	<code>this</code>	The <code>cvecfcn_helper</code> object.
<code>in</code>	<code>jac</code>	The function pointer.

Definition at line 310 of file `nonlin_c_binding.f90`.

5.1.2.17 subroutine `nonlin_c_binding::evaluate_polynomial` (`type(c_polynomial)`, `intent(in) poly`, `integer(i32)`, `intent(in)`, `value n`, `real(dp)`, `dimension(n)`, `intent(in) x`, `real(dp)`, `dimension(n)`, `intent(out) y`)

Evaluates a polynomial at the specified points.

Parameters

in	<i>poly</i>	The c_polynomial object.
in	<i>n</i>	The number of points to evaluate.
in	<i>x</i>	An N-element array containing the points at which to evaluate the polynomial.
out	<i>y</i>	An N-element array where the resulting polynomial outputs will be written.

Definition at line 1100 of file `nonlin_c_binding.f90`.

5.1.2.18 `subroutine nonlin_c_binding::evaluate_polynomial_cmplx (type(c_polynomial), intent(in) poly, integer(i32), intent(in), value n, complex(dp), dimension(n), intent(in) x, complex(dp), dimension(n), intent(out) y)`

Evaluates a polynomial at the specified points.

Parameters

in	<i>poly</i>	The c_polynomial object.
in	<i>n</i>	The number of points to evaluate.
in	<i>x</i>	An N-element array containing the points at which to evaluate the polynomial.
out	<i>y</i>	An N-element array where the resulting polynomial outputs will be written.

Definition at line 1126 of file `nonlin_c_binding.f90`.

5.1.2.19 `subroutine nonlin_c_binding::fit_polynomial (type(c_polynomial), intent(out) poly, integer(i32), intent(in), value n, real(dp), dimension(n), intent(in) x, real(dp), dimension(n), intent(inout) y, integer(i32), intent(in), value order, type(errorhandler), intent(inout) err)`

Fits a polynomial of the specified order to a data set.

Parameters

out	<i>poly</i>	The c_polynomial object to initialize.
in	<i>n</i>	The size of the arrays.
in	<i>x</i>	An N-element array containing the independent variable data points. Notice, must be $N > \text{order}$.
in, out	<i>y</i>	On input, an N-element array containing the dependent variable data points. On output, the contents are overwritten.
in	<i>order</i>	The order of the polynomial (must be ≥ 1).
in, out	<i>err</i>	<p>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.</p> <ul style="list-style-type: none"> • <code>NL_INVALID_INPUT_ERROR</code>: Occurs if a zero or negative polynomial order was specified, or if order is too large for the data set. • <code>NL_OUT_OF_MEMORY_ERROR</code>: Occurs if insufficient memory is available. • <code>NL_ARRAY_SIZE_ERROR</code>: Occurs if <i>x</i> and <i>y</i> are different sizes.

Definition at line 1022 of file `nonlin_c_binding.f90`.

5.1.2.20 `subroutine nonlin_c_binding::fit_polynomial_thru_zero (type(c_polynomial), intent(out) poly, integer(i32), intent(in), value n, real(dp), dimension(n), intent(in) x, real(dp), dimension(n), intent(inout) y, integer(i32), intent(in), value order, type(errorhandler), intent(inout) err)`

Fits a polynomial of the specified order that passes through zero to a data set.

Parameters

out	<i>poly</i>	The <code>c_polynomial</code> object to initialize.
in	<i>n</i>	The size of the arrays.
in	<i>x</i>	An N-element array containing the independent variable data points. Notice, must be $N > \text{order}$.
in, out	<i>y</i>	On input, an N-element array containing the dependent variable data points. On output, the contents are overwritten.
in	<i>order</i>	The order of the polynomial (must be ≥ 1).
in, out	<i>err</i>	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. <ul style="list-style-type: none"> NL_INVALID_INPUT_ERROR: Occurs if a zero or negative polynomial order was specified, or if order is too large for the data set. NL_OUT_OF_MEMORY_ERROR: Occurs if insufficient memory is available. NL_ARRAY_SIZE_ERROR: Occurs if <i>x</i> and <i>y</i> are different sizes.

Definition at line 1066 of file `nonlin_c_binding.f90`.

5.1.2.21 `subroutine nonlin_c_binding::free_polynomial (type(c_polynomial), intent(inout), target obj)`

Frees resources held by a `c_polynomial` object.

Parameters

in, out	<i>obj</i>	The <code>c_polynomial</code> object.
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Definition at line 941 of file `nonlin_c_binding.f90`.

5.1.2.22 `subroutine nonlin_c_binding::get_polynomial (type(c_polynomial), intent(in), target obj, type(polynomial), intent(out), pointer poly)`

Retrieves the polynomial object from the C compatible `c_polynomial` data structure.

Parameters

in	<i>obj</i>	The C compatible <code>c_polynomial</code> data structure.
out	<i>poly</i>	The resulting polynomials object.

Definition at line 965 of file `nonlin_c_binding.f90`.

5.1.2.23 `real(dp) function nonlin_c_binding::get_polynomial_coefficient (type(c_polynomial), intent(in) poly, integer(i32), intent(in), value ind, type(errorhandler), intent(inout) err)`

Gets the requested polynomial coefficient by index. The coefficient index is established as follows: $c(1) + c(2) * x + c(3) * x**2 + \dots c(n) * x**n-1$.

Parameters

in	<i>poly</i>	The c_polynomial object.
in	<i>ind</i>	The polynomial coefficient index ($0 < ind \leq order + 1$).
in, out	<i>err</i>	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. <ul style="list-style-type: none"> NL_INVALID_INPUT_ERROR: Occurs if the requested index is less than or equal to zero, or if the requested index exceeds the number of polynomial coefficients.

Definition at line 1200 of file `nonlin_c_binding.f90`.

5.1.2.24 `integer(i32) function nonlin_c_binding::get_polynomial_order_c (type(c_polynomial), intent(in) poly)`

Gets the order of the polynomial.

Parameters

in	<i>poly</i>	The c_polynomial object.
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Returns

The order of the polynomial object.

Definition at line 988 of file `nonlin_c_binding.f90`.

5.1.2.25 `subroutine nonlin_c_binding::levmarq_c (type(c_funptr), intent(in), value fcn, type(c_funptr), intent(in), value jac, integer(i32), intent(in), value neqn, integer(i32), intent(in), value nvar, real(dp), dimension(nvar), intent(inout) x, real(dp), dimension(neqn), intent(out) fvec, type(solver_control), intent(in) tol, type(iteration_behavior), intent(out) ib, type(errorhandler), intent(inout) err)`

Applies the Levenberg-Marquardt method to solve the nonlinear least-squares problem.

Parameters

in	<i>fcn</i>	A pointer to the routine containing the system of equations to solve.
in	<i>jac</i>	A pointer to a routine used to compute the Jacobian of the system of equations. To let the program compute the Jacobian numerically, simply pass NULL.
in	<i>neqn</i>	The number of equations.
in	<i>nvar</i>	The number of unknowns. This must be less than or equal to <i>neqn</i> .
in, out	<i>x</i>	On input, an N-element array containing an initial estimate to the solution. On output, the updated solution estimate. N is the number of variables.
out	<i>fvec</i>	An N-element array that, on output, will contain the values of each equation as evaluated at the variable values given in <i>x</i> .

Parameters

in	<i>tol</i>	A solver_control object defining the solver control parameters.
out	<i>ib</i>	On output, an <code>iteration_behavior</code> object containing the iteration performance statistics.
in	<i>err</i>	<p>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.</p> <ul style="list-style-type: none"> • <code>NL_INVALID_OPERATION_ERROR</code>: Occurs if no equations have been defined. • <code>NL_INVALID_INPUT_ERROR</code>: Occurs if the number of equations is less than the number of variables. • <code>NL_ARRAY_SIZE_ERROR</code>: Occurs if any of the input arrays are not sized correctly. • <code>NL_CONVERGENCE_ERROR</code>: Occurs if the line search cannot converge within the allowed number of iterations. • <code>NL_OUT_OF_MEMORY_ERROR</code>: Occurs if there is insufficient memory available. • <code>NL_TOLERANCE_TOO_SMALL_ERROR</code>: Occurs if the requested tolerance is too small to be practical for the problem at hand.

Definition at line 685 of file `nonlin_c_binding.f90`.

5.1.2.26 `subroutine nonlin_c_binding::nelder_mead_c (type(c_funptr), intent(in), value fcn, integer(i32), intent(in), value nvar, real(dp), dimension(nvar), intent(inout) x, real(dp), intent(out) f, type(c_ptr), intent(in), value smplx, type(solver_control), intent(in) tol, type(iteration_behavior), intent(out) ib, type(errorhandler), intent(inout) err)`

Utilizes the Nelder-Mead simplex method for finding a minimum value of the specified function.

Parameters

in	<i>fcn</i>	A pointer to the routine containing the function on which to operate.
in	<i>nvar</i>	The dimension of the problem (number of variables).
in, out	<i>x</i>	On input, the initial guess at the optimal point. On output, the updated optimal point estimate.
out	<i>f</i>	An optional output, that if provided, returns the value of the function at <i>x</i> .
in	<i>smplx</i>	An optional NVAR-by-(NVAR + 1) matrix, that if supplied provides an initial simplex geometry (each column is a vertex location). If not provided (NULL), the solver generates its own estimate of a starting simplex geometry.
in	<i>tol</i>	A solver_control object defining the solver control parameters.
out	<i>ib</i>	On output, an <code>iteration_behavior</code> object containing the iteration performance statistics.
in	<i>err</i>	<p>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.</p> <ul style="list-style-type: none"> • <code>NL_INVALID_OPERATION_ERROR</code>: Occurs if no equations have been defined. • <code>NL_INVALID_INPUT_ERROR</code>: Occurs if <i>x</i> is not appropriately sized for the problem as defined in <i>fcn</i>. • <code>NL_OUT_OF_MEMORY_ERROR</code>: Occurs if there is insufficient memory available. • <code>NL_CONVERGENCE_ERROR</code>: Occurs if the algorithm cannot converge within the allowed number of iterations.

Definition at line 788 of file `nonlin_c_binding.f90`.

5.1.2.27 `subroutine nonlin_c_binding::newton_c (type(c_funptr), intent(in), value fcn, type(c_funptr), intent(in), value jac, integer(i32), intent(in), value n, real(dp), dimension(n), intent(inout) x, real(dp), dimension(n), intent(out) fvec, type(solver_control), intent(in) tol, type(c_ptr), intent(in), value lsearch, type(iteration_behavior), intent(out) ib, type(errorhandler), intent(inout) err)`

Applies Newton's method in conjunction with a backtracking type line search to solve N equations of N unknowns.

Parameters

in	<i>fcn</i>	A pointer to the routine containing the system of equations to solve.
in	<i>jac</i>	A pointer to a routine used to compute the Jacobian of the system of equations. To let the program compute the Jacobian numerically, simply pass NULL.
in	<i>n</i>	The number of equations, and the number of unknowns.
in, out	<i>x</i>	On input, an N-element array containing an initial estimate to the solution. On output, the updated solution estimate. N is the number of variables.
out	<i>fvec</i>	An N-element array that, on output, will contain the values of each equation as evaluated at the variable values given in <i>x</i> .
in	<i>tol</i>	A <code>solver_control</code> object defining the solver control parameters.
in	<i>lsearch</i>	A pointer to a <code>line_search_control</code> object defining the line search control parameters. If no line search is desired, simply pass NULL.
out	<i>ib</i>	On output, an <code>iteration_behavior</code> object containing the iteration performance statistics.
in	<i>err</i>	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. <ul style="list-style-type: none"> • <code>NL_INVALID_OPERATION_ERROR</code>: Occurs if no equations have been defined. • <code>NL_INVALID_INPUT_ERROR</code>: Occurs if the number of equations is different than the number of variables. • <code>NL_ARRAY_SIZE_ERROR</code>: Occurs if any of the input arrays are not sized correctly. • <code>NL_DIVERGENT_BEHAVIOR_ERROR</code>: Occurs if the direction vector is pointing in an apparent uphill direction. • <code>NL_CONVERGENCE_ERROR</code>: Occurs if the line search cannot converge within the allowed number of iterations. • <code>NL_OUT_OF_MEMORY_ERROR</code>: Occurs if there is insufficient memory available. • <code>NL_SPURIOUS_CONVERGENCE_ERROR</code>: Occurs as a warning if the slope of the gradient vector becomes sufficiently close to zero.

Definition at line 593 of file `nonlin_c_binding.f90`.

5.1.2.28 `subroutine nonlin_c_binding::polynomial_add (type(c_polynomial), intent(in) p1, type(c_polynomial), intent(in) p2, type(c_polynomial), intent(out) rst)`

Adds two polynomials.

Parameters

in	<i>p1</i>	The left-hand-side argument.
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Parameters

in	<i>p2</i>	The right-hand-side argument.
out	<i>rst</i>	The resulting polynomial.

Definition at line 1267 of file `nonlin_c_binding.f90`.

5.1.2.29 `subroutine nonlin_c_binding::polynomial_copy (type(c_polynomial), intent(in) src, type(c_polynomial), intent(out) dst)`

Copies the contents of one polynomial object to another.

Parameters

in	<i>src</i>	The source polynomial object.
out	<i>dst</i>	The destination polynomial.

Definition at line 1337 of file `nonlin_c_binding.f90`.

5.1.2.30 `subroutine nonlin_c_binding::polynomial_multiply (type(c_polynomial), intent(in) p1, type(c_polynomial), intent(in) p2, type(c_polynomial), intent(out) rst)`

Multiplies two polynomials.

Parameters

in	<i>p1</i>	The left-hand-side argument.
in	<i>p2</i>	The right-hand-side argument.
out	<i>rst</i>	The resulting polynomial.

Definition at line 1315 of file `nonlin_c_binding.f90`.

5.1.2.31 `subroutine nonlin_c_binding::polynomial_roots_c (type(c_polynomial), intent(in) poly, integer(i32), intent(in), value n, complex(dp), dimension(n), intent(out) rts, type(errorhandler), intent(inout) err)`

Computes all the roots of a polynomial by computing the eigenvalues of the polynomial companion matrix.

Parameters

in	<i>poly</i>	The <code>c_polynomial</code> object.
in	<i>n</i>	The size of <code>rts</code> . This value should be the same as the order of the polynomial.
out	<i>rts</i>	An N-element array where the roots of the polynomial will be written.
in, out	<i>err</i>	<p>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.</p> <ul style="list-style-type: none"> LA_OUT_OF_MEMORY_ERROR: Occurs if local memory must be allocated, and there is insufficient memory available. LA_CONVERGENCE_ERROR: Occurs if the algorithm failed to converge.

Definition at line 1159 of file `nonlin_c_binding.f90`.

5.1.2.32 `subroutine nonlin_c_binding::polynomial_subtract (type(c_polynomial), intent(in) p1, type(c_polynomial), intent(in) p2, type(c_polynomial), intent(out) rst)`

Subtracts two polynomials.

Parameters

in	<i>p1</i>	The left-hand-side argument.
in	<i>p2</i>	The right-hand-side argument.
out	<i>rst</i>	The resulting polynomial.

Definition at line 1291 of file `nonlin_c_binding.f90`.

5.1.2.33 `subroutine nonlin_c_binding::quasi_newton_c (type(c_funptr), intent(in), value fcn, type(c_funptr), intent(in), value jac, integer(i32), intent(in), value n, real(dp), dimension(n), intent(inout) x, real(dp), dimension(n), intent(out) fvec, type(solver_control), intent(in) tol, type(c_ptr), intent(in), value lsearch, type(iteration_behavior), intent(out) ib, type(errorhandler), intent(inout) err)`

Applies the quasi-Newton's method developed by Broyden in conjunction with a backtracking type line search to solve N equations of N unknowns.

Parameters

in	<i>fcn</i>	A pointer to the routine containing the system of equations to solve.
in	<i>jac</i>	A pointer to a routine used to compute the Jacobian of the system of equations. To let the program compute the Jacobian numerically, simply pass NULL.
in	<i>n</i>	The number of equations, and the number of unknowns.
in, out	<i>x</i>	On input, an N-element array containing an initial estimate to the solution. On output, the updated solution estimate. N is the number of variables.
out	<i>fvec</i>	An N-element array that, on output, will contain the values of each equation as evaluated at the variable values given in <i>x</i> .
in	<i>tol</i>	A solver_control object defining the solver control parameters.
in	<i>lsearch</i>	A pointer to a line_search_control object defining the line search control parameters. If no line search is desired, simply pass NULL.
out	<i>ib</i>	On output, an iteration_behavior object containing the iteration performance statistics.

Parameters

<code>in</code>	<code>err</code>	<p>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.</p> <ul style="list-style-type: none"> • <code>NL_INVALID_OPERATION_ERROR</code>: Occurs if no equations have been defined. • <code>NL_INVALID_INPUT_ERROR</code>: Occurs if the number of equations is different than the number of variables. • <code>NL_ARRAY_SIZE_ERROR</code>: Occurs if any of the input arrays are not sized correctly. • <code>NL_DIVERGENT_BEHAVIOR_ERROR</code>: Occurs if the direction vector is pointing in an apparent uphill direction. • <code>NL_CONVERGENCE_ERROR</code>: Occurs if the line search cannot converge within the allowed number of iterations. • <code>NL_OUT_OF_MEMORY_ERROR</code>: Occurs if there is insufficient memory available. • <code>NL_SPURIOUS_CONVERGENCE_ERROR</code>: Occurs as a warning if the slope of the gradient vector becomes sufficiently close to zero.
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Definition at line 498 of file `nonlin_c_binding.f90`.

5.1.2.34 subroutine `nonlin_c_binding::set_nonlin_defaults` (`type(solver_control)`, `intent(out) tol`)

Sets defaults for the `solver_control` type.

Parameters

<code>out</code>	<code>tol</code>	The <code>solver_control</code> object.
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Definition at line 728 of file `nonlin_c_binding.f90`.

5.1.2.35 subroutine `nonlin_c_binding::set_nonlin_ls_defaults` (`type(line_search_control)`, `intent(out) ls`)

Sets defaults for the `line_search_control` type.

Parameters

<code>out</code>	<code>ls</code>	The <code>line_search_control</code> object.
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Definition at line 745 of file `nonlin_c_binding.f90`.

5.1.2.36 subroutine `nonlin_c_binding::set_polynomial_set_coefficient` (`type(c_polynomial)`, `intent(inout) poly`, `integer(i32)`, `intent(in)`, `value ind`, `real(dp)`, `intent(in)`, `value x`, `type(errorhandler)`, `intent(inout) err`)

Sets the requested polynomial coefficient by index. The coefficient index is established as follows: $c(1) + c(2) * x + c(3) * x^2 + \dots c(n) * x^{n-1}$.

Parameters

in, out	<i>poly</i>	The c_polynomial object.
in	<i>ind</i>	The polynomial coefficient index ($0 < \text{ind} \leq \text{order} + 1$).
in	<i>x</i>	The polynomial coefficient.
in, out	<i>err</i>	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. <ul style="list-style-type: none"> NL_INVALID_INPUT_ERROR: Occurs if the requested index is less than or equal to zero, or if the requested index exceeds the number of polynomial coefficients.

Definition at line 1239 of file `nonlin_c_binding.f90`.

5.2 `nonlin_least_squares` Module Reference

[nonlin_least_squares](#)

Data Types

- type [least_squares_solver](#)
Defines a Levenberg-Marquardt based solver for unconstrained least-squares problems.

Functions/Subroutines

- pure real(dp) function [lss_get_factor](#) (this)
Gets a factor used to scale the bounds on the initial step.
- subroutine [lss_set_factor](#) (this, x)
Sets a factor used to scale the bounds on the initial step.
- subroutine [lss_solve](#) (this, fcn, x, fvec, ib, err)
Applies the Levenberg-Marquardt method to solve the nonlinear least-squares problem.
- subroutine [lmpar](#) (r, ipvt, diag, qtb, delta, par, x, sdiag, wa1, wa2)
*Completes the solution of the Levenberg-Marquardt problem when provided with a QR factored form of the system Jacobian matrix. The form of the problem at this stage is $J * X = B$ (J = Jacobian), and $D * X = 0$, where D is a diagonal matrix.*
- subroutine [lmfactor](#) (a, pivot, ipvt, rdiag, acnorm, wa)
Computes the QR factorization of an M-by-N matrix.
- subroutine [lmsolve](#) (r, ipvt, diag, qtb, x, sdiag, wa)
*Solves the QR factored system $A * X = B$, coupled with the diagonal system $D * X = 0$ in the least-squares sense.*

5.2.1 Detailed Description

[nonlin_least_squares](#)

Purpose

To provide routines capable of solving the nonlinear least squares problem.

5.2.2 Function/Subroutine Documentation

- 5.2.2.1 subroutine `nonlin_least_squares::lmfactor` (real(dp), dimension(:,:), intent(inout) *a*, logical, intent(in) *pivot*, integer(i32), dimension(:), intent(out) *ipvt*, real(dp), dimension(:), intent(out) *rdiag*, real(dp), dimension(:), intent(out) *acnorm*, real(dp), dimension(:), intent(out) *wa*) [private]

Computes the QR factorization of an M-by-N matrix.

Parameters

in, out	<i>a</i>	On input, the M-by-N matrix to factor. On output, the strict upper triangular portion contains matrix R1 of the factorization, the lower trapezoidal portion contains the factored form of Q1, and the diagonal contains the corresponding elementary reflector.
in	<i>pivot</i>	Set to true to utilize column pivoting; else, set to false for no pivoting.
out	<i>ipvt</i>	An N-element array that is used to contain the pivot indices unless <i>pivot</i> is set to false. In such event, this array is unused.
out	<i>rdiag</i>	An N-element array used to store the diagonal elements of the R1 matrix.
out	<i>acnorm</i>	An N-element array used to contain the norms of each column in the event column pivoting is used. If pivoting is not used, this array is unused.
out	<i>wa</i>	An N-element workspace array.

Remarks

This routines is based upon the MINPACK routine QRFAC.

Definition at line 734 of file `nonlin_least_squares.f90`.

```
5.2.2.2 subroutine nonlin_least_squares::lmpar ( real(dp), dimension(:, :), intent(inout) r, integer(i32), dimension(:), intent(in)
ipvt, real(dp), dimension(:), intent(in) diag, real(dp), dimension(:), intent(in) qtb, real(dp), intent(in) delta, real(dp),
intent(inout) par, real(dp), dimension(:), intent(out) x, real(dp), dimension(:), intent(out) sdiag, real(dp), dimension(:),
intent(out) wa1, real(dp), dimension(:), intent(out) wa2 ) [private]
```

Completes the solution of the Levenberg-Marquardt problem when provided with a QR factored form of the system Jacobian matrix. The form of the problem at this stage is $J \cdot X = B$ (J = Jacobian), and $D \cdot X = 0$, where D is a diagonal matrix.

Parameters

in, out	<i>r</i>	On input, the N-by-N upper triangular matrix R1 of the QR factorization. On output, the upper triangular portion is unaltered, but the strict lower triangle contains the strict upper triangle (transposed) of the matrix S.
in	<i>ipvt</i>	An N-element array tracking the pivoting operations from the original QR factorization.
in	<i>diag</i>	An N-element array containing the diagonal components of the matrix D.
in	<i>qtb</i>	An N-element array containing the first N elements of $Q1^{*T} \cdot B$.
in	<i>delta</i>	A positive input variable that specifies an upper bounds on the Euclidean norm of $D \cdot X$.
in, out	<i>par</i>	On input, the initial estimate of the Levenberg-Marquardt parameter. On output, the final estimate.
out	<i>x</i>	The N-element array that is the solution of $A \cdot X = B$, and of $D \cdot X = 0$.
out	<i>sdiag</i>	An N-element array containing the diagonal elements of the matrix S.
out	<i>wa1</i>	An N-element workspace array.
out	<i>wa2</i>	An N-element workspace array.

Remarks

This routines is based upon the MINPACK routine LMPAR.

Definition at line 567 of file `nonlin_least_squares.f90`.

5.2.2.3 subroutine `nonlin_least_squares::lmsolve` (`real(dp)`, `dimension(:, :)`, `intent(inout)` *r*, `integer(i32)`, `dimension(:)`, `intent(in)` *ipvt*, `real(dp)`, `dimension(:)`, `intent(in)` *diag*, `real(dp)`, `dimension(:)`, `intent(in)` *qtb*, `real(dp)`, `dimension(:)`, `intent(out)` *x*, `real(dp)`, `dimension(:)`, `intent(out)` *sdiag*, `real(dp)`, `dimension(:)`, `intent(out)` *wa*) [`private`]

Solves the QR factored system $A \cdot X = B$, coupled with the diagonal system $D \cdot X = 0$ in the least-squares sense.

Parameters

in, out	<i>r</i>	On input, the N-by-N upper triangular matrix R1 of the QR factorization. On output, the upper triangular portion is unaltered, but the strict lower triangle contains the strict upper triangle (transposed) of the matrix S.
in	<i>ipvt</i>	An N-element array tracking the pivoting operations from the original QR factorization.
in	<i>diag</i>	An N-element array containing the diagonal components of the matrix D.
in	<i>qtb</i>	An N-element array containing the first N elements of $Q1^{**T} * B$.
out	<i>x</i>	The N-element array that is the solution of $A \cdot X = B$, and of $D \cdot X = 0$.
out	<i>sdiag</i>	An N-element array containing the diagonal elements of the matrix S.
out	<i>wa</i>	An N-element workspace array.

Remarks

This routines is based upon the MINPACK routine QRSOLV.

Definition at line 837 of file `nonlin_least_squares.f90`.

5.2.2.4 pure `real(dp)` function `nonlin_least_squares::lss_get_factor` (`class(least_squares_solver)`, `intent(in)` *this*) [`private`]

Gets a factor used to scale the bounds on the initial step.

Parameters

in	<i>this</i>	The <code>least_squares_solver</code> object.
----	-------------	---

Returns

The factor.

Remarks

This factor is used to set the bounds on the initial step such that the initial step is bounded as the product of the factor with the Euclidean norm of the vector resulting from multiplication of the diagonal scaling matrix and the solution estimate. If zero, the factor itself is used.

Definition at line 48 of file `nonlin_least_squares.f90`.

5.2.2.5 subroutine `nonlin_least_squares::lss_set_factor` (`class(least_squares_solver)`, `intent(inout)` *this*, `real(dp)`, `intent(in)` *x*) [`private`]

Sets a factor used to scale the bounds on the initial step.

Parameters

in	<i>this</i>	The least_squares_solver object.
in	<i>x</i>	The factor. Notice, the factor is limited to the interval [0.1, 100].

Remarks

This factor is used to set the bounds on the initial step such that the initial step is bounded as the product of the factor with the Euclidean norm of the vector resulting from multiplication of the diagonal scaling matrix and the solution estimate. If zero, the factor itself is used.

Definition at line 67 of file `nonlin_least_squares.f90`.

5.2.2.6 subroutine `nonlin_least_squares::lss_solve` (`class(least_squares_solver)`, intent(inout) *this*,
`class(vecfcn_helper)`, intent(in) *fcn*, `real(dp)`, `dimension(:)`, intent(inout) *x*, `real(dp)`, `dimension(:)`, intent(out) *fvec*,
`type(iteration_behavior)`, optional *ib*, `class(errors)`, intent(inout), optional, target *err*) [private]

Applies the Levenberg-Marquardt method to solve the nonlinear least-squares problem.

Parameters

in, out	<i>this</i>	The least_squares_solver object.
in	<i>fcn</i>	The <code>vecfcn_helper</code> object containing the equations to solve.
in, out	<i>x</i>	On input, an M-element array containing an initial estimate to the solution. On output, the updated solution estimate. M is the number of variables.
out	<i>fvec</i>	An N-element array that, on output, will contain the values of each equation as evaluated at the variable values given in <i>x</i> . N is the number of equations.
out	<i>ib</i>	An optional output, that if provided, allows the caller to obtain iteration performance statistics.
out	<i>err</i>	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. <ul style="list-style-type: none"> NL_INVALID_OPERATION_ERROR: Occurs if no equations have been defined. NL_INVALID_INPUT_ERROR: Occurs if the number of equations is less than the number of variables. NL_ARRAY_SIZE_ERROR: Occurs if any of the input arrays are not sized correctly. NL_CONVERGENCE_ERROR: Occurs if the line search cannot converge within the allowed number of iterations. NL_OUT_OF_MEMORY_ERROR: Occurs if there is insufficient memory available. NL_TOLERANCE_TOO_SMALL_ERROR: Occurs if the requested tolerance is too small to be practical for the problem at hand.

Remarks

This routine is based upon the MINPACK routine LMDIF.

Example 1

The following code provides an example of how to solve a system of N equations of N unknowns using the

Levenberg-Marquardt method.

```

program main
  use linalg_constants, only : dp
  use nonlin_types, only : vecfcn, vecfcn_helper
  use nonlin_least_squares, only : least_squares_solver

  type(vecfcn_helper) :: obj
  procedure(vecfcn), pointer :: fcn
  type(least_squares_solver) :: solver
  real(dp) :: x(2), f(2)

  ! Set the initial conditions to [1, 1]
  x = 1.0d0

  ! Define the function
  fcn => fcn1
  call obj%set_fcn(fcn, 2, 2)

  ! Solve the system of equations. The solution overwrites X
  call solver%solve(obj, x, f)

  ! Print the output and the residual:
  print '(AF5.3AF5.3A)', "The solution: (", x(1), ", ", x(2), ")"
  print '(AE8.3AE8.3A)', "The residual: (", f(1), ", ", f(2), ")"
contains
  ! System of Equations:
  !
  !  $x^2 + y^2 = 34$ 
  !  $x^2 - 2 * y^2 = 7$ 
  !
  ! Solution:
  !  $x = +/-5$ 
  !  $y = +/-3$ 
  subroutine fcn1(x, f)
    real(dp), intent(in), dimension(:) :: x
    real(dp), intent(out), dimension(:) :: f
    f(1) = x(1)**2 + x(2)**2 - 34.0d0
    f(2) = x(1)**2 - 2.0d0 * x(2)**2 - 7.0d0
  end subroutine
end program

```

The above program returns the following results.

```

The solution: (5.000, 3.000)
The residual: (.000E+00, .000E+00)

```

Example 2

```

program example
  use linalg_constants, only : dp, i32
  use nonlin_types, only : vecfcn_helper, vecfcn
  use nonlin_least_squares, only : least_squares_solver
  implicit none

  ! Local Variables
  type(vecfcn_helper) :: obj
  procedure(vecfcn), pointer :: fcn
  type(least_squares_solver) :: solver
  real(dp) :: x(4), f(21) ! There are 4 coefficients and 21 data points

  ! Locate the routine containing the equations to solve
  fcn => fcns
  call obj%set_fcn(fcn, 21, 4)

  ! Define an initial guess
  x = 1.0d0 ! Equivalent to x = [1.0d0, 1.0d0, 1.0d0, 1.0d0]

  ! Solve
  call solver%solve(obj, x, f)

  ! Display the output
  print "(AF12.8)", "c1: ", x(1)
  print "(AF12.8)", "c2: ", x(2)
  print "(AF12.8)", "c3: ", x(3)
  print "(AF12.8)", "c4: ", x(4)
  print "(AF9.5)", "Max Residual: ", maxval(abs(f))

contains
  ! The function containing the data to fit
  subroutine fcns(x, f)
    ! Arguments
    real(dp), intent(in), dimension(:) :: x ! Contains the coefficients
    real(dp), intent(out), dimension(:) :: f

```

```

! Local Variables
real(dp), dimension(21) :: xp, yp

! Data to fit (21 data points)
xp = [0.0d0, 0.1d0, 0.2d0, 0.3d0, 0.4d0, 0.5d0, 0.6d0, 0.7d0, 0.8d0, &
      0.9d0, 1.0d0, 1.1d0, 1.2d0, 1.3d0, 1.4d0, 1.5d0, 1.6d0, 1.7d0, &
      1.8d0, 1.9d0, 2.0d0]
yp = [1.216737514d0, 1.250032542d0, 1.305579195d0, 1.040182335d0, &
      1.751867738d0, 1.109716707d0, 2.018141531d0, 1.992418729d0, &
      1.807916923d0, 2.078806005d0, 2.698801324d0, 2.644662712d0, &
      3.412756702d0, 4.406137221d0, 4.567156645d0, 4.999550779d0, &
      5.652854194d0, 6.784320119d0, 8.307936836d0, 8.395126494d0, &
      10.30252404d0]

! We'll apply a cubic polynomial model to this data:
! y = c1 * x**3 + c2 * x**2 + c3 * x + c4
f = x(1) * xp**3 + x(2) * xp**2 + x(3) * xp + x(4) - yp

! For reference, the data was generated by adding random errors to
! the following polynomial: y = x**3 - 0.3 * x**2 + 1.2 * x + 0.3
end subroutine
end program

```

The above program returns the following results.

```

c1: 1.06476276
c2: -0.12232029
c3: 0.44661345
c4: 1.18661422
Max Residual: 0.50636

```

See Also

- [Wikipedia](#)
- [MINPACK \(Wikipedia\)](#)

Definition at line 237 of file nonlin_least_squares.f90.

5.3 nonlin_linesearch Module Reference

nonlin_linesearch

Data Types

- type [line_search](#)

Defines a type capable of performing an inexact, backtracking line search to find a point as far along the specified direction vector that is usable for unconstrained minimization problems.

Functions/Subroutines

- pure integer(i32) function [ls_get_max_eval](#) (this)

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

- subroutine [ls_set_max_eval](#) (this, x)

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

- pure real(dp) function [ls_get_scale](#) (this)

*Gets the scaling of the product of the gradient and direction vectors (ALPHA) such that $F(X + LAMBDA * P) \leq F(X) + LAMBDA * ALPHA * P^T * G$, where P is the search direction vector, G is the gradient vector, and $LAMBDA$ is the scaling factor.*

- subroutine [ls_set_scale](#) (this, x)

*sets the scaling of the product of the gradient and direction vectors (ALPHA) such that $F(X + LAMBDA * P) \leq F(X) + LAMBDA * ALPHA * P^T * G$, where P is the search direction vector, G is the gradient vector, and $LAMBDA$ is the scaling factor.*

- pure real(dp) function [ls_get_dist](#) (this)
Gets a distance factor defining the minimum distance along the search direction vector is practical.
- subroutine [ls_set_dist](#) (this, x)
Sets a distance factor defining the minimum distance along the search direction vector is practical.
- subroutine [ls_search_mimo](#) (this, fcn, xold, grad, dir, x, fvec, fold, fx, ib, err)
Utilizes an inexact, backtracking line search to find a point as far along the specified direction vector that is usable for unconstrained minimization problems.
- subroutine [ls_search_miso](#) (this, fcn, xold, grad, dir, x, fold, fx, ib, err)
Utilizes an inexact, backtracking line search to find a point as far along the specified direction vector that is usable for unconstrained minimization problems.
- pure real(dp) function [min_backtrack_search](#) (mode, f0, f, f1, alam, alam1, slope)
Minimizes either the quadratic or cubic representation for a backtracking-type line search.
- subroutine, public [limit_search_vector](#) (x, lim)
Provides a means of scaling the length of the search direction vector.

5.3.1 Detailed Description

[nonlin_linesearch](#)

Purpose

To provide line search routines capable of minimizing nondesireable influences of the nonlinear equation solver model on the convergence of the iteration process.

5.3.2 Function/Subroutine Documentation

5.3.2.1 subroutine, public [nonlin_linesearch::limit_search_vector](#) (real(dp), dimension(:), intent(inout) x, real(dp), intent(in) lim)

Provides a means of scaling the length of the search direction vector.

Parameters

in, out	x	On input, the search direction vector. On output, the search direction vector limited in length to that specified by <code>lim</code> . If the vector is originally shorter than the limit length, no change is made.
in	lim	The length limit value.

Definition at line 643 of file `nonlin_linesearch.f90`.

5.3.2.2 pure real(dp) function [nonlin_linesearch::ls_get_dist](#) (class([line_search](#)), intent(in) this) [private]

Gets a distance factor defining the minimum distance along the search direction vector is practical.

Parameters

in	this	The line_search object.
----	------	---

Returns

The distance factor. A value of 1 indicates the full length of the vector.

Definition at line 146 of file `nonlin_linesearch.f90`.

5.3.2.3 `pure integer(i32) function nonlin_linesearch::ls_get_max_eval (class(line_search), intent(in) this) [private]`

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

Parameters

in	<i>this</i>	The line_search object.
----	-------------	---

Returns

The maximum number of function evaluations.

Definition at line 93 of file `nonlin_linesearch.f90`.

5.3.2.4 `pure real(dp) function nonlin_linesearch::ls_get_scale (class(line_search), intent(in) this) [private]`

Gets the scaling of the product of the gradient and direction vectors (ALPHA) such that $F(X + LAMBDA * P) \leq F(X) + LAMBDA * ALPHA * P^{**T} * G$, where P is the search direction vector, G is the gradient vector, and $LAMBDA$ is the scaling factor.

Parameters

in	<i>this</i>	The line_search object.
----	-------------	---

Returns

The scaling factor.

Definition at line 119 of file `nonlin_linesearch.f90`.

5.3.2.5 `subroutine nonlin_linesearch::ls_search_mimo (class(line_search), intent(in) this, class(vecfcn_helper), intent(in) fcn, real(dp), dimension(:), intent(in) xold, real(dp), dimension(:), intent(in) grad, real(dp), dimension(:), intent(in) dir, real(dp), dimension(:), intent(out) x, real(dp), dimension(:), intent(out) fvec, real(dp), intent(in), optional fold, real(dp), intent(out), optional fx, type(iteration_behavior), optional ib, class(errors), intent(inout), optional, target err) [private]`

Utilizes an inexact, backtracking line search to find a point as far along the specified direction vector that is usable for unconstrained minimization problems.

Parameters

in	<i>this</i>	The line_search object.
in	<i>fcn</i>	A <code>vecfcn_helper</code> object containing the system of equations.
in	<i>xold</i>	An N-element array defining the initial point, where N is the number of variables.
in	<i>grad</i>	An N-element array defining the gradient of <code>fcn</code> evaluated at <code>xold</code> .

Parameters

in	<i>dir</i>	An N-element array defining the search direction.
out	<i>x</i>	An N-element array where the updated solution point will be written.
out	<i>fvec</i>	An M-element array containing the M equation values evaluated at <i>x</i> , where M is the number of equations.
in	<i>fold</i>	An optional input that provides the value resulting from: $1/2 * \text{dot_product}(\text{fcn}(\text{xold}), \text{fcn}(\text{xold}))$. If not provided, <i>fcn</i> is evaluated at <i>xold</i> , and the aforementioned relationship is computed.
out	<i>fx</i>	The result of the operation: $(1/2) * \text{dot_product}(\text{fvec}, \text{fvec})$. Remember <i>fvec</i> is evaluated at <i>x</i> .
out	<i>ib</i>	An optional output, that if provided, allows the caller to obtain iteration performance statistics.
out	<i>err</i>	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. <ul style="list-style-type: none"> • <code>NL_INVALID_OPERATION_ERROR</code>: Occurs if no equations have been defined. • <code>NL_ARRAY_SIZE_ERROR</code>: Occurs if any of the input arrays are not sized correctly. • <code>NL_DIVERGENT_BEHAVIOR_ERROR</code>: Occurs if the direction vector is pointing in an apparent uphill direction. • <code>NL_CONVERGENCE_ERROR</code>: Occurs if the line search cannot converge within the allowed number of iterations.

Definition at line 209 of file `nonlin_linesearch.f90`.

```
5.3.2.6 subroutine nonlin_linesearch::ls_search_miso ( class(line_search), intent(in) this, class(fcnvar_helper),
intent(in) fcn, real(dp), dimension(:), intent(in) xold, real(dp), dimension(:), intent(in) grad, real(dp), dimension(:),
intent(in) dir, real(dp), dimension(:), intent(out) x, real(dp), intent(in), optional fold, real(dp), intent(out), optional fx,
type(iteration_behavior), optional ib, class(errors), intent(inout), optional, target err ) [private]
```

Utilizes an inexact, backtracking line search to find a point as far along the specified direction vector that is usable for unconstrained minimization problems.

Parameters

in	<i>this</i>	The line_search object.
in	<i>fcn</i>	A <code>vecfcn_helper</code> object containing the system of equations.
in	<i>xold</i>	An N-element array defining the initial point, where N is the number of variables.
in	<i>grad</i>	An N-element array defining the gradient of <i>fcn</i> evaluated at <i>xold</i> .
in	<i>dir</i>	An N-element array defining the search direction.
out	<i>x</i>	An N-element array where the updated solution point will be written.
in	<i>fold</i>	An optional input that provides the function value at <i>xold</i> . If not provided, <i>fcn</i> is evaluated at <i>xold</i> .
out	<i>fx</i>	The value of the function as evaluated at <i>x</i> .
out	<i>ib</i>	An optional output, that if provided, allows the caller to obtain iteration performance statistics.

Parameters

out	err	<p>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.</p> <ul style="list-style-type: none"> • <code>NL_INVALID_OPERATION_ERROR</code>: Occurs if no equations have been defined. • <code>NL_ARRAY_SIZE_ERROR</code>: Occurs if any of the input arrays are not sized correctly. • <code>NL_DIVERGENT_BEHAVIOR_ERROR</code>: Occurs if the direction vector is pointing in an apparent uphill direction. • <code>NL_CONVERGENCE_ERROR</code>: Occurs if the line search cannot converge within the allowed number of iterations.
-----	-----	--

Definition at line 412 of file `nonlin_linesearch.f90`.

5.3.2.7 `subroutine nonlin_linesearch::ls_set_dist (class(line_search), intent(inout) this, real(dp), intent(in) x)`
`[private]`

Sets a distance factor defining the minimum distance along the search direction vector is practical.

Parameters

in, out	this	The line_search object.
in	x	The distance factor. A value of 1 indicates the full length of the vector. Notice, this value is restricted to lie in the set [0.1, 1.0)

Definition at line 160 of file `nonlin_linesearch.f90`.

5.3.2.8 `subroutine nonlin_linesearch::ls_set_max_eval (class(line_search), intent(inout) this, integer(i32), intent(in) x)`
`[private]`

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

Parameters

in, out	this	The line_search object.
in	x	The maximum number of function evaluations.

Definition at line 105 of file `nonlin_linesearch.f90`.

5.3.2.9 `subroutine nonlin_linesearch::ls_set_scale (class(line_search), intent(inout) this, real(dp), intent(in) x)`
`[private]`

sets the scaling of the product of the gradient and direction vectors (ALPHA) such that $F(X + LAMBDA * P) \leq F(X) + LAMBDA * ALPHA * P^T * G$, where P is the search direction vector, G is the gradient vector, and LAMBDA is the scaling factor.

Parameters

in, out	<i>this</i>	The line_search object.
in	<i>x</i>	The scaling factor.

Definition at line 133 of file `nonlin_linesearch.f90`.

```
5.3.2.10 pure real(dp) function nonlin_linesearch::min_backtrack_search ( integer(i32), intent(in) mode, real(dp), intent(in) f0,
    real(dp), intent(in) f, real(dp), intent(in) f1, real(dp), intent(in) alam, real(dp), intent(in) alam1, real(dp), intent(in) slope
    ) [private]
```

Minimizes either the quadratic or cubic representation for a backtracking-type line search.

Parameters

in	<i>mode</i>	Set to 1 to apply the quadratic model; else, any other value will apply the cubic model.
in	<i>f0</i>	The previous function value.
in	<i>f</i>	The current function value.
in	<i>f1</i>	The predicted function value.
in	<i>alam</i>	The step length scaling factor at <i>f</i> .
in	<i>alam1</i>	The step length scaling factor at <i>f1</i> .
in	<i>slope</i>	The slope of the direction vector.

Returns

The new step length scaling factor.

Definition at line 592 of file `nonlin_linesearch.f90`.

5.4 nonlin_optimize Module Reference

[nonlin_optimize](#)

Data Types

- type [bfgs](#)
Defines a Broyden–Fletcher–Goldfarb–Shanno (BFGS) solver for minimization of functions of multiple variables.
- type [line_search_optimizer](#)
A class describing equation optimizers that use a line search algorithm to improve convergence behavior.
- type [nelder_mead](#)
Defines a solver based upon Nelder and Mead's simplex algorithm for minimization of functions of multiple variables.

Functions/Subroutines

- subroutine `nm_solve` (this, fcn, x, fout, ib, err)
Utilizes the Nelder-Mead simplex method for finding a minimum value of the specified function.
- real(dp) function `nm_extrapolate` (this, fcn, y, pcent, ihi, fac, neval, work)
Extrapolates by the specified factor through the simplex across from the largest point. If the extrapolation results in a better estimate, the current high point is replaced with the new estimate.
- pure real(dp) function, dimension(:,:), allocatable `nm_get_simplex` (this)
Gets an N-by-(N+1) matrix containing the current simplex.
- subroutine `nm_set_simplex` (this, x)
Sets an N-by-(N+1) matrix as the current simplex. Notice, if this matrix is different in size from the problem dimensionality, the Nelder-Mead routine will replace it with an appropriately sized matrix.
- pure real(dp) function `nm_get_size` (this)
Gets the size of the initial simplex that will be utilized by the Nelder-Mead algorithm in the event that the user does not supply a simplex geometry, or if the user supplies an invalid simplex geometry.
- subroutine `nm_set_size` (this, x)
Sets the size of the initial simplex that will be utilized by the Nelder-Mead algorithm in the event that the user does not supply a simplex geometry, or if the user supplies an invalid simplex geometry.
- subroutine `lso_get_line_search` (this, ls)
Gets the line search module.
- subroutine `lso_set_line_search` (this, ls)
Sets the line search module.
- subroutine `lso_set_default` (this)
Establishes a default line_search object for the line search module.
- pure logical function `lso_is_line_search_defined` (this)
Tests to see if a line search module is defined.
- pure logical function `lso_get_use_search` (this)
Gets a value determining if a line-search should be employed.
- subroutine `lso_set_use_search` (this, x)
Sets a value determining if a line-search should be employed.
- pure real(dp) function `lso_get_var_tol` (this)
Gets the convergence on change in variable tolerance.
- subroutine `lso_set_var_tol` (this, x)
Sets the convergence on change in variable tolerance.
- subroutine `bfgs_solve` (this, fcn, x, fout, ib, err)
Utilizes the Broyden-Fletcher-Goldfarb-Shanno (BFGS) algorithm for finding a minimum value of the specified function.

5.4.1 Detailed Description

`nonlin_optimize`

Purpose

To provide various optimization routines.

5.4.2 Function/Subroutine Documentation

5.4.2.1 subroutine `nonlin_optimize::bfgs_solve` (class(bfgs), intent(inout) this, class(fcnvar_helper), intent(in) fcn, real(dp), dimension(:), intent(inout) x, real(dp), intent(out), optional fout, type(iteration_behavior), optional ib, class(errors), intent(inout), optional, target err) [private]

Utilizes the Broyden-Fletcher-Goldfarb-Shanno (BFGS) algorithm for finding a minimum value of the specified function.

Parameters

in, out	<i>this</i>	The <code>bfgs_mead</code> object.
in	<i>fcn</i>	The <code>fcnvar_helper</code> object containing the equation to optimize.
in, out	<i>x</i>	On input, the initial guess at the optimal point. On output, the updated optimal point estimate.
out	<i>fout</i>	An optional output, that if provided, returns the value of the function at <i>x</i> .
out	<i>ib</i>	An optional output, that if provided, allows the caller to obtain iteration performance statistics.
out	<i>err</i>	<p>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.</p> <ul style="list-style-type: none"> • <code>NL_INVALID_OPERATION_ERROR</code>: Occurs if no equations have been defined. • <code>NL_INVALID_INPUT_ERROR</code>: Occurs if <i>x</i> is not appropriately sized for the problem as defined in <i>fcn</i>. • <code>NL_OUT_OF_MEMORY_ERROR</code>: Occurs if there is insufficient memory available. • <code>NL_CONVERGENCE_ERROR</code>: Occurs if the algorithm cannot converge within the allowed number of iterations.

Usage

The following example illustrates how to find the minimum of Rosenbrock's function using this BFGS solver.

```

program example
  use linalg_constants, only : dp, i32
  use nonlin_optimize, only : bfgs
  use nonlin_types, only : fcnvar, fcnvar_helper,
    iteration_behavior
  implicit none

  ! Local Variables
  type(bfgs) :: solver
  type(fcnvar_helper) :: obj
  procedure(fcnvar), pointer :: fcn
  real(dp) :: x(2), fout
  type(iteration_behavior) :: ib

  ! Initialization
  fcn => rosenbrock
  call obj%set_fcn(fcn, 2)

  ! Define an initial guess - the solution is (1, 1)
  call random_number(x)

  ! Call the solver
  call solver%solve(obj, x, fout, ib)

  ! Display the output
  print '(AF8.5AF8.5A)', "Rosenbrock Minimum: (", x(1), ", ", x(2), ")"
  print '(AE9.3)', "Function Value: ", fout
  print '(AI0)', "Iterations: ", ib%iter_count
  print '(AI0)', "Function Evaluations: ", ib%fcn_count
contains
  ! Rosenbrock's Function
  function rosenbrock(x) result(f)
    real(dp), intent(in), dimension(:) :: x
    real(dp) :: f
    f = 1.0d2 * (x(2) - x(1)**2)**2 + (x(1) - 1.0d0)**2
  end function
end

```

The above program yields the following output:

```

Rosenbrock Minimum: ( 1.00000,  0.99999)
Function Value: 0.200E-10
Iterations: 47
Function Evaluations: 70

```

See Also

- [Wikipedia - BFGS Methods](#)
- [Wikipedia - Quasi-Newton Methods](#)
- [minFunc](#)

Definition at line 731 of file `nonlin_optimize.f90`.

5.4.2.2 subroutine `nonlin_optimize::iso_get_line_search` (class(`line_search_optimizer`), intent(in) *this*,
class(`line_search`), intent(out), allocatable *ls*) [private]

Gets the line search module.

Parameters

in	<i>this</i>	The line_search_optimizer object.
out	<i>ls</i>	The <code>line_search</code> object.

Definition at line 565 of file `nonlin_optimize.f90`.

5.4.2.3 pure logical function `nonlin_optimize::iso_get_use_search` (class(`line_search_optimizer`), intent(in) *this*)
[private]

Gets a value determining if a line-search should be employed.

Parameters

in	<i>this</i>	The line_search_optimizer object.
----	-------------	---

Returns

Returns true if a line search should be used; else, false.

Definition at line 611 of file `nonlin_optimize.f90`.

5.4.2.4 pure real(dp) function `nonlin_optimize::iso_get_var_tol` (class(`line_search_optimizer`), intent(in) *this*)
[private]

Gets the convergence on change in variable tolerance.

Parameters

in	<i>this</i>	The line_search_optimizer object.
----	-------------	---

Returns

The tolerance value.

Definition at line 633 of file `nonlin_optimize.f90`.

5.4.2.5 pure logical function `nonlin_optimize::iso_is_line_search_defined (class(line_search_optimizer), intent(in) this)` `[private]`

Tests to see if a line search module is defined.

Parameters

<code>in</code>	<code>this</code>	The line_search_optimizer object.
-----------------	-------------------	---

Returns

Returns true if a module is defined; else, false.

Definition at line 600 of file `nonlin_optimize.f90`.

5.4.2.6 subroutine `nonlin_optimize::iso_set_default (class(line_search_optimizer), intent(inout) this)` `[private]`

Establishes a default `line_search` object for the line search module.

Parameters

<code>in, out</code>	<code>this</code>	The line_search_optimizer object.
----------------------	-------------------	---

Definition at line 589 of file `nonlin_optimize.f90`.

5.4.2.7 subroutine `nonlin_optimize::iso_set_line_search (class(line_search_optimizer), intent(inout) this, class(line_search), intent(in) ls)` `[private]`

Sets the line search module.

Parameters

<code>in, out</code>	<code>this</code>	The line_search_optimizer object.
<code>in</code>	<code>ls</code>	The <code>line_search</code> object.

Definition at line 577 of file `nonlin_optimize.f90`.

5.4.2.8 subroutine `nonlin_optimize::iso_set_use_search (class(line_search_optimizer), intent(inout) this, logical, intent(in) x)` `[private]`

Sets a value determining if a line-search should be employed.

Parameters

<code>in, out</code>	<code>this</code>	The line_search_optimizer object.
<code>in</code>	<code>x</code>	Set to true if a line search should be used; else, false.

Definition at line 622 of file `nonlin_optimize.f90`.

5.4.2.9 subroutine `nonlin_optimize::iso_set_var_tol` (`class(line_search_optimizer)`, `intent(inout) this`, `real(dp)`, `intent(in) x`) `[private]`

Sets the convergence on change in variable tolerance.

Parameters

<code>in, out</code>	<code>this</code>	The line_search_optimizer object.
<code>in</code>	<code>x</code>	The tolerance value.

Definition at line 644 of file `nonlin_optimize.f90`.

5.4.2.10 `real(dp)` function `nonlin_optimize::nm_extrapolate` (`class(nelder_mead)`, `intent(inout) this`, `class(fcnvar_helper)`, `intent(in) fcn`, `real(dp)`, `dimension(:)`, `intent(inout) y`, `real(dp)`, `dimension(:)`, `intent(inout) pcent`, `integer(i32)`, `intent(in) ihi`, `real(dp)`, `intent(in) fac`, `integer(i32)`, `intent(inout) neval`, `real(dp)`, `dimension(:)`, `intent(out) work`) `[private]`

Extrapolates by the specified factor through the simplex across from the largest point. If the extrapolation results in a better estimate, the current high point is replaced with the new estimate.

Parameters

<code>in, out</code>	<code>this</code>	The nelder_mead object.
<code>in</code>	<code>fcn</code>	The function to evaluate.
<code>in, out</code>	<code>y</code>	An array containing the function values at each vertex.
<code>in, out</code>	<code>pcent</code>	An array containing the centroid of vertex position information.
<code>in</code>	<code>ihi</code>	The index of the largest magnitude vertex.
<code>in, out</code>	<code>neval</code>	The number of function evaluations.
<code>out</code>	<code>work</code>	An N-element workspace array where N is the number of dimensions of the problem.

Returns

The new function estimate.

Definition at line 447 of file `nonlin_optimize.f90`.

5.4.2.11 `pure real(dp)` function, `dimension(:, :)`, allocatable `nonlin_optimize::nm_get_simplex` (`class(nelder_mead)`, `intent(in) this`) `[private]`

Gets an N-by-(N+1) matrix containing the current simplex.

Parameters

<code>in</code>	<code>this</code>	The nelder_mead object.
-----------------	-------------------	---

Returns

The N-by-(N+1) matrix containing the simplex. Each vertex of the simplex is stored as its own column of this matrix.

Definition at line 494 of file `nonlin_optimize.f90`.

5.4.2.12 pure real(dp) function `nonlin_optimize::nm_get_size` (`class(nelder_mead)`, `intent(in) this`) [private]

Gets the size of the initial simplex that will be utilized by the Nelder-Mead algorithm in the event that the user does not supply a simplex geometry, or if the user supplies an invalid simplex geometry.

Parameters

<code>in</code>	<code>this</code>	The <code>nelder_mead</code> object.
-----------------	-------------------	--------------------------------------

Returns

The size of the simplex (length of an edge).

Definition at line 539 of file `nonlin_optimize.f90`.

5.4.2.13 subroutine `nonlin_optimize::nm_set_simplex` (`class(nelder_mead)`, `intent(inout) this`, `real(dp)`, `dimension(:,:) x`) [private]

Sets an N-by-(N+1) matrix as the current simplex. Notice, if this matrix is different in size from the problem dimensionality, the Nelder-Mead routine will replace it with an appropriately sized matrix.

Parameters

<code>in, out</code>	<code>this</code>	The <code>nelder_mead</code> object.
<code>in</code>	<code>x</code>	The simplex matrix. Each column of the matrix must contain the coordinates of each vertex of the simplex.

Definition at line 514 of file `nonlin_optimize.f90`.

5.4.2.14 subroutine `nonlin_optimize::nm_set_size` (`class(nelder_mead)`, `intent(inout) this`, `real(dp)`, `intent(in) x`) [private]

Sets the size of the initial simplex that will be utilized by the Nelder-Mead algorithm in the event that the user does not supply a simplex geometry, or if the user supplies an invalid simplex geometry.

Parameters

<code>in, out</code>	<code>this</code>	The <code>nelder_mead</code> object.
<code>in</code>	<code>x</code>	The size of the simplex (length of an edge).

Definition at line 552 of file `nonlin_optimize.f90`.

5.4.2.15 subroutine `nonlin_optimize::nm_solve` (`class(nelder_mead)`, `intent(inout) this`, `class(fcnnvar_helper)`, `intent(in) fcn`, `real(dp)`, `dimension(:)`, `intent(inout) x`, `real(dp)`, `intent(out)`, optional `fout`, `type(iteration_behavior)`, optional `ib`, `class(errors)`, `intent(inout)`, optional, target `err`) [private]

Utilizes the Nelder-Mead simplex method for finding a minimum value of the specified function.

Parameters

in, out	<i>this</i>	The <code>nelder_mead</code> object.
in	<i>fcn</i>	The <code>fcnvar_helper</code> object containing the equation to optimize.
in, out	<i>x</i>	On input, the initial guess at the optimal point. On output, the updated optimal point estimate.
out	<i>fout</i>	An optional output, that if provided, returns the value of the function at <i>x</i> .
out	<i>ib</i>	An optional output, that if provided, allows the caller to obtain iteration performance statistics.
out	<i>err</i>	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. <ul style="list-style-type: none"> • <code>NL_INVALID_OPERATION_ERROR</code>: Occurs if no equations have been defined. • <code>NL_INVALID_INPUT_ERROR</code>: Occurs if <i>x</i> is not appropriately sized for the problem as defined in <i>fcn</i>. • <code>NL_OUT_OF_MEMORY_ERROR</code>: Occurs if there is insufficient memory available. • <code>NL_CONVERGENCE_ERROR</code>: Occurs if the algorithm cannot converge within the allowed number of iterations.

Usage

The following example illustrates how to find the minimum of Rosenbrock's function using this Nelder-Mead solver.

```

program example
  use linalg_constants, only : dp, i32
  use nonlin_optimize, only : nelder_mead
  use nonlin_types, only : fcnnvar, fcnnvar_helper,
    iteration_behavior
  implicit none

  ! Local Variables
  type(nelder_mead) :: solver
  type(fcnnvar_helper) :: obj
  procedure(fcnnvar), pointer :: fcn
  real(dp) :: x(2), fout
  type(iteration_behavior) :: ib

  ! Initialization
  fcn => rosenbrock
  call obj%set_fcn(fcn, 2)

  ! Define an initial guess - the solution is (1, 1)
  call random_number(x)

  ! Call the solver
  call solver%solve(obj, x, fout, ib)

  ! Display the output
  print '(AF8.5AF8.5A)', "Rosenbrock Minimum: (", x(1), ", ", x(2), ")"
  print '(AE9.3)', "Function Value: ", fout
  print '(AI0)', "Iterations: ", ib%iter_count
  print '(AI0)', "Function Evaluations: ", ib%fcn_count
contains
  ! Rosenbrock's Function
  function rosenbrock(x) result(f)
    real(dp), intent(in), dimension(:) :: x
    real(dp) :: f
    f = 1.0d2 * (x(2) - x(1)**2)**2 + (x(1) - 1.0d0)**2
  end function
end

```

The above program yields the following output:

```

Rosenbrock Minimum: ( 1.00000,  1.00000)
Function Value: 0.264E-12
Iterations: 59
Function Evaluations: 112

```

Remarks

The implementation of the Nelder-Mead algorithm presented here is a slight modification of the original work of Nelder and Mead. The Numerical Recipes implementation is also quite similar. In fact, the Numerical Recipes section relating to reflection, contraction, etc. is leveraged for this implementation.

See Also

- Nelder, John A.; R. Mead (1965). "A simplex method for function minimization". *Computer Journal*. 7: 308–313.
- Gao, Fuchang, Han, Lixing (2010). "Implementing the Nelder-Mead simplex algorithm with adaptive parameters."
- [Wikipedia](#)
- [Numerical Recipes](#)

Definition at line 196 of file `nonlin_optimize.f90`.

5.5 `nonlin_polynomials` Module Reference

`polynomials`

Data Types

- interface `assignment(=)`
Defines polynomial assignment.
- interface `operator(*)`
Defines polynomial multiplication.
- interface `operator(+)`
Defines polynomial addition.
- interface `operator(-)`
Defines polynomial subtraction.
- type `polynomial`
Defines a polynomial, and associated routines for performing polynomial operations.

Functions/Subroutines

- subroutine `init_poly` (this, order, err)
Initializes the polynomial instance, and sets all coefficients to zero.
- pure integer(i32) function `get_poly_order` (this)
Returns the order of the polynomial object.
- subroutine `poly_fit` (this, x, y, order, err)
Fits a polynomial of the specified order to a data set.
- subroutine `poly_fit_thru_zero` (this, x, y, order, err)
Fits a polynomial of the specified order that passes through zero to a data set.
- elemental real(dp) function `poly_eval_double` (this, x)
Evaluates a polynomial at the specified points.
- elemental complex(dp) function `poly_eval_complex` (this, x)
Evaluates a polynomial at the specified points.
- pure real(dp) function, dimension(this%order(), this%order()) `poly_companion_mtx` (this)
Returns the companion matrix for the polynomial.

- `complex(dp)` function, `dimension(this%order())` `poly_roots` (this, err)
Computes all the roots of a polynomial by computing the eigenvalues of the polynomial companion matrix.
- `real(dp)` function `get_poly_coefficient` (this, ind, err)
*Gets the requested polynomial coefficient by index. The coefficient index is established as follows: $c(1) + c(2) * x + c(3) * x**2 + \dots c(n) * x**n-1$.*
- pure `real(dp)` function, `dimension(this%order()+1)` `get_poly_coefficients` (this)
*Gets an array containing all the coefficients of the polynomial. The coefficient index is established as follows: $c(1) + c(2) * x + c(3) * x**2 + \dots c(n) * x**n-1$.*
- subroutine `set_poly_coefficient` (this, ind, c, err)
*Sets the requested polynomial coefficient by index. The coefficient index is established as follows: $c(1) + c(2) * x + c(3) * x**2 + \dots c(n) * x**n-1$.*
- subroutine `poly_equals` (x, y)
Assigns the contents of one polynomial to another.
- subroutine `poly_dbl_equals` (x, y)
Assigns a number to each coefficient of the polynomial.
- type(`polynomial`) function `poly_poly_add` (x, y)
Adds two polynomials.
- type(`polynomial`) function `poly_poly_subtract` (x, y)
Subtracts two polynomials.
- type(`polynomial`) function `poly_poly_mult` (x, y)
Multiplies two polynomials.
- type(`polynomial`) function `poly_dbl_mult` (x, y)
Multiplies a polynomial by a scalar value.
- type(`polynomial`) function `dbl_poly_mult` (x, y)
Multiplies a polynomial by a scalar value.

5.5.1 Detailed Description

polynomials

Purpose

Provides a means of defining and operating on polynomials.

5.5.2 Function/Subroutine Documentation

5.5.2.1 type(`polynomial`) function `nonlin_polynomials::dbl_poly_mult` (`real(dp)`, intent(in) x, `class(polynomial)`, intent(in) y) [private]

Multiplies a polynomial by a scalar value.

Parameters

in	x	The scalar value.
in	y	The polynomial.

Returns

The resulting polynomial.

Definition at line 931 of file `nonlin_polynomials.f90`.

5.5.2.2 `real(dp) function nonlin_polynomials::get_poly_coefficient (class(polynomial), intent(in) this, integer(i32), intent(in) ind, class(errors), intent(inout), optional, target err) [private]`

Gets the requested polynomial coefficient by index. The coefficient index is established as follows: $c(1) + c(2) * x + c(3) * x^2 + \dots c(n) * x^{n-1}$.

Parameters

in	<i>this</i>	The polynomial.
in	<i>ind</i>	The polynomial coefficient index ($0 < ind \leq order + 1$).
out	<i>err</i>	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. <ul style="list-style-type: none"> NL_INVALID_INPUT_ERROR: Occurs if the requested index is less than or equal to zero, or if the requested index exceeds the number of polynomial coefficients.

Returns

The requested coefficient.

Definition at line 610 of file `nonlin_polynomials.f90`.

5.5.2.3 `pure real(dp) function, dimension(this%order() + 1) nonlin_polynomials::get_poly_coefficients (class(polynomial), intent(in) this) [private]`

Gets an array containing all the coefficients of the polynomial. The coefficient index is established as follows: $c(1) + c(2) * x + c(3) * x^2 + \dots c(n) * x^{n-1}$.

Parameters

in	<i>this</i>	The polynomial object.
----	-------------	------------------------

Returns

The array of coefficients.

Definition at line 653 of file `nonlin_polynomials.f90`.

5.5.2.4 `pure integer(i32) function nonlin_polynomials::get_poly_order (class(polynomial), intent(in) this) [private]`

Returns the order of the polynomial object.

Parameters

in	<i>this</i>	The polynomial object.
----	-------------	------------------------

Returns

The order of the polynomial. Returns -1 in the event no polynomial coefficients have been defined.

Definition at line 158 of file `nonlin_polynomials.f90`.

5.5.2.5 `subroutine nonlin_polynomials::init_poly (class(polynomial), intent(inout) this, integer(i32), intent(in) order, class(errors), intent(inout), optional, target err) [private]`

Initializes the polynomial instance, and sets all coefficients to zero.

Parameters

<code>in, out</code>	<code>this</code>	The polynomial object.
<code>in</code>	<code>order</code>	The order of the polynomial (must be ≥ 0).
<code>out</code>	<code>err</code>	<p>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.</p> <ul style="list-style-type: none"> • <code>NL_INVALID_INPUT_ERROR</code>: Occurs if a zero or negative polynomial order was specified. • <code>NL_OUT_OF_MEMORY_ERROR</code>: Occurs if insufficient memory is available.

Definition at line 108 of file `nonlin_polynomials.f90`.

5.5.2.6 `pure real(dp) function, dimension(this%order(), this%order()) nonlin_polynomials::poly_companion_mtx (class(polynomial), intent(in) this) [private]`

Returns the companion matrix for the polynomial.

Parameters

<code>in</code>	<code>this</code>	The polynomial object.
-----------------	-------------------	------------------------

Returns

The companion matrix.

See Also

- [Wikipedia](#)
- [Wolfram MathWorld](#)

Definition at line 484 of file `nonlin_polynomials.f90`.

5.5.2.7 `subroutine nonlin_polynomials::poly_dbl_equals (class(polynomial), intent(inout) x, real(dp), intent(in) y) [private]`

Assigns a number to each coefficient of the polynomial.

Parameters

in, out	x	The assignee.
in	y	The value to assign.

Definition at line 741 of file `nonlin_polynomials.f90`.

5.5.2.8 `type(polynomial) function nonlin_polynomials::poly_dbl_mult (class(polynomial), intent(in) x , real(dp), intent(in) y) [private]`

Multiplies a polynomial by a scalar value.

Parameters

in	x	The polynomial.
in	y	The scalar value.

Returns

The resulting polynomial.

Definition at line 907 of file `nonlin_polynomials.f90`.

5.5.2.9 `subroutine nonlin_polynomials::poly_equals (class(polynomial), intent(inout) x , class(polynomial), intent(in) y) [private]`

Assigns the contents of one polynomial to another.

Parameters

out	x	The assignee.

Definition at line 720 of file `nonlin_polynomials.f90`.

5.5.2.10 `elemental complex(dp) function nonlin_polynomials::poly_eval_complex (class(polynomial), intent(in) this, complex(dp), intent(in) x) [private]`

Evaluates a polynomial at the specified points.

Parameters

in	<i>this</i>	The polynomial object.
in	x	The value(s) at which to evaluate the polynomial.

Returns

The value(s) of the polynomial at x .

Definition at line 444 of file `nonlin_polynomials.f90`.

5.5.2.11 elemental real(dp) function nonlin_polynomials::poly_eval_double (class(polynomial), intent(in) *this*, real(dp), intent(in) *x*) [private]

Evaluates a polynomial at the specified points.

Parameters

in	<i>this</i>	The polynomial object.
in	<i>x</i>	The value(s) at which to evaluate the polynomial.

Returns

The value(s) of the polynomial at *x*.

Definition at line 407 of file nonlin_polynomials.f90.

5.5.2.12 subroutine nonlin_polynomials::poly_fit (class(polynomial), intent(inout) *this*, real(dp), dimension(:), intent(in) *x*, real(dp), dimension(:), intent(inout) *y*, integer(i32), intent(in) *order*, class(errors), intent(inout), optional, target *err*) [private]

Fits a polynomial of the specified order to a data set.

Parameters

in, out	<i>this</i>	The polynomial object.
in	<i>x</i>	An N-element array containing the independent variable data points. Notice, must be $N > \text{order}$.
in, out	<i>y</i>	On input, an N-element array containing the dependent variable data points. On output, the contents are overwritten.
in	<i>order</i>	The order of the polynomial (must be ≥ 1).
out	<i>err</i>	<p>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.</p> <ul style="list-style-type: none"> • NL_INVALID_INPUT_ERROR: Occurs if a zero or negative polynomial order was specified, or if <i>order</i> is too large for the data set. • NL_OUT_OF_MEMORY_ERROR: Occurs if insufficient memory is available. • NL_ARRAY_SIZE_ERROR: Occurs if <i>x</i> and <i>y</i> are different sizes.

Usage

The following code provides an example of how to fit a polynomial to a set of data.

```

program example
  use linalg_constants, only : dp, i32
  use nonlin_polynomials

  ! Local Variables
  real(dp), dimension(21) :: xp, yp, yf, yc, err
  real(dp) :: res
  type(polynomial) :: p

  ! Data to fit
  xp = [0.0d0, 0.1d0, 0.2d0, 0.3d0, 0.4d0, 0.5d0, 0.6d0, 0.7d0, 0.8d0, &

```

```

0.9d0, 1.0d0, 1.1d0, 1.2d0, 1.3d0, 1.4d0, 1.5d0, 1.6d0, 1.7d0, &
1.8d0, 1.9d0, 2.0d0]
yp = [1.216737514d0, 1.250032542d0, 1.305579195d0, 1.040182335d0, &
1.751867738d0, 1.109716707d0, 2.018141531d0, 1.992418729d0, &
1.807916923d0, 2.078806005d0, 2.698801324d0, 2.644662712d0, &
3.412756702d0, 4.406137221d0, 4.567156645d0, 4.999550779d0, &
5.652854194d0, 6.784320119d0, 8.307936836d0, 8.395126494d0, &
10.30252404d0]

! Create a copy of yp as it will be overwritten in the fit command
yc = yp

! Fit the polynomial
call p%fit(xp, yp, 3)

! Evaluate the polynomial at xp, and then determine the residual
yf = p%evaluate(xp)
err = abs(yf - yc)
res = maxval(err)

! Print out the coefficients
print '(A)', "Polynomial Coefficients (c0 + c1*x + c2*x**2 + c3*x**3):"
do i = 1, 4
    print '(AI0AF12.9)', "c", i - 1, " = ", p%get(i)
end do
print '(AE9.4)', "Residual: ", res
end program

```

The above program returns the following results.

```

Polynomial Coefficients (c0 + c1*x + c2*x**2 + c3*x**3):
c0 = 1.186614186
c1 = 0.446613631
c2 = -0.122320499
c3 = 1.064762822
Residual: .5064E+00

```

Definition at line 239 of file `nonlin_polynomials.f90`.

5.5.2.13 subroutine `nonlin_polynomials::poly_fit_thru_zero` (class(**polynomial**), intent(inout) *this*, real(dp), dimension(:), intent(in) *x*, real(dp), dimension(:), intent(inout) *y*, integer(i32), intent(in) *order*, class(errors), intent(inout), optional, target *err*) [private]

Fits a polynomial of the specified order that passes through zero to a data set.

Parameters

in, out	<i>this</i>	The polynomial object.
in	<i>x</i>	An N-element array containing the independent variable data points. Notice, must be $N > \text{order}$.
in, out	<i>y</i>	On input, an N-element array containing the dependent variable data points. On output, the contents are overwritten.
in	<i>order</i>	The order of the polynomial (must be ≥ 1).
out	<i>err</i>	<p>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.</p> <ul style="list-style-type: none"> NL_INVALID_INPUT_ERROR: Occurs if a zero or negative polynomial order was specified, or if order is too large for the data set. NL_OUT_OF_MEMORY_ERROR: Occurs if insufficient memory is available. NL_ARRAY_SIZE_ERROR: Occurs if <i>x</i> and <i>y</i> are different sizes.

Definition at line 330 of file `nonlin_polynomials.f90`.

5.5.2.14 `type(polynomial) function nonlin_polynomials::poly_poly_add (class(polynomial), intent(in) x,
class(polynomial), intent(in) y) [private]`

Adds two polynomials.

Parameters

in	x	The left-hand-side argument.
in	y	The right-hand-side argument.

Returns

The resulting polynomial.

Definition at line 763 of file nonlin_polynomials.f90.

5.5.2.15 `type(polynomial) function nonlin_polynomials::poly_poly_mult (class(polynomial), intent(in) x,
class(polynomial), intent(in) y) [private]`

Multiplies two polynomials.

Parameters

in	x	The left-hand-side argument.
in	y	The right-hand-side argument.

Returns

The resulting polynomial.

Definition at line 877 of file nonlin_polynomials.f90.

5.5.2.16 `type(polynomial) function nonlin_polynomials::poly_poly_subtract (class(polynomial), intent(in) x,
class(polynomial), intent(in) y) [private]`

Subtracts two polynomials.

Parameters

in	x	The left-hand-side argument.
in	y	The right-hand-side argument.

Returns

The resulting polynomial.

Definition at line 820 of file nonlin_polynomials.f90.

5.5.2.17 complex(dp) function, dimension(this%order()) nonlin_polynomials::poly_roots (class(polynomial), intent(in) this, class(errors), intent(inout), optional, target err) [private]

Computes all the roots of a polynomial by computing the eigenvalues of the polynomial companion matrix.

Parameters

in	<i>this</i>	The polynomial object.
out	<i>err</i>	<p>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.</p> <ul style="list-style-type: none"> • NL_OUT_OF_MEMORY_ERROR: Occurs if local memory must be allocated, and there is insufficient memory available. • NL_CONVERGENCE_ERROR: Occurs if the algorithm failed to converge.

Usage

The following code provides an example of how to compute the roots of a polynomial. This examples uses a tenth order polynomial; however, this process is applicable to any order.

```

program example
  use linalg_constants, only : dp, i32
  use nonlin_polynomials

  ! Parameters
  integer(i32), parameter :: order = 10

  ! Local Variables
  integer(i32) :: i
  type(polynomial) :: p
  real(dp), dimension(order+1) :: coeff
  complex(dp), allocatable, dimension(:) :: rts, sol

  ! Define the polynomial
  call random_number(coeff)
  call p%initialize(order)
  do i = 1, size(coeff)
    call p%set(i, coeff(i))
  end do

  ! Compute the roots via the polynomial routine
  rts = p%roots()

  ! Compute the value of the polynomial at each root and ensure it
  ! is sufficiently close to zero.
  sol = p%evaluate(rts)
  do i = 1, size(sol)
    print ' (AE9.3AE9.3A)', "(", real(sol(i)), ", ", aimag(sol(i)), ")"
  end do
end program

```

The above program returns the following results.

```

(-.466E-14, -.161E-14)
(-.466E-14, 0.161E-14)
(-.999E-15, 0.211E-14)
(-.999E-15, -.211E-14)
(0.444E-15, 0.108E-14)
(0.444E-15, -.108E-14)
(-.144E-14, -.433E-14)
(-.144E-14, 0.433E-14)
(0.644E-14, -.100E-13)
(0.644E-14, 0.100E-13)

```

Definition at line 569 of file nonlin_polynomials.f90.

5.5.2.18 subroutine `nonlin_polynomials::set_poly_coefficient` (class(`polynomial`), intent(inout) *this*, integer(i32), intent(in) *ind*, real(dp), intent(in) *c*, class(errors), intent(inout), optional, target *err*) [private]

Sets the requested polynomial coefficient by index. The coefficient index is established as follows: $c(1) + c(2) * x + c(3) * x**2 + \dots c(n) * x**n-1$.

Parameters

in, out	<i>this</i>	The polynomial.
in	<i>ind</i>	The polynomial coefficient index ($0 < ind \leq order + 1$).
in	<i>c</i>	The polynomial coefficient.
out	<i>err</i>	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. <ul style="list-style-type: none"> NL_INVALID_INPUT_ERROR: Occurs if the requested index is less than or equal to zero, or if the requested index exceeds the number of polynomial coefficients.

Definition at line 679 of file `nonlin_polynomials.f90`.

5.6 `nonlin_solve` Module Reference

`nonlin_solve`

Data Types

- type `brent_solver`
Defines a solver based upon Brent's method for solving an equation of one variable without using derivatives.
- type `line_search_solver`
A class describing nonlinear solvers that use a line search algorithm to improve convergence behavior.
- type `newton_solver`
Defines a Newton solver.
- type `quasi_newton_solver`
Defines a quasi-Newton type solver based upon Broyden's method.

Functions/Subroutines

- subroutine `lss_get_line_search` (*this*, *ls*)
Gets the line search module.
- subroutine `lss_set_line_search` (*this*, *ls*)
Sets the line search module.
- subroutine `lss_set_default` (*this*)
Establishes a default line_search object for the line search module.
- pure logical function `lss_is_line_search_defined` (*this*)
Tests to see if a line search module is defined.
- pure logical function `lss_get_use_search` (*this*)
Gets a value determining if a line-search should be employed.
- subroutine `lss_set_use_search` (*this*, *x*)

- Sets a value determining if a line-search should be employed.*

 - subroutine `qns_solve` (this, fcn, x, fvec, ib, err)

Applies the quasi-Newton's method developed by Broyden in conjunction with a backtracking type line search to solve N equations of N unknowns.
 - pure integer(i32) function `qns_get_jac_interval` (this)

Gets the number of iterations that may pass before forcing a recalculation of the Jacobian matrix.
 - subroutine `qns_set_jac_interval` (this, n)

Sets the number of iterations that may pass before forcing a recalculation of the Jacobian matrix.
 - subroutine `ns_solve` (this, fcn, x, fvec, ib, err)

Applies Newton's method in conjunction with a backtracking type line search to solve N equations of N unknowns.
 - subroutine `brent_solve` (this, fcn, x, lim, f, ib, err)

Solves the equation.
 - subroutine `test_convergence` (x, xo, f, g, lg, xtol, ftol, gtol, c, cx, cf, cg, xnorm, fnorm)

Tests for convergence.

5.6.1 Detailed Description

`nonlin_solve`

Purpose

To provide various routines capable of solving systems of nonlinear equations.

5.6.2 Function/Subroutine Documentation

5.6.2.1 subroutine `nonlin_solve::brent_solve` (class(`brent_solver`), intent(inout) *this*, class(`fcn1var_helper`), intent(in) *fcn*, real(dp), intent(inout) *x*, type(value_pair), intent(in) *lim*, real(dp), intent(out), optional *f*, type(iteration_behavior), optional *ib*, class(errors), intent(inout), optional, target *err*) [private]

Solves the equation.

Parameters

in, out	<i>this</i>	The <code>brent_solver</code> object.
in	<i>fcn</i>	The <code>fcn1var_helper</code> object containing the equation to solve.
in, out	<i>x</i>	A parameter used to return the solution. Notice, any input value will be ignored as this routine relies upon the search limits in <i>lim</i> to provide a starting point.
in	<i>lim</i>	A <code>value_pair</code> object defining the search limits.
out	<i>f</i>	An optional parameter used to return the function residual as computed at <i>x</i> .
out	<i>ib</i>	An optional output, that if provided, allows the caller to obtain iteration performance statistics.
out	<i>err</i>	<p>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.</p> <ul style="list-style-type: none"> • <code>NL_INVALID_OPERATION_ERROR</code>: Occurs if no equations have been defined. • <code>NL_INVALID_INPUT_ERROR</code>: Occurs if the number of equations is different than the number of variables. • <code>NL_CONVERGENCE_ERROR</code>: Occurs if the algorithm cannot converge within the allowed number of iterations.

Usage

The following code provides an example of how to solve an equation of one variable using Brent's method.

```

program main
  use linalg_constants, only : dp
  use nonlin_types, only : fcnlvar, fcnlvar_helper,
    value_pair
  use nonlin_solve, only : brent_solver

  type(fcnlvar_helper) :: obj
  procedure(fcnlvar), pointer :: fcn
  type(brent_solver) :: solver
  real(dp) :: x, f
  type(value_pair) :: limits

  ! Define the solution limits
  limits%x1 = 1.5d0
  limits%x2 = 5.0d0

  ! Define the function
  fcn => fcnl
  call obj%set_fcn(fcn)

  ! Solve the equation
  call solver%solve(obj, x, limits, f)

  ! Print the output and the residual:
  print '(AF5.3)', "The solution: ", x
  print '(AE9.3)', "The residual: ", f
contains
  ! f(x) = sin(x) / x, SOLUTION: x = n * pi for n = 1, 2, 3, ...
  function fcnl(x) result(f)
    real(dp), intent(in) :: x
    real(dp) :: f
    f = sin(x) / x
  end function
end program

```

The above program returns the following results.

```

The solution: 3.142
The residual: -.751E-11

```

See Also

- [Wikipedia](#)
- [Numerical Recipes](#)
- R.P. Brent, "Algorithms for Minimization without Derivatives," Dover Publications, January 2002. ISBN 0-486-41998-3. Further information available [here](#).

Definition at line 986 of file nonlin_solve.f90.

5.6.2.2 subroutine nonlin_solve::lss_get_line_search (class(line_search_solver), intent(in) *this*, class(line_search), intent(out), allocatable *ls*) [private]

Gets the line search module.

Parameters

in	<i>this</i>	The line_search_solver object.
out	<i>ls</i>	The line_search object.

Definition at line 95 of file nonlin_solve.f90.

5.6.2.3 pure logical function nonlin_solve::lss_get_use_search (class(line_search_solver), intent(in) *this*) [private]

Gets a value determining if a line-search should be employed.

Parameters

in	<i>this</i>	The line_search_solver object.
----	-------------	--

Returns

Returns true if a line search should be used; else, false.

Definition at line 141 of file `nonlin_solve.f90`.

5.6.2.4 pure logical function `nonlin_solve::lss_is_line_search_defined (class(line_search_solver), intent(in) this)` `[private]`

Tests to see if a line search module is defined.

Parameters

in	<i>this</i>	The line_search_solver object.
----	-------------	--

Returns

Returns true if a module is defined; else, false.

Definition at line 130 of file `nonlin_solve.f90`.

5.6.2.5 subroutine `nonlin_solve::lss_set_default (class(line_search_solver), intent(inout) this)` `[private]`

Establishes a default `line_search` object for the line search module.

Parameters

in, out	<i>this</i>	The line_search_solver object.
---------	-------------	--

Definition at line 119 of file `nonlin_solve.f90`.

5.6.2.6 subroutine `nonlin_solve::lss_set_line_search (class(line_search_solver), intent(inout) this, class(line_search), intent(in) ls)` `[private]`

Sets the line search module.

Parameters

in, out	<i>this</i>	The line_search_solver object.
in	<i>ls</i>	The <code>line_search</code> object.

Definition at line 107 of file `nonlin_solve.f90`.

5.6.2.7 subroutine `nonlin_solve::lss_set_use_search` (class(`line_search_solver`), intent(inout) *this*, logical, intent(in) *x*)
[private]

Sets a value determining if a line-search should be employed.

Parameters

in, out	<i>this</i>	The <code>line_search_solver</code> object.
in	<i>x</i>	Set to true if a line search should be used; else, false.

Definition at line 152 of file `nonlin_solve.f90`.

5.6.2.8 subroutine `nonlin_solve::ns_solve` (class(`newton_solver`), intent(inout) *this*, class(`vecfcn_helper`), intent(in) *fcn*, real(dp), dimension(:), intent(inout) *x*, real(dp), dimension(:), intent(out) *fvec*, type(`iteration_behavior`), optional *ib*, class(`errors`), intent(inout), optional, target *err*) [private]

Applies Newton's method in conjunction with a backtracking type line search to solve N equations of N unknowns.

Parameters

in, out	<i>this</i>	The <code>equation_solver</code> -based object.
in	<i>fcn</i>	The <code>vecfcn_helper</code> object containing the equations to solve.
in, out	<i>x</i>	On input, an N-element array containing an initial estimate to the solution. On output, the updated solution estimate. N is the number of variables.
out	<i>fvec</i>	An N-element array that, on output, will contain the values of each equation as evaluated at the variable values given in <i>x</i> .
out	<i>ib</i>	An optional output, that if provided, allows the caller to obtain iteration performance statistics.
out	<i>err</i>	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. <ul style="list-style-type: none"> • <code>NL_INVALID_OPERATION_ERROR</code>: Occurs if no equations have been defined. • <code>NL_INVALID_INPUT_ERROR</code>: Occurs if the number of equations is different than the number of variables. • <code>NL_ARRAY_SIZE_ERROR</code>: Occurs if any of the input arrays are not sized correctly. • <code>NL_DIVERGENT_BEHAVIOR_ERROR</code>: Occurs if the direction vector is pointing in an apparent uphill direction. • <code>NL_CONVERGENCE_ERROR</code>: Occurs if the line search cannot converge within the allowed number of iterations. • <code>NL_OUT_OF_MEMORY_ERROR</code>: Occurs if there is insufficient memory available. • <code>NL_SPURIOUS_CONVERGENCE_ERROR</code>: Occurs as a warning if the slope of the gradient vector becomes sufficiently close to zero.

Usage

The following code provides an example of how to solve a system of N equations of N unknowns using Newton's method.

```

program main
  use linalg_constants, only : dp
  use nonlin_types, only : vecfcn, vecfcn_helper
  use nonlin_solve, only : newton_solver

  type(vecfcn_helper) :: obj
  procedure(vecfcn), pointer :: fcn
  type(newton_solver) :: solver
  real(dp) :: x(2), f(2)

  ! Set the initial conditions to [1, 1]
  x = 1.0d0

  ! Define the function
  fcn => fcn1
  call obj%set_fcn(fcn, 2, 2)

  ! Solve the system of equations. The solution overwrites X
  call solver%solve(obj, x, f)

  ! Print the output and the residual:
  print '(AF5.3AF5.3A)', "The solution: (", x(1), ", ", x(2), ")"
  print '(AE8.3AE8.3A)', "The residual: (", f(1), ", ", f(2), ")"
contains
  ! System of Equations:
  !
  !  $x^2 + y^2 = 34$ 
  !  $x^2 - 2 * y^2 = 7$ 
  !
  ! Solution:
  !  $x = +/-5$ 
  !  $y = +/-3$ 
  subroutine fcn1(x, f)
    real(dp), intent(in), dimension(:) :: x
    real(dp), intent(out), dimension(:) :: f
    f(1) = x(1)**2 + x(2)**2 - 34.0d0
    f(2) = x(1)**2 - 2.0d0 * x(2)**2 - 7.0d0
  end subroutine
end program

```

The above program returns the following results.

```

The solution: (5.000, 3.000)
The residual: (.000E+00, .000E+00)

```

See Also

- [Wikipedia](#)

Definition at line 671 of file nonlin_solve.f90.

5.6.2.9 pure integer(i32) function nonlin_solve::qns_get_jac_interval (class(quasi_newton_solver), intent(in) *this*)
[private]

Gets the number of iterations that may pass before forcing a recalculation of the Jacobian matrix.

Parameters

in	<i>this</i>	The quasi_newton_solver object.
----	-------------	---

Returns

The number of iterations.

Definition at line 565 of file nonlin_solve.f90.

5.6.2.10 subroutine nonlin_solve::qns_set_jac_interval (class(quasi_newton_solver), intent(inout) *this*, integer(i32),
intent(in) *n*) [private]

Sets the number of iterations that may pass before forcing a recalculation of the Jacobian matrix.

Parameters

<code>in, out</code>	<i>this</i>	The <code>quasi_newton_solver</code> object.
<code>in</code>	<i>n</i>	The number of iterations.

Definition at line 577 of file `nonlin_solve.f90`.

5.6.2.11 `subroutine nonlin_solve::qns_solve (class(quasi_newton_solver), intent(inout) this, class(vecfcn_helper), intent(in) fcn, real(dp), dimension(:), intent(inout) x, real(dp), dimension(:), intent(out) fvec, type(iteration_behavior), optional ib, class(errors), intent(inout), optional, target err) [private]`

Applies the quasi-Newton's method developed by Broyden in conjunction with a backtracking type line search to solve N equations of N unknowns.

Parameters

<code>in, out</code>	<i>this</i>	The equation_solver-based object.
<code>in</code>	<i>fcn</i>	The <code>vecfcn_helper</code> object containing the equations to solve.
<code>in, out</code>	<i>x</i>	On input, an N -element array containing an initial estimate to the solution. On output, the updated solution estimate. N is the number of variables.
<code>out</code>	<i>fvec</i>	An N -element array that, on output, will contain the values of each equation as evaluated at the variable values given in <i>x</i> .
<code>out</code>	<i>ib</i>	An optional output, that if provided, allows the caller to obtain iteration performance statistics.
<code>out</code>	<i>err</i>	<p>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.</p> <ul style="list-style-type: none"> • <code>NL_INVALID_OPERATION_ERROR</code>: Occurs if no equations have been defined. • <code>NL_INVALID_INPUT_ERROR</code>: Occurs if the number of equations is different than the number of variables. • <code>NL_ARRAY_SIZE_ERROR</code>: Occurs if any of the input arrays are not sized correctly. • <code>NL_DIVERGENT_BEHAVIOR_ERROR</code>: Occurs if the direction vector is pointing in an apparent uphill direction. • <code>NL_CONVERGENCE_ERROR</code>: Occurs if the line search cannot converge within the allowed number of iterations. • <code>NL_OUT_OF_MEMORY_ERROR</code>: Occurs if there is insufficient memory available. • <code>NL_SPURIOUS_CONVERGENCE_ERROR</code>: Occurs as a warning if the slope of the gradient vector becomes sufficiently close to zero.

Usage

The following code provides an example of how to solve a system of N equations of N unknowns using this Quasi-Newton method.

```

program main
  use linalg_constants, only : dp
  use nonlin_types, only : vecfcn, vecfcn_helper
  use nonlin_solve, only : quasi_newton_solver

  type(vecfcn_helper) :: obj

```

```

procedure(vecfcn), pointer :: fcn
type(quasi_newton_solver) :: solver
real(dp) :: x(2), f(2)

! Set the initial conditions to [1, 1]
x = 1.0d0

! Define the function
fcn => fcn1
call obj%set_fcn(fcn, 2, 2)

! Solve the system of equations. The solution overwrites X
call solver%solve(obj, x, f)

! Print the output and the residual:
print '(AF5.3AF5.3A)', "The solution: (", x(1), ", ", x(2), ")"
print '(AE8.3AE8.3A)', "The residual: (", f(1), ", ", f(2), ")"
contains
! System of Equations:
!
! x**2 + y**2 = 34
! x**2 - 2 * y**2 = 7
!
! Solution:
! x = +/-5
! y = +/-3
subroutine fcn1(x, f)
    real(dp), intent(in), dimension(:) :: x
    real(dp), intent(out), dimension(:) :: f
    f(1) = x(1)**2 + x(2)**2 - 34.0d0
    f(2) = x(1)**2 - 2.0d0 * x(2)**2 - 7.0d0
end subroutine
end program

```

The above program returns the following results.

```

The solution: (5.000, 3.000)
The residual: (.604E-10, .121E-09)

```

See Also

- [Broyden's Paper](#)
- [Wikipedia](#)
- [Numerical Recipes](#)

Definition at line 249 of file nonlin_solve.f90.

5.6.2.12 subroutine nonlin_solve::test_convergence (real(dp), dimension(:), intent(in) *x*, real(dp), dimension(:), intent(in) *xo*, real(dp), dimension(:), intent(in) *f*, real(dp), dimension(:), intent(in) *g*, logical, intent(in) *lg*, real(dp), intent(in) *xtol*, real(dp), intent(in) *ftol*, real(dp), intent(in) *gtol*, logical, intent(out) *c*, logical, intent(out) *cx*, logical, intent(out) *cf*, logical, intent(out) *cg*, real(dp), intent(out) *xnorm*, real(dp), intent(out) *fnorm*) [private]

Tests for convergence.

Parameters

in	<i>x</i>	The current solution estimate.
in	<i>xo</i>	The previous solution estimate.
in	<i>f</i>	The current residual based upon <i>x</i> .
in	<i>g</i>	The current estimate of the gradient vector at <i>x</i> .
in	<i>lg</i>	Set to true if the gradient slope check should be performed; else, false.
in	<i>xtol</i>	The tolerance on the change in variable.
in	<i>ftol</i>	The tolerance on the residual.
in	<i>gtol</i>	The tolerance on the slope of the gradient.
out	<i>c</i>	True if the solution converged on either the residual or change in variable.
out	<i>cx</i>	True if convergence occurred due to change in variable.
out	<i>cf</i>	True if convergence occurred due to residual.
out	<i>cg</i>	True if convergence occurred due to slope of the gradient.
out	<i>xnorm</i>	The largest magnitude component of the scaled change in variable vector.
out	<i>fnorm</i>	The largest magnitude residual component

Definition at line 1209 of file `nonlin_solve.f90`.

5.7 `nonlin_types` Module Reference

`nonlin_types`

Data Types

- type `equation_optimizer`
A base class for optimization of an equation of multiple variables.
- type `equation_solver`
A base class for various solvers of nonlinear systems of equations.
- type `equation_solver_1var`
A base class for various solvers of equations of one variable.
- interface `fcn1var`
Describes a function of one variable.
- type `fcn1var_helper`
Defines a type capable of encapsulating an equation of one variable of the form: $f(x) = 0$.
- interface `fcnvar`
Describes a function of N variables.
- type `fcnvar_helper`
Defines a type capable of encapsulating an equation of N variables.
- interface `gradientfcn`
Describes a routine capable of computing the gradient vector of an equation of N variables.
- type `iteration_behavior`
Defines a set of parameters that describe the behavior of the iteration process.
- interface `jacobianfcn`
Describes a routine capable of computing the Jacobian matrix of M functions of N unknowns.
- interface `nonlin_optimize`
Describes the interface of a routine for optimizing an equation of N variables.
- interface `nonlin_solver`
Describes the interface of a nonlinear equation solver.
- interface `nonlin_solver_1var`
Describes the interface of a solver for an equation of one variable.
- type `value_pair`
Defines a pair of numeric values.
- interface `vecfcn`
Describes an M -element vector-valued function of N -variables.
- type `vecfcn_helper`
Defines a type capable of encapsulating a system of nonlinear equations of the form: $F(X) = 0$.

Functions/Subroutines

- subroutine [vfh_set_fcn](#) (this, fcn, nfcn, nvar)
Establishes a pointer to the routine containing the system of equations to solve.
- subroutine [vfh_set_jac](#) (this, jac)
Establishes a pointer to the routine for computing the Jacobian matrix of the system of equations. If no routine is defined, the Jacobian matrix will be computed numerically (this is the default state).
- pure logical function [vfh_is_fcn_defined](#) (this)
Tests if the pointer to the subroutine containing the system of equations to solve has been assigned.
- pure logical function [vfh_is_jac_defined](#) (this)
Tests if the pointer to the subroutine containing the system of equations to solve has been assigned.
- subroutine [vfh_fcn](#) (this, x, f)
Executes the routine containing the system of equations to solve. No action is taken if the pointer to the subroutine has not been defined.
- subroutine [vfh_jac_fcn](#) (this, x, jac, fv, work, olwork, err)
Executes the routine containing the Jacobian matrix if supplied. If not supplied, the Jacobian is computed via finite differences.
- pure integer(i32) function [vfh_get_nfcn](#) (this)
Gets the number of equations in this system.
- pure integer(i32) function [vfh_get_nvar](#) (this)
Gets the number of variables in this system.
- real(dp) function [f1h_fcn](#) (this, x)
Executes the routine containing the function to evaluate.
- pure logical function [f1h_is_fcn_defined](#) (this)
Tests if the pointer to the function containing the equation to solve has been assigned.
- subroutine [f1h_set_fcn](#) (this, fcn)
Establishes a pointer to the routine containing the equations to solve.
- real(dp) function [fnh_fcn](#) (this, x)
Executes the routine containing the function to evaluate.
- pure logical function [fnh_is_fcn_defined](#) (this)
Tests if the pointer to the function containing the equation to solve has been assigned.
- subroutine [fnh_set_fcn](#) (this, fcn, nvar)
Establishes a pointer to the routine containing the equations to solve.
- pure integer(i32) function [fnh_get_nvar](#) (this)
Gets the number of variables in this system.
- subroutine [fnh_set_grad](#) (this, fcn)
Establishes a pointer to the routine containing the gradient vector of the function.
- pure logical function [fnh_is_grad_defined](#) (this)
Tests if the pointer to the routine containing the gradient has been assigned.
- subroutine [fnh_grad_fcn](#) (this, x, g, fv, err)
Executes the routine containing the gradient, if supplied. If not supplied, the gradient is computed via finite differences.
- pure integer(i32) function [es_get_max_eval](#) (this)
Gets the maximum number of function evaluations allowed during a single solve.
- subroutine [es_set_max_eval](#) (this, n)
Sets the maximum number of function evaluations allowed during a single solve.
- pure real(dp) function [es_get_fcn_tol](#) (this)
Gets the convergence on function value tolerance.
- subroutine [es_set_fcn_tol](#) (this, x)
Sets the convergence on function value tolerance.
- pure real(dp) function [es_get_var_tol](#) (this)
Gets the convergence on change in variable tolerance.
- subroutine [es_set_var_tol](#) (this, x)

- Sets the convergence on change in variable tolerance.*

 - pure real(`dp`) function `es_get_grad_tol` (this)
- Gets the convergence on slope of the gradient vector tolerance.*

 - subroutine `es_set_grad_tol` (this, x)
- Sets the convergence on slope of the gradient vector tolerance.*

 - pure logical function `es_get_print_status` (this)
- Gets a logical value determining if iteration status should be printed.*

 - subroutine `es_set_print_status` (this, x)
- Sets a logical value determining if iteration status should be printed.*

 - pure integer(`i32`) function `es1_get_max_eval` (this)
- Gets the maximum number of function evaluations allowed during a single solve.*

 - subroutine `es1_set_max_eval` (this, n)
- Sets the maximum number of function evaluations allowed during a single solve.*

 - pure real(`dp`) function `es1_get_fcn_tol` (this)
- Gets the convergence on function value tolerance.*

 - subroutine `es1_set_fcn_tol` (this, x)
- Sets the convergence on function value tolerance.*

 - pure real(`dp`) function `es1_get_var_tol` (this)
- Gets the convergence on change in variable tolerance.*

 - subroutine `es1_set_var_tol` (this, x)
- Sets the convergence on change in variable tolerance.*

 - pure logical function `es1_get_print_status` (this)
- Gets a logical value determining if iteration status should be printed.*

 - subroutine `es1_set_print_status` (this, x)
- Sets a logical value determining if iteration status should be printed.*

 - pure integer(`i32`) function `oe_get_max_eval` (this)
- Gets the maximum number of function evaluations allowed.*

 - subroutine `oe_set_max_eval` (this, n)
- Sets the maximum number of function evaluations allowed.*

 - pure real(`dp`) function `oe_get_tol` (this)
- Gets the tolerance on convergence.*

 - subroutine `oe_set_tol` (this, x)
- Sets the tolerance on convergence.*

 - pure logical function `oe_get_print_status` (this)
- Gets a logical value determining if iteration status should be printed.*

 - subroutine `oe_set_print_status` (this, x)
- Sets a logical value determining if iteration status should be printed.*

 - subroutine, public `print_status` (iter, nfeval, njaceval, xnorm, fnorm)
- Prints the iteration status.*

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 `nl_invalid_input_error` = 201
An error flag denoting an invalid input.
- integer, parameter, public `nl_array_size_error` = 202
An error flag denoting an improperly sized array.

- integer, parameter, public `nl_out_of_memory_error` = `LA_OUT_OF_MEMORY_ERROR`
An error denoting that there is insufficient memory available.
- integer, parameter, public `nl_invalid_operation_error` = `LA_INVALID_OPERATION_ERROR`
An error resulting from an invalid operation.
- integer, parameter, public `nl_convergence_error` = `LA_CONVERGENCE_ERROR`
An error resulting from a lack of convergence.
- integer, parameter, public `nl_divergent_behavior_error` = 206
An error resulting from a divergent condition.
- integer, parameter, public `nl_spurious_convergence_error` = 207
An error indicating a possible spurious convergence condition.
- integer, parameter, public `nl_tolerance_too_small_error` = 208
An error indicating the user-requested tolerance is too small to be practical for the problem at hand.

5.7.1 Detailed Description

`nonlin_types`

Purpose

To provide various types and constants useful in the solution of systems of nonlinear equations.

5.7.2 Function/Subroutine Documentation

5.7.2.1 `pure real(dp) function nonlin_types::es1_get_fcn_tol (class(equation_solver_1var), intent(in) this)`
[private]

Gets the convergence on function value tolerance.

Parameters

in	<i>this</i>	The <code>equation_solver_1var</code> object.
----	-------------	---

Returns

The tolerance value.

Definition at line 1074 of file `nonlin_types.f90`.

5.7.2.2 `pure integer(i32) function nonlin_types::es1_get_max_eval (class(equation_solver_1var), intent(in) this)`
[private]

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

Parameters

in	<i>this</i>	The <code>equation_solver_1var</code> object.
----	-------------	---

Returns

The maximum number of function evaluations.

Definition at line 1051 of file `nonlin_types.f90`.

5.7.2.3 `pure logical function nonlin_types::es1_get_print_status (class(equation_solver_1var), intent(in) this)`
`[private]`

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

Parameters

<code>in</code>	<code>this</code>	The equation_solver_1var object.
-----------------	-------------------	--

Returns

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

Definition at line 1119 of file `nonlin_types.f90`.

5.7.2.4 `pure real(dp) function nonlin_types::es1_get_var_tol (class(equation_solver_1var), intent(in) this)`
`[private]`

Gets the convergence on change in variable tolerance.

Parameters

<code>in</code>	<code>this</code>	The equation_solver_1var object.
-----------------	-------------------	--

Returns

The tolerance value.

Definition at line 1096 of file `nonlin_types.f90`.

5.7.2.5 `subroutine nonlin_types::es1_set_fcn_tol (class(equation_solver_1var), intent(inout) this, real(dp), intent(in) x)`
`[private]`

Sets the convergence on function value tolerance.

Parameters

<code>in, out</code>	<code>this</code>	The equation_solver_1var object.
<code>in</code>	<code>x</code>	The tolerance value.

Definition at line 1085 of file `nonlin_types.f90`.

5.7.2.6 subroutine `nonlin_types::es1_set_max_eval` (`class(equation_solver_1var)`, `intent(inout) this`, `integer(i32)`,
`intent(in) n`) [`private`]

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

Parameters

<code>in, out</code>	<code>this</code>	The equation_solver_1var object.
<code>in</code>	<code>n</code>	The maximum number of function evaluations.

Definition at line 1063 of file `nonlin_types.f90`.

5.7.2.7 subroutine `nonlin_types::es1_set_print_status` (`class(equation_solver_1var)`, `intent(inout) this`, `logical`, `intent(in) x`
`)` [`private`]

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

Parameters

<code>in, out</code>	<code>this</code>	The equation_solver_1var object.
<code>in</code>	<code>x</code>	True if the iteration status should be printed; else, false.

Definition at line 1131 of file `nonlin_types.f90`.

5.7.2.8 subroutine `nonlin_types::es1_set_var_tol` (`class(equation_solver_1var)`, `intent(inout) this`, `real(dp)`, `intent(in) x`)
`[private]`

Sets the convergence on change in variable tolerance.

Parameters

<code>in, out</code>	<code>this</code>	The equation_solver_1var object.
<code>in</code>	<code>x</code>	The tolerance value.

Definition at line 1107 of file `nonlin_types.f90`.

5.7.2.9 pure `real(dp)` function `nonlin_types::es_get_fcn_tol` (`class(equation_solver)`, `intent(in) this`) [`private`]

Gets the convergence on function value tolerance.

Parameters

<code>in</code>	<code>this</code>	The equation_solver object.
-----------------	-------------------	---

Returns

The tolerance value.

Definition at line 958 of file `nonlin_types.f90`.

5.7.2.10 `pure real(dp) function nonlin_types::es_get_grad_tol (class(equation_solver), intent(in) this) [private]`

Gets the convergence on slope of the gradient vector tolerance.

Parameters

<code>in</code>	<code>this</code>	The equation_solver object.
-----------------	-------------------	---

Returns

The tolerance value.

Definition at line 1002 of file `nonlin_types.f90`.

5.7.2.11 `pure integer(i32) function nonlin_types::es_get_max_eval (class(equation_solver), intent(in) this) [private]`

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

Parameters

<code>in</code>	<code>this</code>	The equation_solver object.
-----------------	-------------------	---

Returns

The maximum number of function evaluations.

Definition at line 935 of file `nonlin_types.f90`.

5.7.2.12 `pure logical function nonlin_types::es_get_print_status (class(equation_solver), intent(in) this) [private]`

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

Parameters

<code>in</code>	<code>this</code>	The equation_solver object.
-----------------	-------------------	---

Returns

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

Definition at line 1025 of file `nonlin_types.f90`.

5.7.2.13 `pure real(dp) function nonlin_types::es_get_var_tol (class(equation_solver), intent(in) this) [private]`

Gets the convergence on change in variable tolerance.

Parameters

in	<i>this</i>	The equation_solver object.
----	-------------	---

Returns

The tolerance value.

Definition at line 980 of file `nonlin_types.f90`.

```
5.7.2.14  subroutine nonlin_types::es_set_fcn_tol ( class(equation_solver), intent(inout) this, real(dp), intent(in) x )
           [private]
```

Sets the convergence on function value tolerance.

Parameters

in, out	<i>this</i>	The equation_solver object.
in	<i>x</i>	The tolerance value.

Definition at line 969 of file `nonlin_types.f90`.

```
5.7.2.15  subroutine nonlin_types::es_set_grad_tol ( class(equation_solver), intent(inout) this, real(dp), intent(in) x )
           [private]
```

Sets the convergence on slope of the gradient vector tolerance.

Parameters

in	<i>this</i>	The equation_solver object.
----	-------------	---

Returns

The tolerance value.

Definition at line 1013 of file `nonlin_types.f90`.

```
5.7.2.16  subroutine nonlin_types::es_set_max_eval ( class(equation_solver), intent(inout) this, integer(i32), intent(in) n )
           [private]
```

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

Parameters

in, out	<i>this</i>	The equation_solver object.
in	<i>n</i>	The maximum number of function evaluations.

Definition at line 947 of file `nonlin_types.f90`.

5.7.2.17 `subroutine nonlin_types::es_set_print_status (class(equation_solver), intent(inout) this, logical, intent(in) x)`
`[private]`

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

Parameters

<code>in, out</code>	<code>this</code>	The equation_solver object.
<code>in</code>	<code>x</code>	True if the iteration status should be printed; else, false.

Definition at line 1037 of file `nonlin_types.f90`.

5.7.2.18 `subroutine nonlin_types::es_set_var_tol (class(equation_solver), intent(inout) this, real(dp), intent(in) x)`
`[private]`

Sets the convergence on change in variable tolerance.

Parameters

<code>in, out</code>	<code>this</code>	The equation_solver object.
<code>in</code>	<code>x</code>	The tolerance value.

Definition at line 991 of file `nonlin_types.f90`.

5.7.2.19 `real(dp) function nonlin_types::f1h_fcn (class(fcn1var_helper), intent(in) this, real(dp), intent(in) x)`
`[private]`

Executes the routine containing the function to evaluate.

Parameters

<code>in</code>	<code>this</code>	The fcn1var_helper object.
<code>in</code>	<code>x</code>	The value of the independent variable at which the function should be evaluated.

Returns

The value of the function at `x`.

Definition at line 734 of file `nonlin_types.f90`.

5.7.2.20 `pure logical function nonlin_types::f1h_is_fcn_defined (class(fcn1var_helper), intent(in) this)` `[private]`

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

Parameters

<code>in</code>	<code>this</code>	The fcn1var_helper object.
-----------------	-------------------	--

Returns

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

Definition at line 749 of file `nonlin_types.f90`.

5.7.2.21 `subroutine nonlin_types::f1h_set_fcn (class(fcn1var_helper), intent(inout) this, procedure(fcn1var), intent(in), pointer fcn) [private]`

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

Parameters

<code>in, out</code>	<code>this</code>	The <code>fcn1var_helper</code> object.
<code>in</code>	<code>fcn</code>	The function pointer.

Definition at line 761 of file `nonlin_types.f90`.

5.7.2.22 `real(dp) function nonlin_types::fnh_fcn (class(fcnvar_helper), intent(in) this, real(dp), dimension(:), intent(in) x) [private]`

Executes the routine containing the function to evaluate.

Parameters

<code>in</code>	<code>this</code>	The <code>fcnvar_helper</code> object.
<code>in</code>	<code>x</code>	The value of the independent variable at which the function should be evaluated.

Returns

The value of the function at `x`.

Definition at line 776 of file `nonlin_types.f90`.

5.7.2.23 `pure integer(i32) function nonlin_types::fnh_get_nvar (class(fcnvar_helper), intent(in) this) [private]`

Gets the number of variables in this system.

Parameters

<code>in</code>	<code>this</code>	The <code>fcnvar_helper</code> object.
-----------------	-------------------	--

Returns

The number of variables.

Definition at line 817 of file `nonlin_types.f90`.

5.7.2.24 `subroutine nonlin_types::fnh_grad_fcn (class(fcnvar_helper), intent(in) this, real(dp), dimension(:), intent(inout) x, real(dp), dimension(:), intent(out) g, real(dp), intent(in), optional fv, integer(i32), intent(out), optional err)`
`[private]`

Executes the routine containing the gradient, if supplied. If not supplied, the gradient is computed via finite differences.

Parameters

in	<i>this</i>	The <code>fcnvar_helper</code> object.
in, out	<i>x</i>	An N-element array containing the independent variables defining the point about which the derivatives will be calculated. This array is restored upon output.
out	<i>g</i>	An N-element array where the gradient will be written upon output.
in	<i>fv</i>	An optional input providing the function value at <i>x</i> .
out	<i>err</i>	An optional integer output that can be used to determine error status. If not used, and an error is encountered, the routine simply returns silently. If used, the following error codes identify error status: <ul style="list-style-type: none"> • 0: No error has occurred. • n: A positive integer denoting the index of an invalid input.

Definition at line 864 of file `nonlin_types.f90`.

5.7.2.25 `pure logical function nonlin_types::fnh_is_fcn_defined (class(fcnvar_helper), intent(in) this)` `[private]`

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

Parameters

in	<i>this</i>	The <code>fcnvar_helper</code> object.
----	-------------	--

Returns

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

Definition at line 791 of file `nonlin_types.f90`.

5.7.2.26 `pure logical function nonlin_types::fnh_is_grad_defined (class(fcnvar_helper), intent(in) this)` `[private]`

Tests if the pointer to the routine containing the gradient has been assigned.

Parameters

in	<i>this</i>	The <code>fcnvar_helper</code> object.
----	-------------	--

Returns

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

Definition at line 841 of file `nonlin_types.f90`.

5.7.2.27 subroutine `nonlin_types::fnh_set_fcn` (`class(fcnvar_helper)`, `intent(inout) this`, `procedure(fcnvar)`, `intent(in)`, `pointer fcn`, `integer(i32)`, `intent(in) nvar`) `[private]`

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

Parameters

<code>in, out</code>	<code>this</code>	The <code>fcnvar_helper</code> object.
<code>in</code>	<code>fcn</code>	The function pointer.
<code>in</code>	<code>nvar</code>	The number of variables in the function.

Definition at line 804 of file `nonlin_types.f90`.

5.7.2.28 subroutine `nonlin_types::fnh_set_grad` (`class(fcnvar_helper)`, `intent(inout) this`, `procedure(gradientfcn)`, `intent(in)`, `pointer fcn`) `[private]`

Establishes a pointer to the routine containing the gradient vector of the function.

Parameters

<code>in, out</code>	<code>this</code>	The <code>fcnvar_helper</code> object.
<code>in</code>	<code>fcn</code>	The pointer to the gradient routine.

Definition at line 829 of file `nonlin_types.f90`.

5.7.2.29 pure `integer(i32)` function `nonlin_types::oe_get_max_eval` (`class(equation_optimizer)`, `intent(in) this`) `[private]`

Gets the maximum number of function evaluations allowed.

Parameters

<code>in</code>	<code>this</code>	The <code>equation_optimizer</code> object.
-----------------	-------------------	---

Returns

The maximum number of function evaluations.

Definition at line 1144 of file `nonlin_types.f90`.

5.7.2.30 pure `logical` function `nonlin_types::oe_get_print_status` (`class(equation_optimizer)`, `intent(in) this`) `[private]`

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

Parameters

<code>in</code>	<code>this</code>	The <code>equation_optimizer</code> object.
-----------------	-------------------	---

Returns

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

Definition at line 1189 of file `nonlin_types.f90`.

5.7.2.31 `pure real(dp) function nonlin_types::oe_get_tol (class(equation_optimizer), intent(in) this) [private]`

Gets the tolerance on convergence.

Parameters

<code>in</code>	<code>this</code>	The equation_optimizer object.
-----------------	-------------------	--

Returns

The convergence tolerance.

Definition at line 1166 of file `nonlin_types.f90`.

5.7.2.32 `subroutine nonlin_types::oe_set_max_eval (class(equation_optimizer), intent(inout) this, integer(i32), intent(in) n) [private]`

Sets the maximum number of function evaluations allowed.

Parameters

<code>in, out</code>	<code>this</code>	The equation_optimizer object.
<code>in</code>	<code>n</code>	The maximum number of function evaluations.

Definition at line 1155 of file `nonlin_types.f90`.

5.7.2.33 `subroutine nonlin_types::oe_set_print_status (class(equation_optimizer), intent(inout) this, logical, intent(in) x) [private]`

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

Parameters

<code>in, out</code>	<code>this</code>	The equation_optimizer object.
<code>in</code>	<code>x</code>	True if the iteration status should be printed; else, false.

Definition at line 1201 of file `nonlin_types.f90`.

5.7.2.34 `subroutine nonlin_types::oe_set_tol (class(equation_optimizer), intent(inout) this, real(dp), intent(in) x) [private]`

Sets the tolerance on convergence.

Parameters

in, out	<i>this</i>	The equation_optimizer object.
in	<i>x</i>	The convergence tolerance.

Definition at line 1177 of file `nonlin_types.f90`.

5.7.2.35 `subroutine, public nonlin_types::print_status (integer(i32), intent(in) iter, integer(i32), intent(in) nfeval, integer(i32), intent(in) njaceval, real(dp), intent(in) xnorm, real(dp), intent(in) fnorm)`

Prints the iteration status.

Parameters

in	<i>iter</i>	The iteration number.
in	<i>nfeval</i>	The number of function evaluations.
in	<i>njaceval</i>	The number of Jacobian evaluations.
in	<i>xnorm</i>	The change in variable value.
in	<i>fnorm</i>	The residual.

Definition at line 1217 of file `nonlin_types.f90`.

5.7.2.36 `subroutine nonlin_types::vfh_fcn (class(vecfcn_helper), intent(in) this, real(dp), dimension(:), intent(in) x, real(dp), dimension(:), intent(out) f) [private]`

Executes the routine containing the system of equations to solve. No action is taken if the pointer to the subroutine has not been defined.

Parameters

in	<i>this</i>	The vecfcn_helper object.
in	<i>x</i>	An N-element array containing the independent variables.
out	<i>f</i>	An M-element array that, on output, contains the values of the M functions.

Definition at line 552 of file `nonlin_types.f90`.

5.7.2.37 `pure integer(i32) function nonlin_types::vfh_get_nfcn (class(vecfcn_helper), intent(in) this) [private]`

Gets the number of equations in this system.

Parameters

in	<i>this</i>	The vecfcn_helper object.
----	-------------	---

Returns

The function count.

Definition at line 708 of file `nonlin_types.f90`.

5.7.2.38 pure integer(i32) function `nonlin_types::vfh_get_nvar (class(vecfcn_helper), intent(in) this)` [private]

Gets the number of variables in this system.

Parameters

in	<i>this</i>	The vecfcn_helper object.
----	-------------	---

Returns

The number of variables.

Definition at line 719 of file `nonlin_types.f90`.

5.7.2.39 pure logical function `nonlin_types::vfh_is_fcn_defined (class(vecfcn_helper), intent(in) this)` [private]

Tests if the pointer to the subroutine containing the system of equations to solve has been assigned.

Parameters

in	<i>this</i>	The vecfcn_helper object.
----	-------------	---

Returns

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

Definition at line 526 of file `nonlin_types.f90`.

5.7.2.40 pure logical function `nonlin_types::vfh_is_jac_defined (class(vecfcn_helper), intent(in) this)` [private]

Tests if the pointer to the subroutine containing the system of equations to solve has been assigned.

Parameters

in	<i>this</i>	The vecfcn_helper object.
----	-------------	---

Returns

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

Definition at line 538 of file `nonlin_types.f90`.

5.7.2.41 subroutine `nonlin_types::vfh_jac_fcn (class(vecfcn_helper), intent(in) this, real(dp), dimension(:), intent(inout) x, real(dp), dimension(:, :), intent(out) jac, real(dp), dimension(:), intent(in), optional, target fv, real(dp), dimension(:), intent(out), optional, target work, integer(i32), intent(out), optional olwork, integer(i32), intent(out), optional err)` [private]

Executes the routine containing the Jacobian matrix if supplied. If not supplied, the Jacobian is computed via finite differences.

Parameters

in	<i>this</i>	The vecfcn_helper object.
in	<i>x</i>	An N-element array containing the independent variables defining the point about which the derivatives will be calculated.
out	<i>jac</i>	An M-by-N matrix where, on output, the Jacobian will be written.
in	<i>fv</i>	An optional M-element array containing the function values at <i>x</i> . If not supplied, the function values are computed at <i>x</i> .
out	<i>work</i>	An optional input, that if provided, prevents any local memory allocation. If not provided, the memory required is allocated within. If provided, the length of the array must be at least <code>olwork</code> . Notice, a workspace array is only utilized if the user does not provide a routine for computing the Jacobian.
out	<i>olwork</i>	An optional output used to determine workspace size. If supplied, the routine determines the optimal size for <i>work</i> , and returns without performing any actual calculations.
out	<i>err</i>	An optional integer output that can be used to determine error status. If not used, and an error is encountered, the routine simply returns silently. If used, the following error codes identify error status: <ul style="list-style-type: none"> • 0: No error has occurred. • n: A positive integer denoting the index of an invalid input. • -1: Indicates internal memory allocation failed.

Definition at line 587 of file `nonlin_types.f90`.

5.7.2.42 `subroutine nonlin_types::vfh_set_fcn (class(vecfcn_helper), intent(inout) this, procedure(vecfcn), intent(in), pointer fcn, integer(i32), intent(in) nfcn, integer(i32), intent(in) nvar)`

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

Parameters

in, out	<i>this</i>	The vecfcn_helper object.
in	<i>fcn</i>	The function pointer.
in	<i>nfcn</i>	The number of functions.
in	<i>nvar</i>	The number of variables.

Definition at line 498 of file `nonlin_types.f90`.

5.7.2.43 `subroutine nonlin_types::vfh_set_jac (class(vecfcn_helper), intent(inout) this, procedure(jacobianfcn), intent(in), pointer jac) [private]`

Establishes a pointer to the routine for computing the Jacobian matrix of the system of equations. If no routine is defined, the Jacobian matrix will be computed numerically (this is the default state).

Parameters

in, out	<i>this</i>	The vecfcn_helper object.
in	<i>jac</i>	The function pointer.

Definition at line 514 of file `nonlin_types.f90`.

6 Data Type Documentation

6.1 `nonlin_polynomials::assignment(=)` Interface Reference

Defines polynomial assignment.

Private Member Functions

- subroutine `poly_equals` (`x`, `y`)
Assigns the contents of one polynomial to another.
- subroutine `poly_dbl_equals` (`x`, `y`)
Assigns a number to each coefficient of the polynomial.

6.1.1 Detailed Description

Defines polynomial assignment.

Definition at line 32 of file `nonlin_polynomials.f90`.

6.1.2 Member Function/Subroutine Documentation

6.1.2.1 subroutine `nonlin_polynomials::assignment(=)::poly_dbl_equals` (`class(polynomial)`, `intent(inout)` `x`, `real(dp)`, `intent(in)` `y`) `[private]`

Assigns a number to each coefficient of the polynomial.

Parameters

<code>in, out</code>	<code>x</code>	The assignee.
<code>in</code>	<code>y</code>	The value to assign.

Definition at line 741 of file `nonlin_polynomials.f90`.

6.1.2.2 subroutine `nonlin_polynomials::assignment(=)::poly_equals` (`class(polynomial)`, `intent(inout)` `x`, `class(polynomial)`, `intent(in)` `y`) `[private]`

Assigns the contents of one polynomial to another.

Parameters

<code>out</code>	<code>x</code>	The assignee.

Definition at line 720 of file `nonlin_polynomials.f90`.

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

- `/home/jason/Documents/Code/nonlin/src/nonlin_polynomials.f90`

6.2 `nonlin_optimize::bfgs` Type Reference

Defines a Broyden–Fletcher–Goldfarb–Shanno (BFGS) solver for minimization of functions of multiple variables.

Inheritance diagram for `nonlin_optimize::bfgs`:

Collaboration diagram for `nonlin_optimize::bfgs`:

Public Member Functions

- procedure, public `solve` => `bfgs_solve`
Optimizes the equation.

6.2.1 Detailed Description

Defines a Broyden–Fletcher–Goldfarb–Shanno (BFGS) solver for minimization of functions of multiple variables.

Definition at line 96 of file `nonlin_optimize.f90`.

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

- `/home/jason/Documents/Code/nonlin/src/nonlin_optimize.f90`

6.3 `nonlin_solve::brent_solver` Type Reference

Defines a solver based upon Brent's method for solving an equation of one variable without using derivatives.

Inheritance diagram for `nonlin_solve::brent_solver`:

Collaboration diagram for `nonlin_solve::brent_solver`:

Public Member Functions

- procedure, public `solve` => `brent_solve`
Solves the equation.

6.3.1 Detailed Description

Defines a solver based upon Brent's method for solving an equation of one variable without using derivatives.

Definition at line 79 of file `nonlin_solve.f90`.

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

- `/home/jason/Documents/Code/nonlin/src/nonlin_solve.f90`

6.4 `nonlin_c_binding::c_polynomial` Type Reference

A C compatible type encapsulating a polynomial object.

Public Attributes

- `type(c_ptr)` `ptr`
A pointer to the polynomial object.
- `integer(i32)` `n`
The size of the polynomial object, in bytes.

6.4.1 Detailed Description

A C compatible type encapsulating a polynomial object.

Definition at line 130 of file `nonlin_c_binding.f90`.

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

- `/home/jason/Documents/Code/nonlin/src/nonlin_c_binding.f90`

6.5 `nonlin_c_binding::cfcn1var` Interface Reference

The C-friendly interface to `fcn1var`.

Public Member Functions

- `real(dp)` function **`cfcn1var`** (`x`)

6.5.1 Detailed Description

The C-friendly interface to `fcn1var`.

Parameters

<code>in</code>	<code>x</code>	The independent variable.
-----------------	----------------	---------------------------

Returns

The value of the function x .

Definition at line 29 of file `nonlin_c_binding.f90`.

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

- `/home/jason/Documents/Code/nonlin/src/nonlin_c_binding.f90`

6.6 `nonlin_c_binding::cfcn1var_helper` Type Reference

A type allowing the use of `cfcn1var` in the solver codes.

Inheritance diagram for `nonlin_c_binding::cfcn1var_helper`:

6.7 `nonlin_c_binding::fcnnvar` Interface Reference

The C-friendly interface to `fcnnvar`.

Public Member Functions

- `real(dp)` function **`cfcnvar`** (`nvar`, `x`)

6.7.1 Detailed Description

The C-friendly interface to `fcnnvar`.

Parameters

<code>in</code>	<code>nvar</code>	The number of variables.
<code>in</code>	<code>x</code>	An NVAR-element array containing the independent variables.

Returns

The value of the function at `x`.

Definition at line 68 of file `nonlin_c_binding.f90`.

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

- `/home/jason/Documents/Code/nonlin/src/nonlin_c_binding.f90`

6.8 `nonlin_c_binding::fcnnvar_helper` Type Reference

A type allowing the use of `fcnnvar` in the solver codes.

Inheritance diagram for `nonlin_c_binding::fcnnvar_helper`:

Collaboration diagram for `nonlin_c_binding::fcnnvar_helper`:

Public Member Functions

- procedure, public `fcn` => `cfnh_fcn`
Executes the routine containing the function to evaluate.
- procedure, public `is_fcn_defined` => `cfnh_is_fcn_defined`
Tests if the pointer to the function has been assigned.
- procedure, public `set_cfcn` => `cfnh_set_fcn`
Establishes a pointer to the routine containing the function.
- procedure, public `set_cgradient_fcn` => `cfnh_set_grad`
Establishes a pointer to the routine containing the gradient vector of the function.
- procedure, public `is_gradient_defined` => `cfnh_is_grad_defined`
Tests if the pointer to the routine containing the gradient has been assigned.

Public Attributes

- procedure(`cfcnnvar`), pointer, nopass `m_cfcn` => `null()`
A pointer to the target cfcnnvar routine.
- procedure(`cgradientfcn`), pointer, nopass `m_cgrad` => `null()`
A pointer to the gradient routine.

6.8.1 Detailed Description

A type allowing the use of `cfcnnvar` in the solver codes.

Definition at line 185 of file `nonlin_c_binding.f90`.

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

- `/home/jason/Documents/Code/nonlin/src/nonlin_c_binding.f90`

6.9 `nonlin_c_binding::cgradientfcn` Interface Reference

A C-friendly interface to `gradientfcn`.

Public Member Functions

- subroutine **`cgradientfcn`** (`nvar`, `x`, `g`)

6.9.1 Detailed Description

A C-friendly interface to `gradientfcn`.

Parameters

in	<i>nvar</i>	The number of variables.
in	<i>x</i>	An NVAR-element array containing the independent variables.
out	<i>g</i>	An NVAR-element array where the gradient vector will be written as output.

Definition at line 81 of file `nonlin_c_binding.f90`.

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

- `/home/jason/Documents/Code/nonlin/src/nonlin_c_binding.f90`

6.10 `nonlin_c_binding::cjacobianfcn` Interface Reference

The C-friendly interface to `jacobianfcn`.

Public Member Functions

- subroutine **`cjacobianfcn`** (`neqn`, `nvar`, `x`, `jac`)

6.10.1 Detailed Description

The C-friendly interface to `jacobianfcn`.

Parameters

in	<i>neqn</i>	The number of equations.
in	<i>nvar</i>	The number of variables.
in	<i>x</i>	The NVAR-element array containing the independent variables.
out	<i>jac</i>	An NEQN-byNVAR matrix where the Jacobian will be written.

Definition at line 56 of file `nonlin_c_binding.f90`.

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

- `/home/jason/Documents/Code/nonlin/src/nonlin_c_binding.f90`

6.11 `nonlin_c_binding::cvecfcn` Interface Reference

The C-friendly interface to `vecfcn`.

Public Member Functions

- subroutine **`cvecfcn`** (`neqn`, `nvar`, `x`, `f`)

6.11.1 Detailed Description

The C-friendly interface to `vecfcn`.

Parameters

in	<i>neqn</i>	The number of equations.
in	<i>nvar</i>	The number of variables.
in	<i>x</i>	The NVAR-element array containing the independent variables.
out	<i>f</i>	The NEQN-element array containing the function values.

Definition at line 43 of file `nonlin_c_binding.f90`.

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

- `/home/jason/Documents/Code/nonlin/src/nonlin_c_binding.f90`

6.12 `nonlin_c_binding::cvecfcn_helper` Type Reference

A type allowing the use of `cvecfcn` in the solver codes.

Inheritance diagram for `nonlin_c_binding::cvecfcn_helper`:

Collaboration diagram for `nonlin_c_binding::cvecfcn_helper`:

Public Member Functions

- procedure, public `set_cfcn` => `cvfh_set_fcn`
Establishes a pointer to the routine containing the system of equations to solve.
- procedure, public `set_jacobian` => `cvfh_set_jac`
Establishes a pointer to the routine for computing the Jacobian matrix of the system of equations. If no routine is defined, the Jacobian matrix will be computed numerically (this is the default state).
- procedure, public `is_fcn_defined` => `cvfh_is_fcn_defined`
Tests if the pointer to the subroutine containing the system of equations to solve has been assigned.
- procedure, public `is_jacobian_defined` => `cvfh_is_jac_defined`
Tests if the pointer to the subroutine containing the system of equations to solve has been assigned.
- procedure, public `fcn` => `cvfh_fcn`
Executes the routine containing the system of equations to solve. No action is taken if the pointer to the subroutine has not been defined.

Public Attributes

- procedure(`cvecfcn`), pointer, nopass `m_cfcn` => `null()`
A pointer to the target `cvecfcn` routine.
- procedure(`jacobianfcn`), pointer, nopass `m_cjac` => `null()`
A pointer to the Jacobian routine.

6.12.1 Detailed Description

A type allowing the use of `cvecfcn` in the solver codes.

Definition at line 156 of file `nonlin_c_binding.f90`.

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

- `/home/jason/Documents/Code/nonlin/src/nonlin_c_binding.f90`

6.13 `nonlin_types::equation_optimizer` Type Reference

A base class for optimization of an equation of multiple variables.

Inheritance diagram for `nonlin_types::equation_optimizer`:

Public Member Functions

- procedure, public `get_max_fcn_evals` => `oe_get_max_eval`
Gets the maximum number of function evaluations allowed.
- procedure, public `set_max_fcn_evals` => `oe_set_max_eval`
Sets the maximum number of function evaluations allowed.
- procedure, public `get_tolerance` => `oe_get_tol`
Gets the tolerance on convergence.
- procedure, public `set_tolerance` => `oe_set_tol`
Sets the tolerance on convergence.
- procedure, public `get_print_status` => `oe_get_print_status`
Gets a logical value determining if iteration status should be printed.
- procedure, public `set_print_status` => `oe_set_print_status`
Sets a logical value determining if iteration status should be printed.
- procedure(`nonlin_optimize`), deferred, pass, public `solve`
Optimizes the equation.

Private Attributes

- integer(i32) `m_maxeval` = 500
The maximum number of function evaluations allowed.
- real(dp) `m_tol` = 1.0d-12
The error tolerance used to determine convergence.
- logical `m_printstatus` = .false.
Set to true to print iteration status; else, false.

6.13.1 Detailed Description

A base class for optimization of an equation of multiple variables.

Definition at line 352 of file `nonlin_types.f90`.

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

- `/home/jason/Documents/Code/nonlin/src/nonlin_types.f90`

6.14 `nonlin_types::equation_solver` Type Reference

A base class for various solvers of nonlinear systems of equations.

Inheritance diagram for `nonlin_types::equation_solver`:

Public Member Functions

- procedure, public `get_max_fcn_evals` => `es_get_max_eval`
Gets the maximum number of function evaluations allowed during a single solve.
- procedure, public `set_max_fcn_evals` => `es_set_max_eval`
Sets the maximum number of function evaluations allowed during a single solve.
- procedure, public `get_fcn_tolerance` => `es_get_fcn_tol`
Gets the convergence on function value tolerance.
- procedure, public `set_fcn_tolerance` => `es_set_fcn_tol`
Sets the convergence on function value tolerance.
- procedure, public `get_var_tolerance` => `es_get_var_tol`
Gets the convergence on change in variable tolerance.
- procedure, public `set_var_tolerance` => `es_set_var_tol`
Sets the convergence on change in variable tolerance.
- procedure, public `get_gradient_tolerance` => `es_get_grad_tol`
Gets the convergence on slope of the gradient vector tolerance.
- procedure, public `set_gradient_tolerance` => `es_set_grad_tol`
Sets the convergence on slope of the gradient vector tolerance.
- procedure, public `get_print_status` => `es_get_print_status`
Gets a logical value determining if iteration status should be printed.
- procedure, public `set_print_status` => `es_set_print_status`
Sets a logical value determining if iteration status should be printed.
- procedure(`nonlin_solver`), deferred, pass, public `solve`
Solves the system of equations.

Private Attributes

- integer(i32) `m_maxeval` = 100
The maximum number of function evaluations allowed per solve.
- real(dp) `m_fcntol` = 1.0d-8
The convergence criteria on function values.
- real(dp) `m_xtol` = 1.0d-12
The convergence criteria on change in variable values.
- real(dp) `m_gtol` = 1.0d-12
The convergence criteria for the slope of the gradient vector.
- logical `m_printstatus` = .false.
Set to true to print iteration status; else, false.

6.14.1 Detailed Description

A base class for various solvers of nonlinear systems of equations.

Definition at line 260 of file `nonlin_types.f90`.

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

- `/home/jason/Documents/Code/nonlin/src/nonlin_types.f90`

6.15 `nonlin_types::equation_solver_1var` Type Reference

A base class for various solvers of equations of one variable.

Inheritance diagram for `nonlin_types::equation_solver_1var`:

Public Member Functions

- procedure, public `get_max_fcn_evals` => `es1_get_max_eval`
Gets the maximum number of function evaluations allowed during a single solve.
- procedure, public `set_max_fcn_evals` => `es1_set_max_eval`
Sets the maximum number of function evaluations allowed during a single solve.
- procedure, public `get_fcn_tolerance` => `es1_get_fcn_tol`
Gets the convergence on function value tolerance.
- procedure, public `set_fcn_tolerance` => `es1_set_fcn_tol`
Sets the convergence on function value tolerance.
- procedure, public `get_var_tolerance` => `es1_get_var_tol`
Gets the convergence on change in variable tolerance.
- procedure, public `set_var_tolerance` => `es1_set_var_tol`
Sets the convergence on change in variable tolerance.
- procedure, public `get_print_status` => `es1_get_print_status`
Gets a logical value determining if iteration status should be printed.
- procedure, public `set_print_status` => `es1_set_print_status`
Sets a logical value determining if iteration status should be printed.
- procedure(`nonlin_solver_1var`), deferred, pass, public `solve`
Solves the equation.

Private Attributes

- integer(i32) `m_maxeval` = 100
The maximum number of function evaluations allowed per solve.
- real(dp) `m_fcncol` = 1.0d-8
The convergence criteria on function value.
- real(dp) `m_xtol` = 1.0d-12
The convergence criteria on change in variable value.
- logical `m_printstatus` = .false.
Set to true to print iteration status; else, false.

6.15.1 Detailed Description

A base class for various solvers of equations of one variable.

Definition at line 305 of file `nonlin_types.f90`.

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

- `/home/jason/Documents/Code/nonlin/src/nonlin_types.f90`

6.16 `nonlin_types::fcn1var` Interface Reference

Describes a function of one variable.

Private Member Functions

- `real(dp)` function **`fcn1var`** (x)

6.16.1 Detailed Description

Describes a function of one variable.

Parameters

<code>in</code>	x	The independent variable.
-----------------	-----	---------------------------

Returns

The value of the function at x .

Definition at line 90 of file `nonlin_types.f90`.

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

- `/home/jason/Documents/Code/nonlin/src/nonlin_types.f90`

6.17 `nonlin_types::fcn1var_helper` Type Reference

Defines a type capable of encapsulating an equation of one variable of the form: $f(x) = 0$.

Inheritance diagram for `nonlin_types::fcn1var_helper`:

Public Member Functions

- procedure, public `fcn` => `f1h_fcn`
Executes the routine containing the function to evaluate.
- procedure, public `is_fcn_defined` => `f1h_is_fcn_defined`
Tests if the pointer to the function containing the equation to solve has been assigned.
- procedure, public `set_fcn` => `f1h_set_fcn`
Establishes a pointer to the routine containing the equations to solve.

Private Attributes

- procedure(`fcn1var`), pointer, nopass `m_fcn` => `null()`
A pointer to the target `fcn1var` routine.

6.17.1 Detailed Description

Defines a type capable of encapsulating an equation of one variable of the form: $f(x) = 0$.

Definition at line 188 of file `nonlin_types.f90`.

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

- `/home/jason/Documents/Code/nonlin/src/nonlin_types.f90`

6.18 `nonlin_types::fcnnvar` Interface Reference

Describes a function of N variables.

Private Member Functions

- `real(dp)` function **`fcnnvar`** (`x`)

6.18.1 Detailed Description

Describes a function of N variables.

Parameters

<code>in</code>	<code>x</code>	An N-element array containing the independent variables.
-----------------	----------------	--

Returns

The value of the function at x .

Definition at line 122 of file `nonlin_types.f90`.

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

- `/home/jason/Documents/Code/nonlin/src/nonlin_types.f90`

6.19 `nonlin_types::fcnnvar_helper` Type Reference

Defines a type capable of encapsulating an equation of N variables.

Inheritance diagram for `nonlin_types::fcnnvar_helper`:

Public Member Functions

- procedure, public `fcn` => `fnh_fcn`
Executes the routine containing the function to evaluate.
- procedure, public `is_fcn_defined` => `fnh_is_fcn_defined`
Tests if the pointer to the function has been assigned.
- procedure, public `set_fcn` => `fnh_set_fcn`
Establishes a pointer to the routine containing the function.
- procedure, public `get_variable_count` => `fnh_get_nvar`
Gets the number of variables in this system.
- procedure, public `set_gradient_fcn` => `fnh_set_grad`
Establishes a pointer to the routine containing the gradient vector of the function.
- procedure, public `is_gradient_defined` => `fnh_is_grad_defined`
Tests if the pointer to the routine containing the gradient has been assigned.
- procedure, public `gradient` => `fnh_grad_fcn`
Computes the gradient of the function.

Private Attributes

- procedure(`fcnnvar`), pointer, nopass `m_fcn` => `null()`
A pointer to the target fcnnvar routine.
- procedure(`gradientfcn`), pointer, nopass `m_grad` => `null()`
A pointer to the gradient routine.
- integer(`i32`) `m_nvar` = 0
The number of variables in `m_fcn`.

6.19.1 Detailed Description

Defines a type capable of encapsulating an equation of N variables.

Definition at line 206 of file `nonlin_types.f90`.

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

- `/home/jason/Documents/Code/nonlin/src/nonlin_types.f90`

6.20 `nonlin_types::gradientfcn` Interface Reference

Describes a routine capable of computing the gradient vector of an equation of N variables.

Private Member Functions

- subroutine **`gradientfcn`** (`x`, `g`)

6.20.1 Detailed Description

Describes a routine capable of computing the gradient vector of an equation of N variables.

Parameters

in	x	An N-element array containing the independent variables.
out	g	An N-element array where the gradient vector will be written as output.

Definition at line 134 of file `nonlin_types.f90`.

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

- `/home/jason/Documents/Code/nonlin/src/nonlin_types.f90`

6.21 `nonlin_types::iteration_behavior` Type Reference

Defines a set of parameters that describe the behavior of the iteration process.

Private Attributes

- integer(i32) `iter_count`
Specifies the number of iterations performed.
- integer(i32) `fcn_count`
Specifies the number of function evaluations performed.
- integer(i32) `jacobian_count`
Specifies the number of Jacobian evaluations performed.
- integer(i32) `gradient_count`
Specifies the number of gradient vector evaluations performed.
- logical(c_bool) `converge_on_fcn`
True if the solution converged as a result of a zero-valued function; else, false.
- logical(c_bool) `converge_on_chng`
True if the solution converged as a result of no appreciable change in solution points between iterations; else, false.
- logical(c_bool) `converge_on_zero_diff`
True if the solution appears to have settled on a stationary point such that the gradient of the function is zero-valued; else, false.

6.21.1 Detailed Description

Defines a set of parameters that describe the behavior of the iteration process.

Definition at line 236 of file `nonlin_types.f90`.

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

- `/home/jason/Documents/Code/nonlin/src/nonlin_types.f90`

6.22 `nonlin_types::jacobianfcn` Interface Reference

Describes a routine capable of computing the Jacobian matrix of M functions of N unknowns.

Private Member Functions

- subroutine **jacobianfcn** (x , jac)

6.22.1 Detailed Description

Describes a routine capable of computing the Jacobian matrix of M functions of N unknowns.

Parameters

in	x	An N-element array containing the independent variables.
out	jac	An M-by-N matrix where the Jacobian will be written.

Definition at line 112 of file `nonlin_types.f90`.

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

- `/home/jason/Documents/Code/nonlin/src/nonlin_types.f90`

6.23 `nonlin_least_squares::least_squares_solver` Type Reference

Defines a Levenberg-Marquardt based solver for unconstrained least-squares problems.

Inheritance diagram for `nonlin_least_squares::least_squares_solver`:

Collaboration diagram for `nonlin_least_squares::least_squares_solver`:

Public Member Functions

- procedure, public `get_step_scaling_factor` => `lss_get_factor`
Gets a factor used to scale the bounds on the initial step.
- procedure, public `set_step_scaling_factor` => `lss_set_factor`
Sets a factor used to scale the bounds on the initial step.
- procedure, public `solve` => `lss_solve`
Solves the system of equations.

Private Attributes

- `real(dp) m_factor` = 100.0d0
Initial step bounding factor.

6.23.1 Detailed Description

Defines a Levenberg-Marquardt based solver for unconstrained least-squares problems.

Definition at line 19 of file `nonlin_least_squares.f90`.

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

- `/home/jason/Documents/Code/nonlin/src/nonlin_least_squares.f90`

6.24 `nonlin_linesearch::line_search` Type Reference

Defines a type capable of performing an inexact, backtracking line search to find a point as far along the specified direction vector that is usable for unconstrained minimization problems.

Public Member Functions

- procedure, public [get_max_fcn_evals](#) => [ls_get_max_eval](#)
Gets the maximum number of function evaluations allowed during a single line search.
- procedure, public [set_max_fcn_evals](#) => [ls_set_max_eval](#)
Sets the maximum number of function evaluations allowed during a single line search.
- procedure, public [get_scaling_factor](#) => [ls_get_scale](#)
Gets the scaling of the product of the gradient and direction vectors.
- procedure, public [set_scaling_factor](#) => [ls_set_scale](#)
Sets the scaling of the product of the gradient and direction vectors.
- procedure, public [get_distance_factor](#) => [ls_get_dist](#)
Gets a distance factor defining the minimum distance along the search direction vector is practical.
- procedure, public [set_distance_factor](#) => [ls_set_dist](#)
Sets a distance factor defining the minimum distance along the search direction vector is practical.
- generic, public [search](#) => [ls_search_mimo](#), [ls_search_miso](#)
Utilizes an inexact, backtracking line search based on the Armijo-Goldstein condition to find a point as far along the specified direction vector that is usable for unconstrained minimization problems.

Private Member Functions

- procedure [ls_search_mimo](#)
- procedure [ls_search_miso](#)

Private Attributes

- integer(i32) [m_maxeval](#) = 100
The maximum number of function evaluations allowed during a single line search.
- real(dp) [m_alpha](#) = 1.0d-4
*Defines the scaling of the product of the gradient and direction vectors such that $F(X + \text{LAMBDA} * P) \leq F(X) + \text{LAMBDA} * \text{ALPHA} * P^T * G$, where P is the search direction vector, G is the gradient vector, and LAMBDA is the scaling factor. The parameter must exist on the set $(0, 1)$. A value of $1e-4$ is typically a good starting point.*
- real(dp) [m_factor](#) = 0.1d0
*Defines a minimum factor X used to determine a minimum value LAMBDA such that $\text{MIN}(\text{LAMBDA}) = X * \text{LAMBDA}$, where LAMBDA defines the distance along the line search direction assuming a value of one means the full length of the direction vector is traversed. As such, the value must exist on the set $(0, 1)$; however, for practical considerations, the minimum value should be limited to 0.1 such that the value must exist on the set $[0.1, 1)$.*

6.24.1 Detailed Description

Defines a type capable of performing an inexact, backtracking line search to find a point as far along the specified direction vector that is usable for unconstrained minimization problems.

See Also

- [Wikipedia](#)
- [Oxford Lecture Notes](#)
- [Northwestern University - Line Search](#)
- [Northwestern University - Trust Region Methods](#)
- [Wolfram](#)
- [Numerical Recipes](#)

Definition at line 34 of file `nonlin_linesearch.f90`.

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

- `/home/jason/Documents/Code/nonlin/src/nonlin_linesearch.f90`

6.25 `nonlin_c_binding::line_search_control` Type Reference

Defines a set of line search controls.

Public Attributes

- integer(i32) `max_evals`
The maximum number of function evaluations allowed per search.
- real(dp) `alpha`
*Defines the scaling of the product of the gradient and direction vectors such that $F(X + \text{LAMBDA} * P) \leq F(X) + \text{LAMBDA} * \text{ALPHA} * P^T * G$, where P is the search direction vector, G is the gradient vector, and LAMBDA is the scaling factor. The parameter must exist on the set $(0, 1)$. A value of $1e-4$ is typically a good starting point.*
- real(dp) `factor`
*Defines a minimum factor X used to determine a minimum value LAMBDA such that $\text{MIN}(\text{LAMBDA}) = X * \text{LAMBDA}$, where LAMBDA defines the distance along the line search direction assuming a value of one means the full length of the direction vector is traversed. As such, the value must exist on the set $(0, 1)$; however, for practical considerations, the minimum value should be limited to 0.1 such that the value must exist on the set $[0.1, 1)$.*

6.25.1 Detailed Description

Defines a set of line search controls.

Definition at line 108 of file `nonlin_c_binding.f90`.

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

- `/home/jason/Documents/Code/nonlin/src/nonlin_c_binding.f90`

6.26 `nonlin_optimize::line_search_optimizer` Type Reference

A class describing equation optimizers that use a line search algorithm to improve convergence behavior.

Inheritance diagram for `nonlin_optimize::line_search_optimizer`:

Collaboration diagram for `nonlin_optimize::line_search_optimizer`:

Public Member Functions

- procedure, public `get_line_search` => `Iso_get_line_search`
Gets the line search module.
- procedure, public `set_line_search` => `Iso_set_line_search`
Sets the line search module.
- procedure, public `set_default_line_search` => `Iso_set_default`
Establishes a default line_search object for the line search module.
- procedure, public `is_line_search_defined` => `Iso_is_line_search_defined`
Tests to see if a line search module is defined.
- procedure, public `get_use_line_search` => `Iso_get_use_search`
Gets a value determining if a line-search should be employed.
- procedure, public `set_use_line_search` => `Iso_set_use_search`
Sets a value determining if a line-search should be employed.
- procedure, public `get_var_tolerance` => `Iso_get_var_tol`
Gets the convergence on change in variable tolerance.
- procedure, public `set_var_tolerance` => `Iso_set_var_tol`
Sets the convergence on change in variable tolerance.

Private Attributes

- class([line_search](#)), allocatable [m_linesearch](#)
The line search object.
- logical [m_uselinesearch](#) = .true.
Set to true if a line search should be used regardless of the status of [m_lineSearch](#).
- real(dp) [m_xtol](#) = 1.0d-12
The convergence criteria on change in variable.

6.26.1 Detailed Description

A class describing equation optimizers that use a line search algorithm to improve convergence behavior.

Definition at line 63 of file `nonlin_optimize.f90`.

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

- `/home/jason/Documents/Code/nonlin/src/nonlin_optimize.f90`

6.27 `nonlin_solve::line_search_solver` Type Reference

A class describing nonlinear solvers that use a line search algorithm to improve convergence behavior.

Inheritance diagram for `nonlin_solve::line_search_solver`:

Collaboration diagram for `nonlin_solve::line_search_solver`:

Public Member Functions

- procedure, public [get_line_search](#) => [lss_get_line_search](#)
Gets the line search module.
- procedure, public [set_line_search](#) => [lss_set_line_search](#)
Sets the line search module.
- procedure, public [set_default_line_search](#) => [lss_set_default](#)
Establishes a default [line_search](#) object for the line search module.
- procedure, public [is_line_search_defined](#) => [lss_is_line_search_defined](#)
Tests to see if a line search module is defined.
- procedure, public [get_use_line_search](#) => [lss_get_use_search](#)
Gets a value determining if a line-search should be employed.
- procedure, public [set_use_line_search](#) => [lss_set_use_search](#)
Sets a value determining if a line-search should be employed.

Private Attributes

- class([line_search](#)), allocatable [m_linesearch](#)
The line search module.
- logical [m_uselinesearch](#) = .true.
Set to true if a line search should be used regardless of the status of [m_lineSearch](#).

6.27.1 Detailed Description

A class describing nonlinear solvers that use a line search algorithm to improve convergence behavior.

Definition at line 27 of file `nonlin_solve.f90`.

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

- `/home/jason/Documents/Code/nonlin/src/nonlin_solve.f90`

6.28 `nonlin_optimize::nelder_mead` Type Reference

Defines a solver based upon Nelder and Mead's simplex algorithm for minimization of functions of multiple variables.

Inheritance diagram for `nonlin_optimize::nelder_mead`:

Collaboration diagram for `nonlin_optimize::nelder_mead`:

Public Member Functions

- procedure, public `solve` => `nm_solve`
Optimizes the equation.
- procedure, public `get_simplex` => `nm_get_simplex`
Gets an N-by-(N+1) matrix containing the current simplex.
- procedure, public `set_simplex` => `nm_set_simplex`
Sets an N-by-(N+1) matrix containing the current simplex.
- procedure, public `get_initial_size` => `nm_get_size`
Gets the size of the initial simplex.
- procedure, public `set_initial_size` => `nm_set_size`
Sets the size of the initial simplex.

Private Member Functions

- procedure, private `extrapolate` => `nm_extrapolate`
Extrapolates by the specified factor through the simplex across from the largest point. If the extrapolation results in a better estimate, the current high point is replaced with the new estimate.

Private Attributes

- `real(dp)`, `dimension(:, :)`, allocatable `m_simplex`
The simplex vertices.
- `real(dp)` `m_initsize` = 1.0d0
A scaling parameter used to define the size of the simplex in each coordinate direction.

6.28.1 Detailed Description

Defines a solver based upon Nelder and Mead's simplex algorithm for minimization of functions of multiple variables.

Definition at line 34 of file `nonlin_optimize.f90`.

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

- `/home/jason/Documents/Code/nonlin/src/nonlin_optimize.f90`

6.29 `nonlin_solve::newton_solver` Type Reference

Defines a Newton solver.

Inheritance diagram for `nonlin_solve::newton_solver`:

Collaboration diagram for `nonlin_solve::newton_solver`:

Public Member Functions

- procedure, public `solve` => `ns_solve`
Solves the system of equations.

6.29.1 Detailed Description

Defines a Newton solver.

Definition at line 70 of file `nonlin_solve.f90`.

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

- `/home/jason/Documents/Code/nonlin/src/nonlin_solve.f90`

6.30 `nonlin_types::nonlin_optimize` Interface Reference

Describes the interface of a routine for optimizing an equation of N variables.

Private Member Functions

- subroutine **`nonlin_optimize`** (`this`, `fcn`, `x`, `fout`, `ib`, `err`)

6.30.1 Detailed Description

Describes the interface of a routine for optimizing an equation of N variables.

Parameters

<code>in, out</code>	<i>this</i>	The <code>equation_optimizer</code> -based object.
<code>in</code>	<i>fcn</i>	The <code>fcnvar_helper</code> object containing the equation to optimize.
<code>in, out</code>	<i>x</i>	On input, the initial guess at the optimal point. On output, the updated optimal point estimate.
<code>out</code>	<i>fout</i>	An optional output, that if provided, returns the value of the function at x .
<code>out</code>	<i>ib</i>	An optional output, that if provided, allows the caller to obtain iteration performance statistics.
<code>out</code>	<i>err</i>	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. The possible error codes returned will likely vary from solver to solver.

Definition at line 469 of file `nonlin_types.f90`.

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

- `/home/jason/Documents/Code/nonlin/src/nonlin_types.f90`

6.31 `nonlin_types::nonlin_solver` Interface Reference

Describes the interface of a nonlinear equation solver.

Private Member Functions

- subroutine **`nonlin_solver`** (`this`, `fcn`, `x`, `fvec`, `ib`, `err`)

6.31.1 Detailed Description

Describes the interface of a nonlinear equation solver.

Parameters

<code>in, out</code>	<i>this</i>	The <code>equation_solver</code> -based object.
<code>in</code>	<i>fcn</i>	The <code>vecfcn_helper</code> object containing the equations to solve.
<code>in, out</code>	<i>x</i>	On input, an N-element array containing an initial estimate to the solution. On output, the updated solution estimate. N is the number of variables.
<code>out</code>	<i>fvec</i>	An M-element array that, on output, will contain the values of each equation as evaluated at the variable values given in x .
<code>out</code>	<i>ib</i>	An optional output, that if provided, allows the caller to obtain iteration performance statistics.
<code>out</code>	<i>err</i>	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. The possible error codes returned will likely vary from solver to solver.

Definition at line 402 of file `nonlin_types.f90`.

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

- `/home/jason/Documents/Code/nonlin/src/nonlin_types.f90`

6.32 `nonlin_types::nonlin_solver_1var` Interface Reference

Describes the interface of a solver for an equation of one variable.

Private Member Functions

- subroutine **`nonlin_solver_1var`** (`this`, `fcn`, `x`, `lim`, `f`, `ib`, `err`)

6.32.1 Detailed Description

Describes the interface of a solver for an equation of one variable.

Parameters

<code>in, out</code>	<i>this</i>	The <code>equation_solver_1var</code> -based object.
<code>in</code>	<i>fcn</i>	The fcn1var_helper object containing the equation to solve.
<code>in, out</code>	<i>x</i>	On input the initial guess at the solution. On output the updated solution estimate.
<code>in</code>	<i>lim</i>	A value_pair object defining the search limits.
<code>out</code>	<i>f</i>	An optional parameter used to return the function residual as computed at <code>x</code> .
<code>out</code>	<i>ib</i>	An optional output, that if provided, allows the caller to obtain iteration performance statistics.
<code>out</code>	<i>err</i>	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. The possible error codes returned will likely vary from solver to solver.

Definition at line 435 of file `nonlin_types.f90`.

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

- `/home/jason/Documents/Code/nonlin/src/nonlin_types.f90`

6.33 `nonlin_polynomials::operator(*)` Interface Reference

Defines polynomial multiplication.

Private Member Functions

- type([polynomial](#)) function [poly_poly_mult](#) (`x`, `y`)
Multiplies two polynomials.
- type([polynomial](#)) function [poly_dbl_mult](#) (`x`, `y`)
Multiplies a polynomial by a scalar value.
- type([polynomial](#)) function [dbl_poly_mult](#) (`x`, `y`)
Multiplies a polynomial by a scalar value.

6.33.1 Detailed Description

Defines polynomial multiplication.

Definition at line 48 of file `nonlin_polynomials.f90`.

6.33.2 Member Function/Subroutine Documentation

6.33.2.1 `type(polynomial) function nonlin_polynomials::operator(*)::dbl_poly_mult (real(dp), intent(in) x, class(polynomial), intent(in) y) [private]`

Multiplies a polynomial by a scalar value.

Parameters

in	<i>x</i>	The scalar value.
in	<i>y</i>	The polynomial.

Returns

The resulting polynomial.

Definition at line 931 of file `nonlin_polynomials.f90`.

6.33.2.2 `type(polynomial) function nonlin_polynomials::operator(*)::poly_dbl_mult (class(polynomial), intent(in) x, real(dp), intent(in) y) [private]`

Multiplies a polynomial by a scalar value.

Parameters

in	<i>x</i>	The polynomial.
in	<i>y</i>	The scalar value.

Returns

The resulting polynomial.

Definition at line 907 of file `nonlin_polynomials.f90`.

6.33.2.3 `type(polynomial) function nonlin_polynomials::operator(*)::poly_poly_mult (class(polynomial), intent(in) x, class(polynomial), intent(in) y) [private]`

Multiplies two polynomials.

Parameters

in	<i>x</i>	The left-hand-side argument.
in	<i>y</i>	The right-hand-side argument.

Returns

The resulting polynomial.

Definition at line 877 of file `nonlin_polynomials.f90`.

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

- `/home/jason/Documents/Code/nonlin/src/nonlin_polynomials.f90`

6.34 nonlin_polynomials::operator(+) Interface Reference

Defines polynomial addition.

Private Member Functions

- `type(polynomial)` function `poly_poly_add` (`x`, `y`)
Adds two polynomials.

6.34.1 Detailed Description

Defines polynomial addition.

Definition at line 38 of file `nonlin_polynomials.f90`.

6.34.2 Member Function/Subroutine Documentation

6.34.2.1 `type(polynomial)` function `nonlin_polynomials::operator(+):poly_poly_add` (`class(polynomial)`, `intent(in)` `x`, `class(polynomial)`, `intent(in)` `y`) `[private]`

Adds two polynomials.

Parameters

<code>in</code>	<code>x</code>	The left-hand-side argument.
<code>in</code>	<code>y</code>	The right-hand-side argument.

Returns

The resulting polynomial.

Definition at line 763 of file `nonlin_polynomials.f90`.

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

- `/home/jason/Documents/Code/nonlin/src/nonlin_polynomials.f90`

6.35 `nonlin_polynomials::operator(-)` Interface Reference

Defines polynomial subtraction.

Private Member Functions

- `type(polynomial)` function `poly_poly_subtract` (`x`, `y`)
Subtracts two polynomials.

6.35.1 Detailed Description

Defines polynomial subtraction.

Definition at line 43 of file `nonlin_polynomials.f90`.

6.35.2 Member Function/Subroutine Documentation

6.35.2.1 `type(polynomial)` function `nonlin_polynomials::operator(-)::poly_poly_subtract` (`class(polynomial)`, `intent(in)` `x`, `class(polynomial)`, `intent(in)` `y`) `[private]`

Subtracts two polynomials.

Parameters

<code>in</code>	<code>x</code>	The left-hand-side argument.
<code>in</code>	<code>y</code>	The right-hand-side argument.

Returns

The resulting polynomial.

Definition at line 820 of file `nonlin_polynomials.f90`.

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

- `/home/jason/Documents/Code/nonlin/src/nonlin_polynomials.f90`

6.36 `nonlin_polynomials::polynomial` Type Reference

Defines a polynomial, and associated routines for performing polynomial operations.

Public Member Functions

- procedure, public `initialize` => `init_poly`
Initializes the polynomial instance.
- procedure, public `order` => `get_poly_order`
Returns the order of the polynomial object.
- procedure, public `fit` => `poly_fit`
Fits a polynomial of the specified order to a data set.
- procedure, public `fit_thru_zero` => `poly_fit_thru_zero`
Fits a polynomial of the specified order that passes through zero to a data set.
- generic, public `evaluate` => `evaluate_real`, `evaluate_complex`
Evaluates a polynomial at the specified points.
- procedure, public `companion_mtx` => `poly_companion_mtx`
Returns the companion matrix for the polynomial.
- procedure, public `roots` => `poly_roots`
Computes all the roots of a polynomial.
- procedure, public `get` => `get_poly_coefficient`
Gets the requested polynomial coefficient.
- procedure, public `get_all` => `get_poly_coefficients`
Gets an array containing all the coefficients of the polynomial.
- procedure, public `set` => `set_poly_coefficient`
Sets the requested polynomial coefficient by index.

Private Member Functions

- procedure `evaluate_real` => `poly_eval_double`
- procedure `evaluate_complex` => `poly_eval_complex`

Private Attributes

- `real(dp)`, `dimension(:)`, allocatable `m_coeffs`
An array that contains the polynomial coefficients in ascending order.

6.36.1 Detailed Description

Defines a polynomial, and associated routines for performing polynomial operations.

Definition at line 59 of file `nonlin_polynomials.f90`.

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

- `/home/jason/Documents/Code/nonlin/src/nonlin_polynomials.f90`

6.37 `nonlin_solve::quasi_newton_solver` Type Reference

Defines a quasi-Newton type solver based upon Broyden's method.

Inheritance diagram for `nonlin_solve::quasi_newton_solver`:

Collaboration diagram for `nonlin_solve::quasi_newton_solver`:

Public Member Functions

- procedure, public `solve` => `qns_solve`
Solves the system of equations.
- procedure, public `get_jacobian_interval` => `qns_get_jac_interval`
Gets the number of iterations that may pass before forcing a recalculation of the Jacobian matrix.
- procedure, public `set_jacobian_interval` => `qns_set_jac_interval`
Sets the number of iterations that may pass before forcing a recalculation of the Jacobian matrix.

Private Attributes

- integer(i32) `m_delta` = 5
The number of iterations that may pass between Jacobian calculation.

6.37.1 Detailed Description

Defines a quasi-Newton type solver based upon Broyden's method.

Definition at line 53 of file `nonlin_solve.f90`.

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

- `/home/jason/Documents/Code/nonlin/src/nonlin_solve.f90`

6.38 `nonlin_c_binding::solver_control` Type Reference

Defines a set of solver control information.

Public Attributes

- integer(i32) `max_evals`
The maximum number of function evaluations allowed.
- real(dp) `fcn_tolerance`
The convergence criteria on function values.
- real(dp) `var_tolerance`
The convergence criteria on change in variable values.
- real(dp) `grad_tolerance`
The convergence criteria for the slope of the gradient vector.
- logical(c_bool) `print_status`
Controls whether iteration status is printed.

6.38.1 Detailed Description

Defines a set of solver control information.

Definition at line 93 of file `nonlin_c_binding.f90`.

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

- `/home/jason/Documents/Code/nonlin/src/nonlin_c_binding.f90`

6.39 `nonlin_types::value_pair` Type Reference

Defines a pair of numeric values.

Private Attributes

- `real(dp) x1`
Value 1.
- `real(dp) x2`
Value 2.

6.39.1 Detailed Description

Defines a pair of numeric values.

Definition at line 342 of file `nonlin_types.f90`.

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

- `/home/jason/Documents/Code/nonlin/src/nonlin_types.f90`

6.40 `nonlin_types::vecfcn` Interface Reference

Describes an M-element vector-valued function of N-variables.

Private Member Functions

- subroutine **vecfcn** (*x*, *f*)

6.40.1 Detailed Description

Describes an M-element vector-valued function of N-variables.

Parameters

<i>in</i>	<i>x</i>	An N-element array containing the independent variables.
<i>out</i>	<i>f</i>	An M-element array that, on output, contains the values of the M functions.

Definition at line 101 of file `nonlin_types.f90`.

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

- `/home/jason/Documents/Code/nonlin/src/nonlin_types.f90`

6.41 `nonlin_types::vecfcn_helper` Type Reference

Defines a type capable of encapsulating a system of nonlinear equations of the form: $F(X) = 0$.

Inheritance diagram for `nonlin_types::vecfcn_helper`:

Public Member Functions

- procedure, public `set_fcn` => `vfh_set_fcn`
Establishes a pointer to the routine containing the system of equations to solve.
- procedure, public `set_jacobian` => `vfh_set_jac`
Establishes a pointer to the routine for computing the Jacobian matrix of the system of equations. If no routine is defined, the Jacobian matrix will be computed numerically (this is the default state).
- procedure, public `is_fcn_defined` => `vfh_is_fcn_defined`
Tests if the pointer to the subroutine containing the system of equations to solve has been assigned.
- procedure, public `is_jacobian_defined` => `vfh_is_jac_defined`
Tests if the pointer to the subroutine containing the system of equations to solve has been assigned.
- procedure, public `fcn` => `vfh_fcn`
Executes the routine containing the system of equations to solve. No action is taken if the pointer to the subroutine has not been defined.
- procedure, public `jacobian` => `vfh_jac_fcn`
Executes the routine containing the Jacobian matrix if supplied. If not supplied, the Jacobian is computed via finite differences.
- procedure, public `get_equation_count` => `vfh_get_nfcn`
Gets the number of equations in this system.
- procedure, public `get_variable_count` => `vfh_get_nvar`
Gets the number of variables in this system.

Private Attributes

- procedure(`vecfcn`), pointer, nopass `m_fcn` => `null()`
A pointer to the target vecfcn routine.
- procedure(`jacobianfcn`), pointer, nopass `m_jac` => `null()`
A pointer to the jacobian routine - null if no routine is supplied.
- integer(`i32`) `m_nfcn` = 0
The number of functions in m_fcn.
- integer(`i32`) `m_nvar` = 0
The number of variables in m_fcn.

6.41.1 Detailed Description

Defines a type capable of encapsulating a system of nonlinear equations of the form: $F(X) = 0$.

Definition at line 146 of file `nonlin_types.f90`.

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

- `/home/jason/Documents/Code/nonlin/src/nonlin_types.f90`

Index

- alloc_polynomial
 - nonlin_c_binding, 8
- bfgs_c
 - nonlin_c_binding, 9
- bfgs_solve
 - nonlin_optimize, 33
- brent_solve
 - nonlin_solve, 50
- brent_solver_c
 - nonlin_c_binding, 9
- cf1h_fcn
 - nonlin_c_binding, 10
- cf1h_is_fcn_defined
 - nonlin_c_binding, 10
- cf1h_set_fcn
 - nonlin_c_binding, 10
- cfnh_fcn
 - nonlin_c_binding, 11
- cfnh_is_fcn_defined
 - nonlin_c_binding, 11
- cfnh_is_grad_defined
 - nonlin_c_binding, 11
- cfnh_set_fcn
 - nonlin_c_binding, 12
- cfnh_set_grad
 - nonlin_c_binding, 12
- cvfh_fcn
 - nonlin_c_binding, 12
- cvfh_is_fcn_defined
 - nonlin_c_binding, 12
- cvfh_is_jac_defined
 - nonlin_c_binding, 13
- cvfh_set_fcn
 - nonlin_c_binding, 13
- cvfh_set_jac
 - nonlin_c_binding, 13
- dbl_poly_mult
 - nonlin_polynomials, 41
 - nonlin_polynomials::operator(*), 95
- es1_get_fcn_tol
 - nonlin_types, 60
- es1_get_max_eval
 - nonlin_types, 60
- es1_get_print_status
 - nonlin_types, 61
- es1_get_var_tol
 - nonlin_types, 61
- es1_set_fcn_tol
 - nonlin_types, 61
- es1_set_max_eval
 - nonlin_types, 61
- es1_set_print_status
 - nonlin_types, 62
- es1_set_var_tol
 - nonlin_types, 62
- es_get_fcn_tol
 - nonlin_types, 62
- es_get_grad_tol
 - nonlin_types, 62
- es_get_max_eval
 - nonlin_types, 63
- es_get_print_status
 - nonlin_types, 63
- es_get_var_tol
 - nonlin_types, 63
- es_set_fcn_tol
 - nonlin_types, 64
- es_set_grad_tol
 - nonlin_types, 64
- es_set_max_eval
 - nonlin_types, 64
- es_set_print_status
 - nonlin_types, 64
- es_set_var_tol
 - nonlin_types, 65
- evaluate_polynomial
 - nonlin_c_binding, 13
- evaluate_polynomial_cmplx
 - nonlin_c_binding, 14
- f1h_fcn
 - nonlin_types, 65
- f1h_is_fcn_defined
 - nonlin_types, 65
- f1h_set_fcn
 - nonlin_types, 66
- fit_polynomial
 - nonlin_c_binding, 14
- fit_polynomial_thru_zero
 - nonlin_c_binding, 14
- fnh_fcn
 - nonlin_types, 66
- fnh_get_nvar
 - nonlin_types, 66
- fnh_grad_fcn
 - nonlin_types, 66
- fnh_is_fcn_defined
 - nonlin_types, 67
- fnh_is_grad_defined
 - nonlin_types, 67
- fnh_set_fcn
 - nonlin_types, 67
- fnh_set_grad
 - nonlin_types, 68
- free_polynomial
 - nonlin_c_binding, 15
- get_poly_coefficient

- nonlin_polynomials, 42
- get_poly_coefficients
 - nonlin_polynomials, 42
- get_poly_order
 - nonlin_polynomials, 42
- get_polynomial
 - nonlin_c_binding, 15
- get_polynomial_coefficient
 - nonlin_c_binding, 15
- get_polynomial_order_c
 - nonlin_c_binding, 16
- init_poly
 - nonlin_polynomials, 43
- levmarq_c
 - nonlin_c_binding, 16
- limit_search_vector
 - nonlin_linesearch, 28
- lmfactor
 - nonlin_least_squares, 22
- lmpar
 - nonlin_least_squares, 23
- lmsolve
 - nonlin_least_squares, 23
- ls_get_dist
 - nonlin_linesearch, 28
- ls_get_max_eval
 - nonlin_linesearch, 29
- ls_get_scale
 - nonlin_linesearch, 29
- ls_search_mimo
 - nonlin_linesearch, 29
- ls_search_miso
 - nonlin_linesearch, 30
- ls_set_dist
 - nonlin_linesearch, 31
- ls_set_max_eval
 - nonlin_linesearch, 31
- ls_set_scale
 - nonlin_linesearch, 31
- lso_get_line_search
 - nonlin_optimize, 35
- lso_get_use_search
 - nonlin_optimize, 35
- lso_get_var_tol
 - nonlin_optimize, 35
- lso_is_line_search_defined
 - nonlin_optimize, 35
- lso_set_default
 - nonlin_optimize, 36
- lso_set_line_search
 - nonlin_optimize, 36
- lso_set_use_search
 - nonlin_optimize, 36
- lso_set_var_tol
 - nonlin_optimize, 36
- lss_get_factor
 - nonlin_least_squares, 24
- lss_get_line_search
 - nonlin_solve, 51
- lss_get_use_search
 - nonlin_solve, 51
- lss_is_line_search_defined
 - nonlin_solve, 52
- lss_set_default
 - nonlin_solve, 52
- lss_set_factor
 - nonlin_least_squares, 24
- lss_set_line_search
 - nonlin_solve, 52
- lss_set_use_search
 - nonlin_solve, 52
- lss_solve
 - nonlin_least_squares, 25
- min_backtrack_search
 - nonlin_linesearch, 32
- nelder_mead_c
 - nonlin_c_binding, 17
- newton_c
 - nonlin_c_binding, 18
- nm_extrapolate
 - nonlin_optimize, 37
- nm_get_simplex
 - nonlin_optimize, 37
- nm_get_size
 - nonlin_optimize, 37
- nm_set_simplex
 - nonlin_optimize, 38
- nm_set_size
 - nonlin_optimize, 38
- nm_solve
 - nonlin_optimize, 38
- nonlin_c_binding, 6
 - alloc_polynomial, 8
 - bfgs_c, 9
 - brent_solver_c, 9
 - cf1h_fcn, 10
 - cf1h_is_fcn_defined, 10
 - cf1h_set_fcn, 10
 - cfnh_fcn, 11
 - cfnh_is_fcn_defined, 11
 - cfnh_is_grad_defined, 11
 - cfnh_set_fcn, 12
 - cfnh_set_grad, 12
 - cvfh_fcn, 12
 - cvfh_is_fcn_defined, 12
 - cvfh_is_jac_defined, 13
 - cvfh_set_fcn, 13
 - cvfh_set_jac, 13
 - evaluate_polynomial, 13
 - evaluate_polynomial_cmplx, 14
 - fit_polynomial, 14
 - fit_polynomial_thru_zero, 14
 - free_polynomial, 15
 - get_polynomial, 15

- get_polynomial_coefficient, 15
- get_polynomial_order_c, 16
- levmarq_c, 16
- nelder_mead_c, 17
- newton_c, 18
- polynomial_add, 18
- polynomial_copy, 19
- polynomial_multiply, 19
- polynomial_roots_c, 19
- polynomial_subtract, 20
- quasi_newton_c, 20
- set_nonlin_defaults, 21
- set_nonlin_ls_defaults, 21
- set_polynomial_set_coefficient, 21
- nonlin_c_binding::c_polynomial, 75
- nonlin_c_binding::cfcn1var, 75
- nonlin_c_binding::cfcn1var_helper, 76
- nonlin_c_binding::cfcnnvar, 76
- nonlin_c_binding::cfcnnvar_helper, 76
- nonlin_c_binding::cgradientfcn, 77
- nonlin_c_binding::cjacobianfcn, 78
- nonlin_c_binding::cvecfcn, 78
- nonlin_c_binding::cvecfcn_helper, 79
- nonlin_c_binding::line_search_control, 89
- nonlin_c_binding::solver_control, 99
- nonlin_least_squares, 22
 - lmfactor, 22
 - lmpar, 23
 - lmsolve, 23
 - lss_get_factor, 24
 - lss_set_factor, 24
 - lss_solve, 25
- nonlin_least_squares::least_squares_solver, 87
- nonlin_linesearch, 27
 - limit_search_vector, 28
 - ls_get_dist, 28
 - ls_get_max_eval, 29
 - ls_get_scale, 29
 - ls_search_mimo, 29
 - ls_search_miso, 30
 - ls_set_dist, 31
 - ls_set_max_eval, 31
 - ls_set_scale, 31
 - min_backtrack_search, 32
- nonlin_linesearch::line_search, 87
- nonlin_optimize, 32
 - bfgs_solve, 33
 - iso_get_line_search, 35
 - iso_get_use_search, 35
 - iso_get_var_tol, 35
 - iso_is_line_search_defined, 35
 - iso_set_default, 36
 - iso_set_line_search, 36
 - iso_set_use_search, 36
 - iso_set_var_tol, 36
 - nm_extrapolate, 37
 - nm_get_simplex, 37
 - nm_get_size, 37
 - nm_set_simplex, 38
 - nm_set_size, 38
 - nm_solve, 38
- nonlin_optimize::bfgs, 74
- nonlin_optimize::line_search_optimizer, 89
- nonlin_optimize::nelder_mead, 91
- nonlin_polynomials, 40
 - dbl_poly_mult, 41
 - get_poly_coefficient, 42
 - get_poly_coefficients, 42
 - get_poly_order, 42
 - init_poly, 43
 - poly_companion_mtx, 43
 - poly_dbl_equals, 43
 - poly_dbl_mult, 44
 - poly_equals, 44
 - poly_eval_complex, 44
 - poly_eval_double, 44
 - poly_fit, 45
 - poly_fit_thru_zero, 46
 - poly_poly_add, 46
 - poly_poly_mult, 47
 - poly_poly_subtract, 47
 - poly_roots, 47
 - set_poly_coefficient, 48
- nonlin_polynomials::assignment(=), 73
 - poly_dbl_equals, 73
 - poly_equals, 73
- nonlin_polynomials::operator(*), 94
 - dbl_poly_mult, 95
 - poly_dbl_mult, 95
 - poly_poly_mult, 95
- nonlin_polynomials::operator(+), 96
 - poly_poly_add, 96
- nonlin_polynomials::operator(-), 97
 - poly_poly_subtract, 97
- nonlin_polynomials::polynomial, 97
- nonlin_solve, 49
 - brent_solve, 50
 - lss_get_line_search, 51
 - lss_get_use_search, 51
 - lss_is_line_search_defined, 52
 - lss_set_default, 52
 - lss_set_line_search, 52
 - lss_set_use_search, 52
 - ns_solve, 53
 - qns_get_jac_interval, 54
 - qns_set_jac_interval, 54
 - qns_solve, 55
 - test_convergence, 56
- nonlin_solve::brent_solver, 74
- nonlin_solve::line_search_solver, 90
- nonlin_solve::newton_solver, 92
- nonlin_solve::quasi_newton_solver, 98
- nonlin_types, 57
 - es1_get_fcn_tol, 60
 - es1_get_max_eval, 60
 - es1_get_print_status, 61

- es1_get_var_tol, 61
- es1_set_fcn_tol, 61
- es1_set_max_eval, 61
- es1_set_print_status, 62
- es1_set_var_tol, 62
- es_get_fcn_tol, 62
- es_get_grad_tol, 62
- es_get_max_eval, 63
- es_get_print_status, 63
- es_get_var_tol, 63
- es_set_fcn_tol, 64
- es_set_grad_tol, 64
- es_set_max_eval, 64
- es_set_print_status, 64
- es_set_var_tol, 65
- f1h_fcn, 65
- f1h_is_fcn_defined, 65
- f1h_set_fcn, 66
- fnh_fcn, 66
- fnh_get_nvar, 66
- fnh_grad_fcn, 66
- fnh_is_fcn_defined, 67
- fnh_is_grad_defined, 67
- fnh_set_fcn, 67
- fnh_set_grad, 68
- oe_get_max_eval, 68
- oe_get_print_status, 68
- oe_get_tol, 69
- oe_set_max_eval, 69
- oe_set_print_status, 69
- oe_set_tol, 69
- poly_companion_mtx
 - nonlin_polynomials, 43
- poly_dbl_equals
 - nonlin_polynomials, 43
 - nonlin_polynomials::assignment(=), 73
- poly_dbl_mult
 - nonlin_polynomials, 44
 - nonlin_polynomials::operator(*), 95
- poly_equals
 - nonlin_polynomials, 44
 - nonlin_polynomials::assignment(=), 73
- poly_eval_complex
 - nonlin_polynomials, 44
- poly_eval_double
 - nonlin_polynomials, 44
- poly_fit
 - nonlin_polynomials, 45
- poly_fit_thru_zero
 - nonlin_polynomials, 46
- poly_poly_add
 - nonlin_polynomials, 46
 - nonlin_polynomials::operator(+), 96
- poly_poly_mult
 - nonlin_polynomials, 47
 - nonlin_polynomials::operator(*), 95
- poly_poly_subtract
 - nonlin_polynomials, 47
 - nonlin_polynomials::operator(-), 97
- poly_roots
 - nonlin_polynomials, 47
- polynomial_add
 - nonlin_c_binding, 18
- polynomial_copy
 - nonlin_c_binding, 19
- polynomial_multiply
 - nonlin_c_binding, 19
- polynomial_roots_c
 - nonlin_c_binding, 19
- polynomial_subtract
 - nonlin_c_binding, 20
- print_status
 - nonlin_types, 70
- qns_get_jac_interval
 - nonlin_solve, 54
- qns_set_jac_interval
- ns_solve
 - nonlin_solve, 53
- nonlin_types::equation_optimizer, 80
- nonlin_types::equation_solver, 80
- nonlin_types::equation_solver_1var, 82
- nonlin_types::fcn1var, 83
- nonlin_types::fcn1var_helper, 83
- nonlin_types::fcnnvar, 84
- nonlin_types::fcnnvar_helper, 84
- nonlin_types::gradientfcn, 85
- nonlin_types::iteration_behavior, 86
- nonlin_types::jacobianfcn, 86
- nonlin_types::nonlin_optimize, 92
- nonlin_types::nonlin_solver, 93
- nonlin_types::nonlin_solver_1var, 94
- nonlin_types::value_pair, 100
- nonlin_types::vecfcn, 100
- nonlin_types::vecfcn_helper, 101

- nonlin_solve, [54](#)
- qns_solve
 - nonlin_solve, [55](#)
- quasi_newton_c
 - nonlin_c_binding, [20](#)
- set_nonlin_defaults
 - nonlin_c_binding, [21](#)
- set_nonlin_ls_defaults
 - nonlin_c_binding, [21](#)
- set_poly_coefficient
 - nonlin_polynomials, [48](#)
- set_polynomial_set_coefficient
 - nonlin_c_binding, [21](#)
- test_convergence
 - nonlin_solve, [56](#)
- vfh_fcn
 - nonlin_types, [70](#)
- vfh_get_nfcn
 - nonlin_types, [70](#)
- vfh_get_nvar
 - nonlin_types, [70](#)
- vfh_is_fcn_defined
 - nonlin_types, [71](#)
- vfh_is_jac_defined
 - nonlin_types, [71](#)
- vfh_jac_fcn
 - nonlin_types, [71](#)
- vfh_set_fcn
 - nonlin_types, [72](#)
- vfh_set_jac
 - nonlin_types, [72](#)