

linalg

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Chapter 1

Main Page

1.1 Introduction

LINALG is a linear algebra library that provides a user-friendly interface to several BLAS and LAPACK routines.

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Version

1.0

Chapter 2

Modules Index

2.1 Modules List

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

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Chapter 3

Data Type Index

3.1 Data Types List

Here are the data types with brief descriptions:

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lapack::DLAMCH	74
linalg_eigen::eigen	Computes the eigenvalues, and optionally the eigenvectors, of a matrix	74
linalg_factor::form_lu	Extracts the L and U matrices from the condensed [L\U] storage format used by the lu_factor .	78
linalg_factor::form_qr	Forms the full M-by-M orthogonal matrix Q from the elementary reflectors returned by the base QR factorization algorithm	79
linalg_core::mtx_mult	Performs the matrix operation: $C = \alpha * op(A) * op(B) + \beta * C$	82
linalg_factor::mult_qr	Multiplies a general matrix by the orthogonal matrix Q from a QR factorization	83
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linalg_solve::solve_least_squares	Solves the overdetermined or underdetermined system ($A*X = B$) of M equations of N unknowns	92
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linalg_solve::solve_qr	Solves a system of M QR-factored equations of N unknowns	100
linalg_solve::solve_triangular_system	Solves a triangular system of equations	103

Chapter 4

Module Documentation

4.1 lapack Module Reference

lapack

Data Types

- interface [DLAMCH](#)

4.1.1 Detailed Description

lapack

Purpose

Provides interfaces to various LAPACK routines.

4.2 linalg_c_binding Module Reference

[linalg_c_binding](#)

Functions/Subroutines

- subroutine [mtx_mult_c](#) (transa, transb, m, n, k, alpha, a, lda, b, ldb, beta, c)
*Performs the matrix operation: $C = \alpha * op(A) * op(B) + \beta * C$.*
- subroutine [diag_mtx_mult_c](#) (trans, m, n, alpha, na, a, mb, nb, b, beta, c, err)
*Computes the matrix operation: $C = \alpha * A * op(B) + \beta * C$.*
- subroutine [diag_mtx_mult_cmplx_c](#) (trans, m, n, alpha, na, a, mb, nb, b, beta, c, err)
*Computes the matrix operation: $C = \alpha * A * op(B) + \beta * C$, where A and C are complex-valued.*
- subroutine [rank1_update_c](#) (m, n, alpha, x, y, a)
*Performs the rank-1 update to matrix A such that: $A = \alpha * X * Y^{**T} + A$, where A is an M -by- N matrix, α is a scalar, X is an M -element array, and N is an N -element array.*

- pure real(dp) function [trace_c](#) (m, n, x)
Computes the trace of a matrix (the sum of the main diagonal elements).
- integer(i32) function [mtx_rank_c](#) (m, n, a, err)
Computes the rank of a matrix.
- real(dp) function [det_c](#) (n, a, err)
Computes the determinant of a square matrix.
- subroutine [swap_c](#) (n, x, y)
Swaps the contents of two arrays.
- subroutine [lu_factor_c](#) (m, n, a, ni, ipvt, err)
Computes the LU factorization of an M-by-N matrix.
- subroutine [form_lu_c](#) (n, lu, ipvt, u, p)
Extracts the L, U, and P matrices from the output of the lu_factor routine.
- subroutine [qr_factor_c](#) (m, n, a, nt, tau, err)
Computes the QR factorization of an M-by-N matrix without pivoting.
- subroutine [qr_factor_pivot_c](#) (m, n, a, nt, tau, jpvt, err)
*Computes the QR factorization of an M-by-N matrix with column pivoting such that $A * P = Q * R$.*
- subroutine [form_qr_c](#) (m, n, r, nt, tau, q, err)
Forms the full M-by-M orthogonal matrix Q from the elementary reflectors returned by the base QR factorization algorithm.
- subroutine [form_qr_pivot_c](#) (m, n, r, nt, tau, pvt, q, p, err)
Forms the full M-by-M orthogonal matrix Q from the elementary reflectors returned by the base QR factorization algorithm.
- subroutine [mult_qr_c](#) (trans, m, n, q, nt, tau, c, err)
*Multiplies a general matrix by the orthogonal matrix Q from a QR factorization such that: $C = op(Q) * C$.*
- subroutine [qr_rank1_update_c](#) (m, n, q, r, u, v, err)
*Computes the rank 1 update to an M-by-N QR factored matrix A ($M \geq N$) where $A = Q * R$, and $A1 = A + U * V^{**T}$ such that $A1 = Q1 * R1$.*
- subroutine [cholesky_factor_c](#) (n, a, upper, err)
Computes the Cholesky factorization of a symmetric, positive definite matrix.
- subroutine [cholesky_rank1_update_c](#) (n, r, u, err)
Computes the rank 1 update to a Cholesky factored matrix (upper triangular).
- subroutine [rz_factor_c](#) (m, n, a, tau, err)
*Factors an upper trapezoidal matrix by means of orthogonal transformations such that $A = R * Z = (R \ 0) * Z$. Z is an orthogonal matrix of dimension N-by-N, and R is an M-by-M upper triangular matrix.*
- subroutine [mult_rz_c](#) (trans, m, n, l, a, tau, c, err)
*Multiplies a general matrix by the orthogonal matrix Z from an RZ factorization such that: $C = op(Z) * C$.*
- subroutine [svd_c](#) (m, n, a, ns, s, u, vt, err)
*Computes the singular value decomposition of a matrix A. The SVD is defined as: $A = U * S * V^{**T}$, where U is an M-by-M orthogonal matrix, S is an M-by-N diagonal matrix, and V is an N-by-N orthogonal matrix.*
- subroutine [solve_tri_mtx_c](#) (upper, trans, nounit, n, nrhs, alpha, a, b)
*Solves one of the matrix equations: $op(A) * X = alpha * B$, where A is a triangular matrix.*
- subroutine [solve_lu_c](#) (n, nrhs, a, ipvt, b)
Solves a system of LU-factored equations.
- subroutine [solve_qr_c](#) (m, n, nrhs, a, tau, b, err)
Solves a system of M QR-factored equations of N unknowns where $M \geq N$.
- subroutine [solve_qr_pivot_c](#) (m, n, nrhs, a, nt, tau, jpvt, mb, b, err)
Solves a system of M QR-factored equations of N unknowns where the QR factorization made use of column pivoting.
- subroutine [solve_cholesky_c](#) (upper, n, nrhs, a, b)
Solves a system of Cholesky factored equations.
- subroutine [mtx_inverse_c](#) (n, a, err)
Computes the inverse of a square matrix.
- subroutine [mtx_pinverse_c](#) (m, n, a, ainvt, err)

Computes the Moore-Penrose pseudo-inverse of a M-by-N matrix using the singular value decomposition of the matrix.

- subroutine [solve_least_squares_c](#) (m, n, nrhs, a, mb, b, err)

Solves the overdetermined or underdetermined system ($A \cdot X = B$) of M equations of N unknowns using a complete orthogonal factorization of matrix A.

- subroutine [eigen_symm_c](#) (n, vecs, a, vals, err)

Computes the eigenvalues, and optionally the eigenvectors of a real, symmetric matrix.

- subroutine [eigen_asymm_c](#) (n, a, vals, vecs, err)

Computes the eigenvalues, and the right eigenvectors of a square matrix.

- subroutine [eigen_gen_c](#) (n, a, b, alpha, beta, vecs, err)

Computes the eigenvalues, and optionally the right eigenvectors of a square matrix assuming the structure of the eigenvalue problem is $A \cdot X = \lambda B \cdot X$.

4.2.1 Detailed Description

[linalg_c_binding](#)

Purpose

Provides a C friendly interface to the LINALG library.

4.2.2 Function/Subroutine Documentation

- 4.2.2.1 subroutine [linalg_c_binding::cholesky_factor_c](#) (integer(i32), intent(in), value *n*, real(dp), dimension(n,n), intent(inout) *a*, logical(c_bool), intent(in), value *upper*, type(c_ptr), intent(in), value *err*)

Computes the Cholesky factorization of a symmetric, positive definite matrix.

Parameters

in	<i>n</i>	The dimension of the matrix.
in, out	<i>a</i>	On input, the N-by-N matrix to factor. On output, the factored matrix is returned in either the upper or lower triangular portion of the matrix, dependent upon the value of <i>upper</i> .
in	<i>upper</i>	An optional input that, if specified, provides control over whether the factorization is computed as $A = U \cdot U^T$ (set to true), or as $A = L \cdot L^T$ (set to false). The default value is true such that $A = U \cdot U^T$.
in	<i>err</i>	A pointer to the C error handler 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"> • LA_MATRIX_FORMAT_ERROR: Occurs if <i>a</i> is not positive definite.

Definition at line 670 of file [linalg_c_binding.f90](#).

- 4.2.2.2 subroutine [linalg_c_binding::cholesky_rank1_update_c](#) (integer(i32), intent(in), value *n*, real(dp), dimension(n,n), intent(inout) *r*, real(dp), dimension(n), intent(inout) *u*, type(c_ptr), intent(in), value *err*)

Computes the rank 1 update to a Cholesky factored matrix (upper triangular).

Parameters

in	<i>n</i>	The dimension of the matrix.
in, out	<i>r</i>	On input, the N-by-N upper triangular matrix R. On output, the updated matrix R1.
in, out	<i>u</i>	On input, the N-element update vector U. On output, the rotation sines used to transform R to R1.
in	<i>err</i>	A pointer to the C error handler 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"> LA_OUT_OF_MEMORY_ERROR: Occurs if local memory must be allocated, and there is insufficient memory available.

Definition at line 705 of file linalg_c_binding.f90.

4.2.2.3 `real(dp) function linalg_c_binding::det_c (integer(i32), intent(in), value n, real(dp), dimension(n,n), intent(inout) a, type(c_ptr), intent(in), value err)`

Computes the determinant of a square matrix.

Parameters

in	<i>n</i>	The dimension of the matrix.
in, out	<i>a</i>	On input, the N-by-N matrix on which to operate. On output the contents are overwritten by the LU factorization of the original matrix.
in	<i>err</i>	A pointer to the C error handler 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"> LA_ARRAY_SIZE_ERROR: Occurs if the input matrix is not square. LA_OUT_OF_MEMORY_ERROR: Occurs if local memory must be allocated, and there is insufficient memory available.

Definition at line 264 of file linalg_c_binding.f90.

4.2.2.4 `subroutine linalg_c_binding::diag_mtx_mult_c (logical(c_bool), intent(in), value trans, integer(i32), intent(in), value m, integer(i32), intent(in), value n, real(dp), intent(in), value alpha, integer(i32), intent(in), value na, real(dp), dimension(na), intent(in) a, integer(i32), intent(in), value mb, integer(i32), intent(in), value nb, real(dp), dimension(mb, nb), intent(in) b, real(dp), intent(in), value beta, real(dp), dimension(m, n), intent(inout) c, type(c_ptr), intent(in), value err)`

Computes the matrix operation: $C = \alpha * A * \text{op}(B) + \beta * C$.

Parameters

in	<i>trans</i>	Set to true if $\text{op}(B) == B^{**T}$; else, set to false if $\text{op}(B) == B$.
in	<i>m</i>	The number of rows in matrix C.
in	<i>n</i>	The number of columns in matrix C.
in	<i>alpha</i>	The scalar multiplier to matrix A.
in	<i>na</i>	The length of <i>a</i> .

Parameters

in	<i>a</i>	A MIN(M,P)-element array containing the diagonal elements of matrix A.
in	<i>mb</i>	The number of rows in matrix B.
in	<i>nb</i>	The number of columns in matrix B.
in	<i>b</i>	The LDB-by-TDB matrix B where (LDB = leading dimension of B, and TDB = trailing dimension of B): <ul style="list-style-type: none"> • <code>trans == true</code>: LDB = N, TDB = P • <code>trans == false</code>: LDB = P, TDB = N
in	<i>beta</i>	The scalar multiplier to matrix C.
in, out	<i>c</i>	The M-by-N matrix C.
in	<i>err</i>	A pointer to the C error handler 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>LA_ARRAY_SIZE_ERROR</code>: Occurs if any of the input arrays are not sized appropriately.

Definition at line 94 of file `linalg_c_binding.f90`.

4.2.2.5 subroutine `linalg_c_binding::diag_mtx_mult_cmplx_c` (`logical(c_bool)`, intent(in), value *trans*, integer(i32), intent(in), value *m*, integer(i32), intent(in), value *n*, real(dp), intent(in), value *alpha*, integer(i32), intent(in), value *na*, complex(dp), dimension(*na*), intent(in) *a*, integer(i32), intent(in), value *mb*, integer(i32), intent(in), value *nb*, real(dp), dimension(*mb*, *nb*), intent(in) *b*, real(dp), intent(in), value *beta*, complex(dp), dimension(*m*, *n*), intent(inout) *c*, type(*c_ptr*), intent(in), value *err*)

Computes the matrix operation: $C = \alpha * A * \text{op}(B) + \beta * C$, where A and C are complex-valued.

Parameters

in	<i>trans</i>	Set to true if $\text{op}(B) == B^{**T}$; else, set to false if $\text{op}(B) == B$.
in	<i>m</i>	The number of rows in matrix C.
in	<i>n</i>	The number of columns in matrix C.
in	<i>alpha</i>	The scalar multiplier to matrix A.
in	<i>na</i>	The length of <i>a</i> .
in	<i>a</i>	A MIN(M,P)-element array containing the diagonal elements of matrix A.
in	<i>mb</i>	The number of rows in matrix B.
in	<i>nb</i>	The number of columns in matrix B.
in	<i>b</i>	The LDB-by-TDB matrix B where (LDB = leading dimension of B, and TDB = trailing dimension of B): <ul style="list-style-type: none"> • <code>trans == true</code>: LDB = N, TDB = P • <code>trans == false</code>: LDB = P, TDB = N
in	<i>beta</i>	The scalar multiplier to matrix C.
in, out	<i>c</i>	The M-by-N matrix C.
in	<i>err</i>	A pointer to the C error handler 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>LA_ARRAY_SIZE_ERROR</code>: Occurs if any of the input arrays are not sized appropriately.

Definition at line 143 of file linalg_c_binding.f90.

4.2.2.6 subroutine linalg_c_binding::eigen_asymm_c (integer(i32), intent(in), value *n*, real(dp), dimension(n,n), intent(inout) *a*, complex(dp), dimension(n), intent(out) *vals*, complex(dp), dimension(n,n), intent(out) *vecs*, type(c_ptr), intent(in), value *err*)

Computes the eigenvalues, and the right eigenvectors of a square matrix.

Parameters

in	<i>n</i>	The dimension of the matrix.
in, out	<i>a</i>	On input, the N-by-N matrix on which to operate. On output, the contents of this matrix are overwritten.
out	<i>vals</i>	An N-element array containing the eigenvalues of the matrix on output. The eigenvalues are not sorted.
out	<i>vecs</i>	An N-by-N matrix containing the right eigenvectors (one per column) on output.
in	<i>err</i>	A pointer to the C error handler 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"> 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 1196 of file linalg_c_binding.f90.

4.2.2.7 subroutine linalg_c_binding::eigen_gen_c (integer(i32), intent(in), value *n*, real(dp), dimension(n, n), intent(inout) *a*, real(dp), dimension(n, n), intent(inout) *b*, complex(dp), dimension(n), intent(out) *alpha*, real(dp), dimension(n), intent(out) *beta*, complex(dp), dimension(n,n), intent(out) *vecs*, type(c_ptr), intent(in), value *err*)

Computes the eigenvalues, and optionally the right eigenvectors of a square matrix assuming the structure of the eigenvalue problem is $A*X = \lambda*B*X$.

Parameters

in	<i>n</i>	The dimension of the matrix.
in, out	<i>a</i>	On input, the N-by-N matrix A. On output, the contents of this matrix are overwritten.
in, out	<i>b</i>	On input, the N-by-N matrix B. On output, the contents of this matrix are overwritten.
out	<i>alpha</i>	An N-element array that, on output, contains the numerator of the eigenvalue ration ALPHA / BETA. Computation of this ratio isn't necessarily as trivial as it seems as it is entirely possible, and likely, that ALPHA / BETA can overflow or underflow. With that said, the values in ALPHA will always be less than and usually comparable with the NORM(A).
out	<i>beta</i>	An N-element array that, on output, contains the denominator used to determine the eigenvalues as ALPHA / BETA. The values in this array will always be less than and usually comparable with the NORM(B).
out	<i>vecs</i>	An N-by-N matrix containing the right eigenvectors (one per column) on output.

Parameters

in	err	<p>A pointer to the C error handler 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.
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Definition at line 1245 of file linalg_c_binding.f90.

4.2.2.8 subroutine linalg_c_binding::eigen_symm_c (integer(i32), intent(in), value *n*, logical(c_bool), intent(in), value *vecs*, real(dp), dimension(n,n), intent(inout) *a*, real(dp), dimension(n), intent(out) *vals*, type(c_ptr), intent(in), value *err*)

Computes the eigenvalues, and optionally the eigenvectors of a real, symmetric matrix.

Parameters

in	<i>n</i>	The dimension of the matrix.
in	<i>vecs</i>	Set to true to compute the eigenvectors as well as the eigenvalues; else, set to false to just compute the eigenvalues.
in, out	<i>a</i>	On input, the N-by-N symmetric matrix on which to operate. On output, and if <i>vecs</i> is set to true, the matrix will contain the eigenvectors (one per column) corresponding to each eigenvalue in <i>vals</i> . If <i>vecs</i> is set to false, the lower triangular portion of the matrix is overwritten.
out	<i>vals</i>	An N-element array that will contain the eigenvalues sorted into ascending order.
in	err	<p>A pointer to the C error handler 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 1157 of file linalg_c_binding.f90.

4.2.2.9 subroutine linalg_c_binding::form_lu_c (integer(i32), intent(in), value *n*, real(dp), dimension(n,n), intent(inout) *lu*, integer(i32), dimension(n), intent(in) *ipvt*, real(dp), dimension(n,n), intent(out) *u*, real(dp), dimension(n,n), intent(out) *p*)

Extracts the L, U, and P matrices from the output of the lu_factor routine.

Parameters

in	<i>n</i>	The dimension of the original matrix.
in, out	<i>lu</i>	On input, the N-by-N matrix as output by lu_factor. On output, the N-by-N lower triangular matrix L.
in	<i>ipvt</i>	The N-element pivot array as output by lu_factor.
out	<i>u</i>	An N-by-N matrix where the U matrix will be written.
out	<i>p</i>	An N-by-N matrix where the row permutation matrix will be written.

Remarks

This routine allows extraction of the actual "L", "U", and "P" matrices of the decomposition. To use these matrices to solve the system $A \cdot X = B$, the following approach is used.

1. First, solve the linear system: $L \cdot Y = P \cdot B$ for Y .
2. Second, solve the linear system: $U \cdot X = Y$ for X .

Notice, as both L and U are triangular in structure, the above equations can be solved by forward and backward substitution.

See Also

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

Definition at line 367 of file `linalg_c_binding.f90`.

4.2.2.10 `subroutine linalg_c_binding::form_qr_c (integer(i32), intent(in), value m, integer(i32), intent(in), value n, real(dp), dimension(m,n), intent(inout) r, integer(i32), intent(in), value nt, real(dp), dimension(nt), intent(in) tau, real(dp), dimension(m,m), intent(out) q, type(c_ptr), intent(in), value err)`

Forms the full M -by- M orthogonal matrix Q from the elementary reflectors returned by the base QR factorization algorithm.

Parameters

<code>in</code>	<code>m</code>	The number of rows in the original matrix.
<code>in</code>	<code>n</code>	The number of columns in the original matrix.
<code>in, out</code>	<code>r</code>	On input, an M -by- N matrix where the elements below the diagonal contain the elementary reflectors generated from the QR factorization. On and above the diagonal, the matrix contains the matrix R . On output, the elements below the diagonal are zeroed such that the remaining matrix is simply the M -by- N matrix R .
<code>in</code>	<code>nt</code>	The number of elements in the scalar factor array <code>tau</code> . This value must be equal to $\text{MIN}(M, N)$.
<code>in</code>	<code>tau</code>	A $\text{MIN}(M, N)$ -element array containing the scalar factors of each elementary reflector defined in <code>r</code> .
<code>out</code>	<code>q</code>	An M -by- M matrix where the full orthogonal matrix Q will be written. In the event that $M > N$, Q may be supplied as M -by- N , and therefore only return the useful submatrix Q_1 ($Q = [Q_1, Q_2]$) as the factorization can be written as $Q * R = [Q_1, Q_2] * [R_1; 0]$.
<code>in</code>	<code>err</code>	A pointer to the C error handler object. If no error handling is desired, simply pass <code>NULL</code> , 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>LA_ARRAY_SIZE_ERROR</code>: Occurs if the scalar factor array is not sized appropriately. • <code>LA_OUT_OF_MEMORY_ERROR</code>: Occurs if local memory must be allocated, and there is insufficient memory available.

Definition at line 495 of file `linalg_c_binding.f90`.

4.2.2.11 subroutine `linalg_c_binding::form_qr_pivot_c` (integer(i32), intent(in), value *m*, integer(i32), intent(in), value *n*, real(dp), dimension(m,n), intent(inout) *r*, integer(i32), intent(in), value *nt*, real(dp), dimension(nt), intent(in) *tau*, integer(i32), dimension(n), intent(in) *pvt*, real(dp), dimension(m,m), intent(out) *q*, real(dp), dimension(n,n), intent(out) *p*, type(c_ptr), intent(in), value *err*)

Forms the full M-by-M orthogonal matrix Q from the elementary reflectors returned by the base QR factorization algorithm.

Parameters

in	<i>m</i>	The number of rows in the original matrix.
in	<i>n</i>	The number of columns in the original matrix.
in, out	<i>r</i>	On input, an M-by-N matrix where the elements below the diagonal contain the elementary reflectors generated from the QR factorization. On and above the diagonal, the matrix contains the matrix R. On output, the elements below the diagonal are zeroed such that the remaining matrix is simply the M-by-N matrix R.
in	<i>nt</i>	The number of elements in the scalar factor array <i>tau</i> . This value must be equal to MIN(M, N).
in	<i>tau</i>	A MIN(M, N)-element array containing the scalar factors of each elementary reflector defined in <i>r</i> .
in	<i>pvt</i>	An N-element column pivot array as returned by the QR factorization.
out	<i>q</i>	An M-by-M matrix where the full orthogonal matrix Q will be written. In the event that $M > N$, Q may be supplied as M-by-N, and therefore only return the useful submatrix Q1 ($Q = [Q1, Q2]$) as the factorization can be written as $Q * R = [Q1, Q2] * [R1; 0]$.
out	<i>p</i>	An N-by-N matrix where the pivot matrix will be written.
in	<i>err</i>	A pointer to the C error handler 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"> LA_ARRAY_SIZE_ERROR: Occurs if the scalar factor array is not sized appropriately. LA_OUT_OF_MEMORY_ERROR: Occurs if local memory must be allocated, and there is insufficient memory available.

Definition at line 546 of file `linalg_c_binding.f90`.

4.2.2.12 subroutine `linalg_c_binding::lu_factor_c` (integer(i32), intent(in), value *m*, integer(i32), intent(in), value *n*, real(dp), dimension(m,n), intent(inout) *a*, integer(i32), intent(in), value *ni*, integer(i32), dimension(ni), intent(out) *ipvt*, type(c_ptr), intent(in), value *err*)

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

Parameters

in	<i>m</i>	The number of rows in the matrix.
in	<i>n</i>	The number of columns in the matrix.
in, out	<i>a</i>	On input, the M-by-N matrix on which to operate. On output, the LU factored matrix in the form [L\U] where the unit diagonal elements of L are not stored.
in	<i>ni</i>	The number of elements in the pivot array <i>ipvt</i> . This value must be equal to MIN(M, N).
out	<i>ipvt</i>	An MIN(M, N)-element array used to track row-pivot operations. The array stored pivot information such that row <i>i</i> is interchanged with row IPVT(<i>i</i>).

Parameters

in	err	<p>A pointer to the C error handler 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_ARRAY_SIZE_ERROR: Occurs if the pivot array is not sized appropriately. LA_SINGULAR_MATRIX_ERROR: Occurs as a warning if <i>a</i> is found to be singular.
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Definition at line 321 of file `linalg_c_binding.f90`.

4.2.2.13 subroutine `linalg_c_binding::mtx_inverse_c` (integer(i32), intent(in), value *n*, real(dp), dimension(n,n), intent(inout) *a*, type(c_ptr), intent(in), value *err*)

Computes the inverse of a square matrix.

Parameters

in	<i>n</i>	The dimension of the matrix.
in, out	<i>a</i>	On input, the N-by-N matrix to invert. On output, the inverted matrix.
in	err	<p>A pointer to the C error handler 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_SINGULAR_MATRIX_ERROR: Occurs if the input matrix is singular.

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

4.2.2.14 subroutine `linalg_c_binding::mtx_mult_c` (logical(c_bool), intent(in), value *transa*, logical(c_bool), intent(in), value *transb*, integer(i32), intent(in), value *m*, integer(i32), intent(in), value *n*, integer(i32), intent(in), value *k*, real(dp), intent(in), value *alpha*, real(dp), dimension(lda,*), intent(in) *a*, integer(i32), intent(in), value *lda*, real(dp), dimension(ldb,*), intent(in) *b*, integer(i32), intent(in), value *ldb*, real(dp), intent(in), value *beta*, real(dp), dimension(m,n), intent(inout) *c*)

Performs the matrix operation: $C = \alpha * \text{op}(A) * \text{op}(B) + \beta * C$.

Parameters

in	<i>transa</i>	Set to true if $\text{op}(A) == A^T$; else, set to false if $\text{op}(A) == A$.
in	<i>transb</i>	Set to true if $\text{op}(B) == B^T$; else, set to false if $\text{op}(B) == B$.
in	<i>m</i>	The number of rows in matrix <i>C</i> , and the number of rows in matrix $\text{op}(A)$.
in	<i>n</i>	The number of columns in matrix <i>C</i> , and the number of columns in matrix $\text{op}(B)$.
in	<i>k</i>	The number of columns in matrix $\text{op}(A)$, and the number of rows in the matrix $\text{op}(B)$.
in	<i>alpha</i>	The scalar multiplier to matrix <i>A</i> .
in	<i>a</i>	The M-by-K matrix <i>A</i> .
in	<i>lda</i>	The leading dimension of matrix <i>A</i> . If <i>transa</i> is true, this value must be at least MAX(1, K); else, if <i>transa</i> is false, this value must be at least MAX(1, M).

Parameters

in	<i>b</i>	The K-by-N matrix B.
in	<i>ldb</i>	The leading dimension of matrix B. If <code>transb</code> is true, this value must be at least MAX(1, N); else, if <code>transb</code> is false, this value must be at least MAX(1, K).
in	<i>beta</i>	The scalar multiplier to matrix C.
in, out	<i>c</i>	The M-by-N matrix C.

Definition at line 45 of file `linalg_c_binding.f90`.

4.2.2.15 subroutine `linalg_c_binding::mtx_pinverse_c` (integer(i32), intent(in), value *m*, integer(i32), intent(in), value *n*, real(dp), dimension(m,n), intent(inout) *a*, real(dp), dimension(n,m), intent(out) *ainv*, type(c_ptr), intent(in), value *err*)

Computes the Moore-Penrose pseudo-inverse of a M-by-N matrix using the singular value decomposition of the matrix.

Parameters

in	<i>m</i>	The number of rows in the matrix to invert.
in	<i>n</i>	The number of columns in the matrix to invert.
in, out	<i>a</i>	On input, the M-by-N matrix to invert. The matrix is overwritten on output.
out	<i>ainv</i>	The N-by-M matrix where the pseudo-inverse of <i>a</i> will be written.
in	<i>err</i>	A pointer to the C error handler 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"> LA_OUT_OF_MEMORY_ERROR: Occurs if local memory must be allocated, and there is insufficient memory available. LA_CONVERGENCE_ERROR: Occurs as a warning if the QR iteration process could not converge to a zero value.

Definition at line 1073 of file `linalg_c_binding.f90`.

4.2.2.16 integer(i32) function `linalg_c_binding::mtx_rank_c` (integer(i32), intent(in), value *m*, integer(i32), intent(in), value *n*, real(dp), dimension(m,n), intent(inout) *a*, type(c_ptr), intent(in), value *err*)

Computes the rank of a matrix.

Parameters

in	<i>m</i>	The number of rows in the matrix.
in	<i>n</i>	The number of columns in the matrix.
in, out	<i>a</i>	On input, the M-by-N matrix of interest. On output, the contents of the matrix are overwritten.

Parameters

in	err	<p>A pointer to the C error handler 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_ARRAY_SIZE_ERROR: Occurs if any of the input arrays are not sized appropriately. • LA_OUT_OF_MEMORY_ERROR: Occurs if local memory must be allocated, and there is insufficient memory available. • LA_CONVERGENCE_ERROR: Occurs as a warning if the QR iteration process could not converge to a zero value.
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Definition at line 231 of file linalg_c_binding.f90.

4.2.2.17 subroutine linalg_c_binding::mult_qr_c (logical(c_bool), intent(in), value *trans*, integer(i32), intent(in), value *m*, integer(i32), intent(in), value *n*, real(dp), dimension(m,m), intent(inout) *q*, integer(i32), intent(in), value *nt*, real(dp), dimension(nt), intent(in) *tau*, real(dp), dimension(m,n), intent(inout) *c*, type(c_ptr), intent(in), value *err*)

Multiplies a general matrix by the orthogonal matrix Q from a QR factorization such that: $C = \text{op}(Q) * C$.

Parameters

in	<i>trans</i>	Set to true to apply Q^{**T} ; else, set to false.
in	<i>m</i>	The number of rows in the matrix <i>c</i> .
in	<i>n</i>	The number of columns in the matrix <i>c</i> .
in	<i>q</i>	On input, an M-by-M matrix containing the elementary reflectors output from the QR factorization. Notice, the contents of this matrix are restored on exit. that the remaining matrix is simply the M-by-N matrix R.
in	<i>nt</i>	The number of elements in the scalar factor array <i>tau</i> . This value must be equal to MIN(M, N).
in	<i>tau</i>	A MIN(M,N)-element array containing the scalar factors of each elementary reflector defined in <i>a</i> .
in, out	<i>c</i>	On input, the M-by-N matrix C. On output, the product of the orthogonal matrix Q and the original matrix C.
in	err	<p>A pointer to the C error handler 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_ARRAY_SIZE_ERROR: Occurs if the scalar factor array is not sized appropriately. • LA_OUT_OF_MEMORY_ERROR: Occurs if local memory must be allocated, and there is insufficient memory available.

Definition at line 593 of file linalg_c_binding.f90.

4.2.2.18 subroutine `linalg_c_binding::mult_rz_c` (`logical(c_bool)`, `intent(in)`, `value trans`, `integer(i32)`, `intent(in)`, `value m`, `integer(i32)`, `intent(in)`, `value n`, `integer(i32)`, `intent(in)`, `value l`, `real(dp)`, `dimension(m,m)`, `intent(inout) a`, `real(dp)`, `dimension(m)`, `intent(in) tau`, `real(dp)`, `dimension(m,n)`, `intent(inout) c`, `type(c_ptr)`, `intent(in)`, `value err`)

Multiplies a general matrix by the orthogonal matrix Z from an RZ factorization such that: $C = \text{op}(Z) * C$.

Parameters

<code>in</code>	<code>trans</code>	Set to true to apply Z^{**T} ; else, set to false.
<code>in</code>	<code>m</code>	The number of rows in the matrix <code>c</code> .
<code>in</code>	<code>n</code>	The number of columns in the matrix <code>c</code> .
<code>in</code>	<code>l</code>	The number of columns in matrix <code>a</code> containing the meaningful part of the Householder vectors ($M \geq L \geq 0$).
<code>in, out</code>	<code>a</code>	On input, the M-by-M matrix Z as output by <code>rz_factor</code> . The matrix is used as in-place storage during execution; however, the contents of the matrix are restored on exit.
<code>in</code>	<code>tau</code>	An M-element array containing the scalar factors of the elementary reflectors found in <code>a</code> .
<code>in, out</code>	<code>c</code>	On input, the M-by-N matrix C. On output, the product of the orthogonal matrix Z and the original matrix C.
<code>in</code>	<code>err</code>	A pointer to the C error handler 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"> LA_OUT_OF_MEMORY_ERROR: Occurs if local memory must be allocated, and there is insufficient memory available.

Definition at line 786 of file `linalg_c_binding.f90`.

4.2.2.19 subroutine `linalg_c_binding::qr_factor_c` (`integer(i32)`, `intent(in)`, `value m`, `integer(i32)`, `intent(in)`, `value n`, `real(dp)`, `dimension(m,n)`, `intent(inout) a`, `integer(i32)`, `intent(in)`, `value nt`, `real(dp)`, `dimension(nt)`, `intent(out) tau`, `type(c_ptr)`, `intent(in)`, `value err`)

Computes the QR factorization of an M-by-N matrix without pivoting.

Parameters

<code>in</code>	<code>m</code>	The number of rows in the matrix.
<code>in</code>	<code>n</code>	The number of columns in the matrix.
<code>in, out</code>	<code>a</code>	On input, the M-by-N matrix to factor. On output, the elements on and above the diagonal contain the MIN(M, N)-by-N upper trapezoidal matrix R (R is upper triangular if $M \geq N$). The elements below the diagonal, along with the array <code>tau</code> , represent the orthogonal matrix Q as a product of elementary reflectors.
<code>in</code>	<code>nt</code>	The number of elements in the scalar factor array <code>tau</code> . This value must be equal to MIN(M, N).
<code>out</code>	<code>tau</code>	A MIN(M, N)-element array used to store the scalar factors of the elementary reflectors.
<code>in</code>	<code>err</code>	A pointer to the C error handler 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"> LA_ARRAY_SIZE_ERROR: Occurs if the scalar factor array is not sized appropriately. LA_OUT_OF_MEMORY_ERROR: Occurs if local memory must be allocated, and there is insufficient memory available.

Definition at line 401 of file linalg_c_binding.f90.

4.2.2.20 subroutine linalg_c_binding::qr_factor_pivot_c (integer(i32), intent(in), value *m*, integer(i32), intent(in), value *n*, real(dp), dimension(m,n), intent(inout) *a*, integer(i32), intent(in), value *nt*, real(dp), dimension(nt), intent(out) *tau*, integer(i32), dimension(n), intent(inout) *jpvt*, type(c_ptr), intent(in), value *err*)

Computes the QR factorization of an M-by-N matrix with column pivoting such that $A * P = Q * R$.

Parameters

in	<i>m</i>	The number of rows in the matrix.
in	<i>n</i>	The number of columns in the matrix.
in, out	<i>a</i>	On input, the M-by-N matrix to factor. On output, the elements on and above the diagonal contain the MIN(M, N)-by-N upper trapezoidal matrix R (R is upper triangular if $M \geq N$). The elements below the diagonal, along with the array <i>tau</i> , represent the orthogonal matrix Q as a product of elementary reflectors.
in	<i>nt</i>	The number of elements in the scalar factor array <i>tau</i> . This value must be equal to MIN(M, N).
out	<i>tau</i>	A MIN(M, N)-element array used to store the scalar factors of the elementary reflectors.
in, out	<i>jpvt</i>	On input, an N-element array that if JPVT(I) .ne. 0, the I-th column of A is permuted to the front of $A * P$; if JPVT(I) = 0, the I-th column of A is a free column. On output, if JPVT(I) = K, then the I-th column of $A * P$ was the K-th column of A.
in	<i>err</i>	A pointer to the C error handler 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"> LA_ARRAY_SIZE_ERROR: Occurs if the scalar factor array is not sized appropriately. LA_OUT_OF_MEMORY_ERROR: Occurs if local memory must be allocated, and there is insufficient memory available.

Definition at line 448 of file linalg_c_binding.f90.

4.2.2.21 subroutine linalg_c_binding::qr_rank1_update_c (integer(i32), intent(in), value *m*, integer(i32), intent(in), value *n*, real(dp), dimension(m,m), intent(inout) *q*, real(dp), dimension(m,n), intent(inout) *r*, real(dp), dimension(m), intent(inout) *u*, real(dp), dimension(n), intent(inout) *v*, type(c_ptr), intent(in), value *err*)

Computes the rank 1 update to an M-by-N QR factored matrix A ($M \geq N$) where $A = Q * R$, and $A1 = A + U * V^{**T}$ such that $A1 = Q1 * R1$.

Parameters

in	<i>m</i>	The number of rows in the original matrix.
in	<i>n</i>	The number of columns in the original matrix.
in, out	<i>q</i>	On input, the original M-by-M orthogonal matrix Q. On output, the updated matrix Q1.
in, out	<i>r</i>	On input, the M-by-N matrix R. On output, the updated matrix R1.
in, out	<i>u</i>	On input, the M-element U update vector. On output, the original content of the array is overwritten.
in, out	<i>v</i>	On input, the N-element V update vector. On output, the original content of the array is overwritten.

Parameters

in	err	A pointer to the C error handler 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"> LA_OUT_OF_MEMORY_ERROR: Occurs if local memory must be allocated, and there is insufficient memory available.
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Definition at line 634 of file linalg_c_binding.f90.

4.2.2.22 subroutine linalg_c_binding::rank1_update_c (integer(i32), intent(in), value *m*, integer(i32), intent(in), value *n*, real(dp), intent(in), value *alpha*, real(dp), dimension(m), intent(in) *x*, real(dp), dimension(n), intent(in) *y*, real(dp), dimension(m,n), intent(inout) *a*)

Performs the rank-1 update to matrix A such that: $A = \alpha * X * Y^{**T} + A$, where A is an M-by-N matrix, alpha is a scalar, X is an M-element array, and Y is an N-element array.

Parameters

in	<i>m</i>	The number of elements in <i>x</i> , and the number of rows in matrix <i>a</i> .
in	<i>n</i>	The number of elements in <i>y</i> , and the number of columns in matrix <i>a</i> .
in	<i>alpha</i>	The scalar multiplier.
in	<i>x</i>	An M-element array.
in	<i>y</i>	An N-element array.
in, out	<i>a</i>	On input, the M-by-N matrix to update. On output, the updated M-by-N matrix.

Notes

This routine is based upon the BLAS routine DGER.

Definition at line 184 of file linalg_c_binding.f90.

4.2.2.23 subroutine linalg_c_binding::rz_factor_c (integer(i32), intent(in), value *m*, integer(i32), intent(in), value *n*, real(dp), dimension(m,n), intent(inout) *a*, real(dp), dimension(m), intent(out) *tau*, type(c_ptr), intent(in), value *err*)

Factors an upper trapezoidal matrix by means of orthogonal transformations such that $A = R * Z = (R \ 0) * Z$. Z is an orthogonal matrix of dimension N-by-N, and R is an M-by-M upper triangular matrix.

Parameters

in	<i>m</i>	The number of rows in the original matrix.
in	<i>n</i>	The number of columns in the original matrix.
in, out	<i>a</i>	On input, the M-by-N upper trapezoidal matrix to factor. On output, the leading M-by-M upper triangular part of the matrix contains the upper triangular matrix R, and elements N-L+1 to N of the first M rows of A, with the array <i>tau</i> , represent the orthogonal matrix Z as a product of M elementary reflectors.
out	<i>tau</i>	An M-element array used to store the scalar factors of the elementary reflectors.

Parameters

in	err	A pointer to the C error handler 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"> LA_OUT_OF_MEMORY_ERROR: Occurs if local memory must be allocated, and there is insufficient memory available.
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Definition at line 744 of file linalg_c_binding.f90.

4.2.2.24 subroutine linalg_c_binding::solve_cholesky_c (logical(c_bool), intent(in), value *upper*, integer(i32), intent(in), value *n*, integer(i32), intent(in), value *nrhs*, real(dp), dimension(n,n), intent(in) *a*, real(dp), dimension(n,nrhs), intent(inout) *b*)

Solves a system of Cholesky factored equations.

Parameters

in	<i>upper</i>	Set to true if the original matrix A was factored such that $A = U^{**T} * U$; else, set to false if the factorization of A was $A = L^{**T} * L$.
in	<i>n</i>	The dimension of the original matrix a.
in	<i>nrhs</i>	The number of right-hand-side vectors (number of columns in matrix b).
in	<i>a</i>	The N-by-N Cholesky factored matrix.
in, out	<i>b</i>	On input, the N-by-NRHS right-hand-side matrix B. On output, the solution matrix X.

Definition at line 1013 of file linalg_c_binding.f90.

4.2.2.25 subroutine linalg_c_binding::solve_least_squares_c (integer(i32), intent(in), value *m*, integer(i32), intent(in), value *n*, integer(i32), intent(in), value *nrhs*, real(dp), dimension(m, n), intent(inout) *a*, integer(i32), intent(in), value *mb*, real(dp), dimension(mb, nrhs), intent(inout) *b*, type(c_ptr), intent(in), value *err*)

Solves the overdetermined or underdetermined system ($A * X = B$) of M equations of N unknowns using a complete orthogonal factorization of matrix A.

Parameters

in	<i>m</i>	The number of rows in the original coefficient matrix A.
in	<i>n</i>	The number of columns in the original coefficient matrix A.
in	<i>nrhs</i>	The number of right-hand-side vectors (number of columns in matrix b).
in, out	<i>a</i>	On input, the M-by-N matrix A. On output, the matrix is overwritten by the details of its complete orthogonal factorization.
in	<i>mb</i>	The number of rows in the matrix b. This value must be equal to MAX(M, N).
in, out	<i>b</i>	If $M \geq N$, the M-by-NRHS matrix B. On output, the first N rows contain the N-by-NRHS solution matrix X. If $M < N$, an N-by-NRHS matrix with the first M rows containing the matrix B. On output, the N-by-NRHS solution matrix X.
in	err	A pointer to the C error handler 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"> LA_OUT_OF_MEMORY_ERROR: Occurs if local memory must be allocated, and there is insufficient memory available.

Definition at line 1116 of file linalg_c_binding.f90.

4.2.2.26 subroutine `linalg_c_binding::solve_lu_c` (integer(i32), intent(in), value *n*, integer(i32), intent(in), value *nrhs*, real(dp), dimension(n,n), intent(in) *a*, integer(i32), dimension(n), intent(in) *ipvt*, real(dp), dimension(n,nrhs), intent(inout) *b*)

Solves a system of LU-factored equations.

Parameters

in	<i>n</i>	The dimension of the original matrix <i>a</i> .
in	<i>nrhs</i>	The number of right-hand-side vectors (number of columns in matrix <i>b</i>).
in	<i>a</i>	The N-by-N LU factored matrix as output by <code>lu_factor</code> .
in	<i>ipvt</i>	The N-element pivot array as output by <code>lu_factor</code> .
in, out	<i>b</i>	On input, the N-by-NRHS right-hand-side matrix. On output, the N-by-NRHS solution matrix.

Definition at line 898 of file linalg_c_binding.f90.

4.2.2.27 subroutine `linalg_c_binding::solve_qr_c` (integer(i32), intent(in), value *m*, integer(i32), intent(in), value *n*, integer(i32), intent(in), value *nrhs*, real(dp), dimension(m,n), intent(inout) *a*, real(dp), dimension(n), intent(in) *tau*, real(dp), dimension(m,nrhs), intent(inout) *b*, type(c_ptr), intent(in), value *err*)

Solves a system of M QR-factored equations of N unknowns where $M \geq N$.

Parameters

in	<i>m</i>	The number of rows in the original coefficient matrix <i>A</i> .
in	<i>n</i>	The number of columns in the original coefficient matrix <i>A</i> .
in	<i>nrhs</i>	The number of right-hand-side vectors (number of columns in matrix <i>b</i>).
in	<i>a</i>	On input, the M-by-N QR factored matrix as returned by <code>qr_factor</code> . On output, the contents of this matrix are restored. Notice, M must be greater than or equal to N.
in	<i>tau</i>	A MIN(M, N)-element array containing the scalar factors of the elementary reflectors as returned by <code>qr_factor</code> .
in	<i>b</i>	On input, the M-by-NRHS right-hand-side matrix. On output, the first N columns are overwritten by the solution matrix <i>X</i> .
in	<i>err</i>	A pointer to the C error handler 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"> LA_OUT_OF_MEMORY_ERROR: Occurs if local memory must be allocated, and there is insufficient memory available.

Definition at line 931 of file linalg_c_binding.f90.

4.2.2.28 subroutine `linalg_c_binding::solve_qr_pivot_c` (integer(i32), intent(in), value *m*, integer(i32), intent(in), value *n*, integer(i32), intent(in), value *nrhs*, real(dp), dimension(m,n), intent(inout) *a*, integer(i32), intent(in), value *nt*, real(dp), dimension(nt), intent(in) *tau*, integer(i32), dimension(n), intent(in) *jpvt*, integer(i32), intent(in), value *mb*, real(dp), dimension(mb,nrhs), intent(inout) *b*, type(c_ptr), intent(in), value *err*)

Solves a system of M QR-factored equations of N unknowns where the QR factorization made use of column pivoting.

Parameters

in	<i>m</i>	The number of rows in the original coefficient matrix A.
in	<i>n</i>	The number of columns in the original coefficient matrix A.
in	<i>nrhs</i>	The number of right-hand-side vectors (number of columns in matrix b).
in	<i>a</i>	On input, the M-by-N QR factored matrix as returned by <code>qr_factor</code> . On output, the contents of this matrix are altered.
in	<i>nt</i>	The number of elements in the scalar factor array <code>tau</code> . This value must be equal to MIN(M, N).
in	<i>tau</i>	A MIN(M, N)-element array containing the scalar factors of the elementary reflectors as returned by <code>qr_factor</code> .
in	<i>jpvt</i>	An N-element array, as output by <code>qr_factor</code> , used to track the column pivots.
in	<i>mb</i>	The number of rows in the matrix b. This value must be equal to MAX(M, N).
in	<i>b</i>	On input, the MAX(M, N)-by-NRHS matrix where the first M rows contain the right-hand-side matrix B. On output, the first N rows are overwritten by the solution matrix X.
in	<i>err</i>	A pointer to the C error handler 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"> LA_ARRAY_SIZE_ERROR: Occurs if any of the input arrays are not sized appropriately. LA_OUT_OF_MEMORY_ERROR: Occurs if local memory must be allocated, and there is insufficient memory available.

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

4.2.2.29 subroutine `linalg_c_binding::solve_tri_mtx_c` (logical(c_bool), intent(in), value *upper*, logical(c_bool), intent(in), value *trans*, logical(c_bool), intent(in), value *nounit*, integer(i32), intent(in), value *n*, integer(i32), intent(in), value *nrhs*, real(dp), intent(in), value *alpha*, real(dp), dimension(n,n), intent(in) *a*, real(dp), dimension(n,nrhs), intent(inout) *b*)

Solves one of the matrix equations: $op(A) * X = \alpha * B$, where A is a triangular matrix.

Parameters

in	<i>upper</i>	Set to true if A is an upper triangular matrix; else, set to false if A is a lower triangular matrix.
in	<i>trans</i>	Set to true if $op(A) = A**T$; else, set to false if $op(A) = A$.
in	<i>nounit</i>	Set to true if A is not a unit-diagonal matrix (ones on every diagonal element); else, set to false if A is a unit-diagonal matrix.
in	<i>n</i>	The dimension of the triangular matrix a.
in	<i>nrhs</i>	The number of right-hand-side vectors (number of columns in matrix b).
in	<i>alpha</i>	The scalar multiplier to B.
in	<i>a</i>	N-by-N triangular matrix on which to operate.
in, out	<i>b</i>	On input, the N-by-NRHS right-hand-side. On output, the N-by-NRHS solution.

Definition at line 875 of file linalg_c_binding.f90.

4.2.2.30 subroutine linalg_c_binding::svd_c (integer(i32), intent(in), value *m*, integer(i32), intent(in), value *n*, real(dp), dimension(m,n), intent(inout) *a*, integer(i32), intent(in), value *ns*, real(dp), dimension(ns), intent(out) *s*, real(dp), dimension(m,m), intent(out) *u*, real(dp), dimension(n,n), intent(out) *vt*, type(c_ptr), intent(in), value *err*)

Computes the singular value decomposition of a matrix A. The SVD is defined as: $A = U * S * V^{**T}$, where U is an M-by-M orthogonal matrix, S is an M-by-N diagonal matrix, and V is an N-by-N orthogonal matrix.

Parameters

in	<i>m</i>	The number of rows in the original matrix.
in	<i>n</i>	The number of columns in the original matrix.
in, out	<i>a</i>	On input, the M-by-N matrix to factor. The matrix is overwritten on output. that the remaining matrix is simply the M-by-N matrix R.
in	<i>ns</i>	The number of elements in the singular value array <i>s</i> . This value must be equal to MIN(M, N).
out	<i>s</i>	A MIN(M, N)-element array containing the singular values of <i>a</i> sorted in descending order.
out	<i>u</i>	An M-by-M matrix that on output contains the left singular vectors (matrix U in the decomposition: $A = U * S * V^{**T}$)
out	<i>vt</i>	An N-by-N matrix that on output contains the right singular vectors (matrix V^{**T} in the decomposition: $A = U * S * V^{**T}$).
in	<i>err</i>	A pointer to the C error handler 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"> LA_ARRAY_SIZE_ERROR: Occurs if the singular value array is not sized appropriately. LA_OUT_OF_MEMORY_ERROR: Occurs if local memory must be allocated, and there is insufficient memory available. LA_CONVERGENCE_ERROR: Occurs as a warning if the QR iteration process could not converge to a zero value.

Definition at line 835 of file linalg_c_binding.f90.

4.2.2.31 subroutine linalg_c_binding::swap_c (integer(i32), intent(in), value *n*, real(dp), dimension(n), intent(inout) *x*, real(dp), dimension(n), intent(inout) *y*)

Swaps the contents of two arrays.

Parameters

in	<i>n</i>	The number of elements either array.
in, out	<i>x</i>	One of the N-element arrays.
in, out	<i>y</i>	The other N-element array.

Definition at line 289 of file linalg_c_binding.f90.

4.2.2.32 pure real(dp) function linalg_c_binding::trace_c (integer(i32), intent(in), value *m*, integer(i32), intent(in), value *n*, real(dp), dimension(m,n), intent(in) *x*)

Computes the trace of a matrix (the sum of the main diagonal elements).

Parameters

in	<i>m</i>	The number of rows in the matrix.
in	<i>n</i>	The number of columns in the matrix.
in	<i>x</i>	The matrix on which to operate.

Returns

The trace of *x*.

Definition at line 204 of file linalg_c_binding.f90.

4.3 linalg_constants Module Reference

[linalg_constants](#)

Variables

- integer, parameter [dp](#) = c_double
Defines a double-precision (64-bit) floating-point type.
- integer, parameter [i32](#) = c_int
Defines a 32-bit signed integer type.
- integer, parameter [la_invalid_input_error](#) = 101
An error flag denoting an invalid input.
- integer, parameter [la_array_size_error](#) = 102
An error flag denoting an improperly sized array.
- integer, parameter [la_singular_matrix_error](#) = 103
An error flag denoting a singular matrix.
- integer, parameter [la_matrix_format_error](#) = 104
An error flag denoting an issue with the matrix format.
- integer, parameter [la_out_of_memory_error](#) = 105
An error flag denoting that there is insufficient memory available.
- integer, parameter [la_convergence_error](#) = 106
An error flag denoting a convergence failure.
- integer, parameter [la_invalid_operation_error](#) = 107
An error resulting from an invalid operation.

4.3.1 Detailed Description

[linalg_constants](#)

Purpose

Provides a set of constants and error flags for the library.

4.4 linalg_core Module Reference

linalg_core

Data Types

- interface [diag_mtx_mult](#)
Multiplies a diagonal matrix with another matrix or array.
- interface [mtx_mult](#)
*Performs the matrix operation: $C = \alpha * op(A) * op(B) + \beta * C$.*

Functions/Subroutines

- subroutine [mtx_mult_mtx](#) (transa, transb, alpha, a, b, beta, c, err)
*Performs the matrix operation: $C = \alpha * op(A) * op(B) + \beta * C$.*
- subroutine [mtx_mult_vec](#) (trans, alpha, a, b, beta, c, err)
*Performs the matrix-vector operation: $c = \alpha * op(A) * b + \beta * c$.*
- subroutine, public [rank1_update](#) (alpha, x, y, a, err)
*Performs the rank-1 update to matrix A such that: $A = \alpha * X * Y^{**T} + A$, where A is an M-by-N matrix, alpha is a scalar, X is an M-element array, and N is an N-element array.*
- subroutine [diag_mtx_mult_mtx](#) (lside, trans, alpha, a, b, beta, c, err)
*Computes the matrix operation: $C = \alpha * A * op(B) + \beta * C$, or $C = \alpha * op(B) * A + \beta * C$.*
- subroutine [diag_mtx_mult_mtx2](#) (lside, alpha, a, b, err)
*Computes the matrix operation: $B = \alpha * A * op(B)$, or $B = \alpha * op(B) * A$.*
- subroutine [diag_mtx_mult_mtx3](#) (lside, trans, alpha, a, b, beta, c, err)
*Computes the matrix operation: $C = \alpha * A * op(B) + \beta * C$, or $C = \alpha * op(B) * A + \beta * C$, where A and C are complex-valued.*
- subroutine [diag_mtx_mult_mtx4](#) (lside, trans, alpha, a, b, beta, c, err)
*Computes the matrix operation: $C = \alpha * A * op(B) + \beta * C$, or $C = \alpha * op(B) * A + \beta * C$, where A, B, and C are complex-valued.*
- pure real(dp) function, public [trace](#) (x)
Computes the trace of a matrix (the sum of the main diagonal elements).
- integer(i32) function, public [mtx_rank](#) (a, tol, work, olwork, err)
Computes the rank of a matrix.
- real(dp) function, public [det](#) (a, iwork, err)
Computes the determinant of a square matrix.
- subroutine, public [swap](#) (x, y, err)
Swaps the contents of two arrays.
- subroutine, public [recip_mult_array](#) (a, x)
Multiplies a vector by the reciprocal of a real scalar.

4.4.1 Detailed Description

linalg_core

Purpose

Provides common "core" linear algebra routines.

4.4.2 Function/Subroutine Documentation

4.4.2.1 `real(dp) function, public linalg_core::det (real(dp), dimension(:, :), intent(inout) a, integer(i32), dimension(:), intent(out), optional, pointer iwork, class(errors), intent(inout), optional, target err)`

Computes the determinant of a square matrix.

Parameters

in, out	<i>a</i>	On input, the N-by-N matrix on which to operate. On output the contents are overwritten by the LU factorization of the original matrix.
out	<i>iwork</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 N-elements.
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"> • LA_ARRAY_SIZE_ERROR: Occurs if any of the input arrays are not sized appropriately. • LA_OUT_OF_MEMORY_ERROR: Occurs if local memory must be allocated, and there is insufficient memory available.

Returns

The determinant of *a*.

Definition at line 1085 of file linalg_core.f90.

4.4.2.2 subroutine linalg_core::diag_mtx_mult_mtx (logical, intent(in) *lside*, logical, intent(in) *trans*, real(dp) *alpha*, real(dp), dimension(:), intent(in) *a*, real(dp), dimension(:, :), intent(in) *b*, real(dp) *beta*, real(dp), dimension(:, :), intent(inout) *c*, class(errors), intent(inout), optional, target *err*) [private]

Computes the matrix operation: $C = \alpha * A * \text{op}(B) + \beta * C$, or $C = \alpha * \text{op}(B) * A + \beta * C$.

Parameters

in	<i>lside</i>	Set to true to apply matrix A from the left; else, set to false to apply matrix A from the left.
in	<i>trans</i>	Set to true if $\text{op}(B) == B^*T$; else, set to false if $\text{op}(B) == B$.
in	<i>alpha</i>	A scalar multiplier.
in	<i>a</i>	A K-element array containing the diagonal elements of A where $K = \text{MIN}(M,P)$ if <i>lside</i> is true; else, if <i>lside</i> is false, $K = \text{MIN}(N,P)$.
in	<i>b</i>	The LDB-by-TDB matrix B where (LDB = leading dimension of B, and TDB = trailing dimension of B): <ul style="list-style-type: none"> • <i>lside</i> == true & <i>trans</i> == true: LDB = N, TDB = P • <i>lside</i> == true & <i>trans</i> == false: LDB = P, TDB = N • <i>lside</i> == false & <i>trans</i> == true: LDB = P, TDB = M • <i>lside</i> == false & <i>trans</i> == false: LDB = M, TDB = P
in	<i>beta</i>	A scalar multiplier.
in, out	<i>c</i>	On input, the M-by-N matrix C. On output, the resulting M-by-N matrix.
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"> • LA_ARRAY_SIZE_ERROR: Occurs if any of the input array sizes are incorrect.

Definition at line 326 of file linalg_core.f90.

4.4.2.3 subroutine linalg_core::diag_mtx_mult_mtx2 (logical, intent(in) *lside*, real(dp), intent(in) *alpha*, real(dp), dimension(:), intent(in) *a*, real(dp), dimension(:,:), intent(inout) *b*, class(errors), intent(inout), optional, target *err*) [private]

Computes the matrix operation: $B = \alpha * A * \text{op}(B)$, or $B = \alpha * \text{op}(B) * A$.

Parameters

in	<i>lside</i>	Set to true to apply matrix A from the left; else, set to false to apply matrix A from the left.
in	<i>alpha</i>	A scalar multiplier.
in	<i>a</i>	A K-element array containing the diagonal elements of A where $K = \text{MIN}(M,P)$ if <i>lside</i> is true; else, if <i>lside</i> is false, $K = \text{MIN}(N,P)$.
in	<i>b</i>	On input, the M-by-N matrix B. On output, the resulting M-by-N matrix.
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"> LA_ARRAY_SIZE_ERROR: Occurs if any of the input array sizes are incorrect.

Definition at line 493 of file linalg_core.f90.

4.4.2.4 subroutine linalg_core::diag_mtx_mult_mtx3 (logical, intent(in) *lside*, logical, intent(in) *trans*, real(dp) *alpha*, complex(dp), dimension(:), intent(in) *a*, real(dp), dimension(:,:), intent(in) *b*, real(dp) *beta*, complex(dp), dimension(:,:), intent(inout) *c*, class(errors), intent(inout), optional, target *err*) [private]

Computes the matrix operation: $C = \alpha * A * \text{op}(B) + \beta * C$, or $C = \alpha * \text{op}(B) * A + \beta * C$, where A and C are complex-valued.

Parameters

in	<i>lside</i>	Set to true to apply matrix A from the left; else, set to false to apply matrix A from the left.
in	<i>trans</i>	Set to true if $\text{op}(B) == B^*T$; else, set to false if $\text{op}(B) == B$.
in	<i>alpha</i>	A scalar multiplier.
in	<i>a</i>	A K-element array containing the diagonal elements of A where $K = \text{MIN}(M,P)$ if <i>lside</i> is true; else, if <i>lside</i> is false, $K = \text{MIN}(N,P)$.
in	<i>b</i>	The LDB-by-TDB matrix B where (LDB = leading dimension of B, and TDB = trailing dimension of B): <ul style="list-style-type: none"> <i>lside</i> == true & <i>trans</i> == true: LDB = N, TDB = P <i>lside</i> == true & <i>trans</i> == false: LDB = P, TDB = N <i>lside</i> == false & <i>trans</i> == true: LDB = P, TDB = M <i>lside</i> == false & <i>trans</i> == false: LDB = M, TDB = P
in	<i>beta</i>	A scalar multiplier.
in, out	<i>c</i>	On input, the M-by-N matrix C. On output, the resulting M-by-N matrix.

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"> LA_ARRAY_SIZE_ERROR: Occurs if any of the input array sizes are incorrect.
-----	-----	--

Definition at line 576 of file linalg_core.f90.

4.4.2.5 subroutine linalg_core::diag_mtx_mult_mtx4 (logical, intent(in) *lside*, logical, intent(in) *trans*, real(dp) *alpha*, complex(dp), dimension(:), intent(in) *a*, complex(dp), dimension(:, :), intent(in) *b*, real(dp) *beta*, complex(dp), dimension(:, :), intent(inout) *c*, class(errors), intent(inout), optional, target *err*) [private]

Computes the matrix operation: $C = \alpha * A * \text{op}(B) + \beta * C$, or $C = \alpha * \text{op}(B) * A + \beta * C$, where *A*, *B*, and *C* are complex-valued.

Parameters

in	<i>lside</i>	Set to true to apply matrix <i>A</i> from the left; else, set to false to apply matrix <i>A</i> from the right.
in	<i>trans</i>	Set to true if $\text{op}(B) == B^{**T}$; else, set to false if $\text{op}(B) == B$.
in	<i>alpha</i>	A scalar multiplier.
in	<i>a</i>	A <i>K</i> -element array containing the diagonal elements of <i>A</i> where $K = \text{MIN}(M, P)$ if <i>lside</i> is true; else, if <i>lside</i> is false, $K = \text{MIN}(N, P)$.
in	<i>b</i>	<p>The LDB-by-TDB matrix <i>B</i> where:</p> <ul style="list-style-type: none"> <i>lside</i> == true & <i>trans</i> == true: LDA = <i>N</i>, TDB = <i>P</i> <i>lside</i> == true & <i>trans</i> == false: LDA = <i>P</i>, TDB = <i>N</i> <i>lside</i> == false & <i>trans</i> == true: LDA = <i>P</i>, TDB = <i>M</i> <i>lside</i> == false & <i>trans</i> == false: LDA = <i>M</i>, TDB = <i>P</i>
in	<i>beta</i>	A scalar multiplier.
in, out	<i>c</i>	On input, the <i>M</i> -by- <i>N</i> matrix <i>C</i> . On output, the resulting <i>M</i> -by- <i>N</i> matrix.
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"> LA_ARRAY_SIZE_ERROR: Occurs if any of the input array sizes are incorrect.

Definition at line 752 of file linalg_core.f90.

4.4.2.6 subroutine linalg_core::mtx_mult_mtx (logical, intent(in) *transa*, logical, intent(in) *transb*, real(dp), intent(in) *alpha*, real(dp), dimension(:, :), intent(in) *a*, real(dp), dimension(:, :), intent(in) *b*, real(dp), intent(in) *beta*, real(dp), dimension(:, :), intent(inout) *c*, class(errors), intent(inout), optional, target *err*) [private]

Performs the matrix operation: $C = \alpha * \text{op}(A) * \text{op}(B) + \beta * C$.

Parameters

in	<i>transa</i>	Set to true if $\text{op}(A) = A^{**T}$; else, set to false for $\text{op}(A) = A$.
in	<i>transb</i>	Set to true if $\text{op}(B) = B^{**T}$; else, set to false for $\text{op}(B) = B$.
in	<i>alpha</i>	A scalar multiplier.
in	<i>a</i>	If <i>transa</i> is set to true, an K-by-M matrix; else, if <i>transa</i> is set to false, an M-by-K matrix.
in	<i>b</i>	If <i>transb</i> is set to true, an N-by-K matrix; else, if <i>transb</i> is set to false, a K-by-N matrix.
in	<i>beta</i>	A scalar multiplier.
in, out	<i>c</i>	On input, the M-by-N matrix C. On output, the M-by-N result.
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"> LA_ARRAY_SIZE_ERROR: Occurs if any of the input array sizes are incorrect.

Notes

This routine utilizes the BLAS routine DGEMM.

Definition at line 82 of file linalg_core.f90.

4.4.2.7 subroutine linalg_core::mtx_mult_vec (logical, intent(in) *trans*, real(dp), intent(in) *alpha*, real(dp), dimension(:, :), intent(in) *a*, real(dp), dimension(:), intent(in) *b*, real(dp), intent(in) *beta*, real(dp), dimension(:), intent(inout) *c*, class(errors), intent(inout), optional, target *err*) [private]

Performs the matrix-vector operation: $c = \alpha * \text{op}(A) * b + \beta * c$.

Parameters

in	<i>trans</i>	Set to true if $\text{op}(A) = A^{**T}$; else, set to false for $\text{op}(A) = A$.
in	<i>alpha</i>	A scalar multiplier.
in	<i>a</i>	The M-by-N matrix A.
in	<i>b</i>	If <i>trans</i> is set to true, an M-element array; else, if <i>trans</i> is set to false, an N-element array.
in	<i>beta</i>	A scalar multiplier.
in, out	<i>c</i>	On input, if <i>trans</i> is set to true, an N-element array; else, if <i>trans</i> is set to false, an M-element array. On output, the results of the operation.
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"> LA_ARRAY_SIZE_ERROR: Occurs if any of the input array sizes are incorrect.

Notes

This routine utilizes the BLAS routine DGEMV.

Definition at line 176 of file linalg_core.f90.

4.4.2.8 `integer(i32) function, public linalg_core::mtx_rank (real(dp), dimension(:,:), intent(inout) a, real(dp), intent(in), optional tol, real(dp), dimension(:), intent(out), optional, pointer work, integer(i32), intent(out), optional olwork, class(errors), intent(inout), optional, target err)`

Computes the rank of a matrix.

Parameters

in, out	<i>a</i>	On input, the M-by-N matrix of interest. On output, the contents of the matrix are overwritten.
in	<i>tol</i>	An optional input, that if supplied, overrides the default tolerance on singular values such that singular values less than this tolerance are treated as zero. The default tolerance is: $\text{MAX}(M, N) * \text{EPS} * \text{MAX}(S)$. If the supplied value is less than the smallest value that causes an overflow if inverted, the tolerance reverts back to its default value, and the operation continues; however, a warning message is issued.
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> .
out	<i>olwork</i>	An optional output used to determine workspace size. If supplied, the routine determines the optimal size for <code>work</code> , and returns without performing any actual calculations.
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>LA_ARRAY_SIZE_ERROR</code>: Occurs if any of the input arrays are not sized appropriately. • <code>LA_OUT_OF_MEMORY_ERROR</code>: Occurs if local memory must be allocated, and there is insufficient memory available. • <code>LA_CONVERGENCE_ERROR</code>: Occurs as a warning if the QR iteration process could not converge to a zero value.

See Also

- [Wolfram MathWorld](#)

Definition at line 965 of file linalg_core.f90.

4.4.2.9 `subroutine, public linalg_core::rank1_update (real(dp), intent(in) alpha, real(dp), dimension(:), intent(in) x, real(dp), dimension(:), intent(in) y, real(dp), dimension(:,:), intent(inout) a, class(errors), intent(inout), optional, target err)`

Performs the rank-1 update to matrix *A* such that: $A = \alpha * X * Y^T + A$, where *A* is an M-by-N matrix, *alpha* is a scalar, *X* is an M-element array, and *N* is an N-element array.

Parameters

in	<i>alpha</i>	The scalar multiplier.
in	<i>x</i>	An M-element array.

Parameters

<code>in</code>	<code>y</code>	An N-element array.
<code>in, out</code>	<code>a</code>	On input, the M-by-N matrix to update. On output, the updated M-by-N matrix.
<code>out</code>	<code>err</code>	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>LA_ARRAY_SIZE_ERROR</code>: Occurs if the size of <code>a</code> does not match with <code>x</code> and <code>y</code>.

Notes

This routine is based upon the BLAS routine DGER.

Definition at line 254 of file `linalg_core.f90`.

4.4.2.10 `subroutine, public linalg_core::recip_mult_array (real(dp), intent(in) a, real(dp), dimension(:), intent(inout) x)`

Multiplies a vector by the reciprocal of a real scalar.

Parameters

<code>in</code>	<code>a</code>	The scalar which is used to divide each component of <code>x</code> . The value must be ≥ 0 , or the subroutine will divide by zero.
<code>in, out</code>	<code>x</code>	The vector.

Notes

This routine is based upon the LAPACK routine DRSCL.

Definition at line 1236 of file `linalg_core.f90`.

4.4.2.11 `subroutine, public linalg_core::swap (real(dp), dimension(:), intent(inout) x, real(dp), dimension(:), intent(inout) y, class(errors), intent(inout), optional, target err)`

Swaps the contents of two arrays.

Parameters

<code>in, out</code>	<code>x</code>	One of the N-element arrays.
<code>in, out</code>	<code>y</code>	The other N-element array.
<code>out</code>	<code>err</code>	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>LA_ARRAY_SIZE_ERROR</code>: Occurs if <code>x</code> and <code>y</code> are not the same size.

Definition at line 1190 of file linalg_core.f90.

4.4.2.12 pure real(dp) function, public linalg_core::trace (real(dp), dimension(:,:), intent(in) x)

Computes the trace of a matrix (the sum of the main diagonal elements).

Parameters

in	x	The matrix on which to operate.
----	---	---------------------------------

Returns

The trace of x.

Definition at line 909 of file linalg_core.f90.

4.5 linalg_eigen Module Reference

[linalg_eigen](#)

Data Types

- interface [eigen](#)
Computes the eigenvalues, and optionally the eigenvectors, of a matrix.

Functions/Subroutines

- subroutine [eigen_symm](#) (vecs, a, vals, work, olwork, err)
Computes the eigenvalues, and optionally the eigenvectors of a real, symmetric matrix.
- subroutine [eigen_asymm](#) (a, vals, vecs, work, olwork, err)
Computes the eigenvalues, and optionally the right eigenvectors of a square matrix.
- subroutine [eigen_gen](#) (a, b, alpha, beta, vecs, work, olwork, err)
*Computes the eigenvalues, and optionally the right eigenvectors of a square matrix assuming the structure of the eigenvalue problem is $A*X = \lambda*B*X$.*

4.5.1 Detailed Description

[linalg_eigen](#)

Purpose

Provides routines for computing the eigenvalues and eigenvectors of matrices.

4.5.2 Function/Subroutine Documentation

4.5.2.1 subroutine linalg_eigen::eigen_asymm (real(dp), dimension(:,:), intent(inout) a, complex(dp), dimension(:), intent(out) vals, complex(dp), dimension(:,:), intent(out), optional vecs, real(dp), dimension(:), intent(out), optional, pointer work, integer(i32), intent(out), optional olwork, class(errors), intent(inout), optional, target err) [private]

Computes the eigenvalues, and optionally the right eigenvectors of a square matrix.

Parameters

in, out	<i>a</i>	On input, the N-by-N matrix on which to operate. On output, the contents of this matrix are overwritten.
out	<i>vals</i>	An N-element array containing the eigenvalues of the matrix. The eigenvalues are not sorted.
out	<i>vecs</i>	An optional N-by-N matrix, that if supplied, signals to compute the right eigenvectors (one per column). If not provided, only the eigenvalues will be computed.
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> .
out	<i>olwork</i>	An optional output used to determine workspace size. If supplied, the routine determines the optimal size for <code>work</code> , and returns without performing any actual calculations.
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"> LA_ARRAY_SIZE_ERROR: Occurs if any of the input arrays are not sized appropriately. 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.

Notes

This routine utilizes the LAPACK routine DGEEV.

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

```
4.5.2.2 subroutine linalg_eigen::eigen_gen ( real(dp), dimension(:,:), intent(inout) a, real(dp), dimension(:,:), intent(inout)
      b, complex(dp), dimension(:), intent(out) alpha, real(dp), dimension(:), intent(out), optional beta, complex(dp),
      dimension(:,:), intent(out), optional vecs, real(dp), dimension(:), intent(out), optional, pointer work, integer(i32),
      intent(out), optional olwork, class(errors), intent(inout), optional, target err ) [private]
```

Computes the eigenvalues, and optionally the right eigenvectors of a square matrix assuming the structure of the eigenvalue problem is $A \cdot X = \lambda B \cdot X$.

Parameters

in, out	<i>a</i>	On input, the N-by-N matrix A. On output, the contents of this matrix are overwritten.
in, out	<i>b</i>	On input, the N-by-N matrix B. On output, the contents of this matrix are overwritten.
out	<i>alpha</i>	An N-element array that, if <code>beta</code> is not supplied, contains the eigenvalues. If <code>beta</code> is supplied however, the eigenvalues must be computed as $\text{ALPHA} / \text{BETA}$. This however, is not as trivial as it seems as it is entirely possible, and likely, that $\text{ALPHA} / \text{BETA}$ can overflow or underflow. With that said, the values in ALPHA will always be less than and usually comparable with the $\text{NORM}(A)$.
out	<i>beta</i>	An optional N-element array that if provided forces <code>alpha</code> to return the numerator, and this array contains the denominator used to determine the eigenvalues as $\text{ALPHA} / \text{BETA}$. If used, the values in this array will always be less than and usually comparable with the $\text{NORM}(B)$.

Parameters

out	<i>vecs</i>	An optional N-by-N matrix, that if supplied, signals to compute the right eigenvectors (one per column). If not provided, only the eigenvalues will be computed.
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> .
out	<i>olwork</i>	An optional output used to determine workspace size. If supplied, the routine determines the optimal size for <code>work</code> , and returns without performing any actual calculations.
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>LA_ARRAY_SIZE_ERROR</code>: Occurs if any of the input arrays are not sized appropriately. • <code>LA_OUT_OF_MEMORY_ERROR</code>: Occurs if local memory must be allocated, and there is insufficient memory available. • <code>LA_CONVERGENCE_ERROR</code>: Occurs if the algorithm failed to converge.

Usage

As an example, consider the eigenvalue problem arising from a mechanical system of masses and springs such that the masses are described by a mass matrix M , and the arrangement of springs are described by a stiffness matrix K .

```
! Parameters
real(dp), parameter :: pi = 3.141592653589793d0

! Variables
real(dp), dimension(n, n) :: m, k
complex(dp), dimension(n, n) :: mode_shapes
complex(dp), dimension(n) :: vals
real(dp), dimension(n) :: nat_freq

! Initialize the mass matrix (m) and the stiffness matrix (k)...

! Solve the eigenvalue problem. The eigenvectors define the mode shapes
! for the system (each eigenvector defines a different mode shape, and
! are stored one per column).
call eigen(k, m, vals, vecs = mode_shapes)

! The eigenvalues represent the square of the system natural frequencies.
! Also, a properly constrained mechanical system will exhibit only real
! eigenvalues; therefore, the following relationship will return the
! natural frequencies with units of Hz.
nat_freq = sqrt(real(vals, dp)) / (2.0d0 * pi)
```

Notes

This routine utilizes the LAPACK routine DGGEV.

Definition at line 426 of file `linalg_eigen.f90`.

4.5.2.3 `subroutine linalg_eigen::eigen_symm (logical, intent(in) vecs, real(dp), dimension(:, :), intent(inout) a, real(dp), dimension(:, :), intent(out) vals, real(dp), dimension(:, :), intent(out), optional, pointer work, integer(i32), intent(out), optional olwork, class(errors), intent(inout), optional, target err) [private]`

Computes the eigenvalues, and optionally the eigenvectors of a real, symmetric matrix.

Parameters

in	<i>vecs</i>	Set to true to compute the eigenvectors as well as the eigenvalues; else, set to false to just compute the eigenvalues.
in, out	<i>a</i>	On input, the N-by-N symmetric matrix on which to operate. On output, and if <i>vecs</i> is set to true, the matrix will contain the eigenvectors (one per column) corresponding to each eigenvalue in <i>vals</i> . If <i>vecs</i> is set to false, the lower triangular portion of the matrix is overwritten.
out	<i>vals</i>	An N-element array that will contain the eigenvalues sorted into ascending order.
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 <i>olwork</i> .
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 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>LA_ARRAY_SIZE_ERROR</code>: Occurs if any of the input arrays are not sized appropriately. • <code>LA_OUT_OF_MEMORY_ERROR</code>: Occurs if local memory must be allocated, and there is insufficient memory available. • <code>LA_CONVERGENCE_ERROR</code>: Occurs if the algorithm failed to converge.

Notes

This routine utilizes the LAPACK routine DSYEV.

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

4.6 linalg_factor Module Reference

[linalg_factor](#)

Data Types

- interface [form_lu](#)
Extracts the L and U matrices from the condensed [L\U] storage format used by the [lu_factor](#).
- interface [form_qr](#)
Forms the full M-by-M orthogonal matrix Q from the elementary reflectors returned by the base QR factorization algorithm.
- interface [mult_qr](#)
Multiplies a general matrix by the orthogonal matrix Q from a QR factorization.
- interface [mult_rz](#)
Multiplies a general matrix by the orthogonal matrix Z from an RZ factorization.
- interface [qr_factor](#)
Computes the QR factorization of an M-by-N matrix.

Functions/Subroutines

- subroutine, public [lu_factor](#) (a, ipvt, err)
Computes the LU factorization of an M-by-N matrix.
- subroutine [form_lu_all](#) (lu, ipvt, u, p, err)
Extracts the L, U, and P matrices from the output of the [lu_factor](#) routine.
- subroutine [form_lu_only](#) (lu, u, err)
Extracts the L, and U matrices from the output of the [lu_factor](#) routine.
- subroutine [qr_factor_no_pivot](#) (a, tau, work, olwork, err)
Computes the QR factorization of an M-by-N matrix without pivoting.
- subroutine [qr_factor_pivot](#) (a, tau, jpvt, work, olwork, err)
*Computes the QR factorization of an M-by-N matrix with column pivoting such that $A * P = Q * R$.*
- subroutine [form_qr_no_pivot](#) (r, tau, q, work, olwork, err)
Forms the full M-by-M orthogonal matrix Q from the elementary reflectors returned by the base QR factorization algorithm.
- subroutine [form_qr_pivot](#) (r, tau, pvt, q, p, work, olwork, err)
Forms the full M-by-M orthogonal matrix Q from the elementary reflectors returned by the base QR factorization algorithm.
- subroutine [mult_qr_mtx](#) (lside, trans, a, tau, c, work, olwork, err)
*Multiplies a general matrix by the orthogonal matrix Q from a QR factorization such that: $C = op(Q) * C$, or $C = C * op(Q)$.*
- subroutine [mult_qr_vec](#) (trans, a, tau, c, work, olwork, err)
*Multiplies a vector by the orthogonal matrix Q from a QR factorization such that: $C = op(Q) * C$.*
- subroutine, public [qr_rank1_update](#) (q, r, u, v, work, err)
*Computes the rank 1 update to an M-by-N QR factored matrix A ($M \geq N$) where $A = Q * R$, and $A1 = A + U * V^{**}T$ such that $A1 = Q1 * R1$.*
- subroutine, public [cholesky_factor](#) (a, upper, err)
Computes the Cholesky factorization of a symmetric, positive definite matrix.
- subroutine, public [cholesky_rank1_update](#) (r, u, work, err)
Computes the rank 1 update to a Cholesky factored matrix (upper triangular).
- subroutine, public [rz_factor](#) (a, tau, work, olwork, err)
*Factors an upper trapezoidal matrix by means of orthogonal transformations such that $A = R * Z = (R \ 0) * Z$. Z is an orthogonal matrix of dimension N-by-N, and R is an M-by-M upper triangular matrix.*
- subroutine [mult_rz_mtx](#) (lside, trans, l, a, tau, c, work, olwork, err)
*Multiplies a general matrix by the orthogonal matrix Z from an RZ factorization such that: $C = op(Z) * C$, or $C = C * op(Z)$.*
- subroutine [mult_rz_vec](#) (trans, l, a, tau, c, work, olwork, err)
*Multiplies a vector by the orthogonal matrix Z from an RZ factorization such that: $C = op(Z) * C$.*
- subroutine, public [svd](#) (a, s, u, vt, work, olwork, err)
*Computes the singular value decomposition of a matrix A. The SVD is defined as: $A = U * S * V^{**}T$, where U is an M-by-M orthogonal matrix, S is an M-by-N diagonal matrix, and V is an N-by-N orthogonal matrix.*

4.6.1 Detailed Description

[linalg_factor](#)

Purpose

Provides a set of matrix factorization routines.

4.6.2 Function/Subroutine Documentation

4.6.2.1 subroutine, public `linalg_factor::cholesky_factor` (`real(dp)`, `dimension(:, :)`, intent(inout) *a*, `logical`, intent(in), optional *upper*, `class(errors)`, intent(inout), optional, target *err*)

Computes the Cholesky factorization of a symmetric, positive definite matrix.

Parameters

in, out	<i>a</i>	On input, the N-by-N matrix to factor. On output, the factored matrix is returned in either the upper or lower triangular portion of the matrix, dependent upon the value of <code>upper</code> .
in	<i>upper</i>	An optional input that, if specified, provides control over whether the factorization is computed as $A = U^{**T} * U$ (set to true), or as $A = L * L^{**T}$ (set to false). The default value is true such that $A = U^{**T} * U$.
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>LA_ARRAY_SIZE_ERROR</code>: Occurs if <i>a</i> is not square. • <code>LA_MATRIX_FORMAT_ERROR</code>: Occurs if <i>a</i> is not positive definite.

Usage

To solve a system of N equations of N unknowns using Cholesky factorization, the following code will suffice. Notice, the system of equations must be positive definite.

```
! Solve the system: A*X = B, where A is an N-by-N matrix, and B and X are
! N-by-NRHS in size.

! Variables
real(dp), dimension(n, n) :: a
real(dp), dimension(n, nrhs) :: b
logical :: upper

! Initialize A and B...

! Specify that we're using the upper portion of A (remember positive
! definite matrices are symmetric)
upper = .true.

! Compute the factorization of A.
call cholesky_factor(a, upper)

! Solve A*X = B for X - Note: X overwrites B.
call solve_cholesky(upper, a, b)
```

Notes

This routine utilizes the LAPACK routine DPOTRF.

Definition at line 1307 of file `linalg_factor.f90`.

4.6.2.2 subroutine, public `linalg_factor::cholesky_rank1_update` (`real(dp), dimension(:, :), intent(inout) r`, `real(dp), dimension(:), intent(inout) u`, `real(dp), dimension(:), intent(out)`, optional, target *work*, `class(errors), intent(inout)`, optional, target *err*)

Computes the rank 1 update to a Cholesky factored matrix (upper triangular).

Parameters

in, out	<i>r</i>	On input, the N-by-N upper triangular matrix R. On output, the updated matrix R1.
in, out	<i>u</i>	On input, the N-element update vector U. On output, the rotation sines used to transform R to R1.
out	<i>work</i>	An optional argument that if supplied prevents local memory allocation. If provided, the array must have at least N elements. Additionally, this workspace array is used to contain the rotation cosines used to transform R to R1.

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"> • LA_ARRAY_SIZE_ERROR: Occurs if any of the input array sizes are incorrect. • LA_OUT_OF_MEMORY_ERROR: Occurs if local memory must be allocated, and there is insufficient memory available.
-----	-----	---

Notes

This routine utilizes the QRUPDATE routine DCH1UP.

See Also

[Source](#)

Definition at line 1399 of file linalg_factor.f90.

4.6.2.3 subroutine linalg_factor::form_lu_all (real(dp), dimension(:,:), intent(inout) *lu*, integer(i32), dimension(:), intent(in) *ipvt*, real(dp), dimension(:,:), intent(out) *u*, real(dp), dimension(:,:), intent(out) *p*, class(errors), intent(inout), optional, target *err*) [private]

Extracts the L, U, and P matrices from the output of the [lu_factor](#) routine.

Parameters

in, out	lu	On input, the N-by-N matrix as output by lu_factor . On output, the N-by-N lower triangular matrix L.
in	ipvt	The N-element pivot array as output by lu_factor .
out	u	An N-by-N matrix where the U matrix will be written.
out	p	An N-by-N matrix where the row permutation matrix will be written.
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"> • LA_ARRAY_SIZE_ERROR: Occurs if any of the input array sizes are incorrect.

Remarks

This routine allows extraction of the actual "L", "U", and "P" matrices of the decomposition. To use these matrices to solve the system $A \cdot X = B$, the following approach is used.

1. First, solve the linear system: $L \cdot Y = P \cdot B$ for Y.
2. Second, solve the linear system: $U \cdot X = Y$ for X.

Notice, as both L and U are triangular in structure, the above equations can be solved by forward and backward substitution.

See Also

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

Definition at line 210 of file linalg_factor.f90.

4.6.2.4 subroutine linalg_factor::form_lu_only (real(dp), dimension(:, :), intent(inout) *lu*, real(dp), dimension(:, :), intent(out) *u*, class(errors), intent(inout), optional, target *err*) [private]

Extracts the L, and U matrices from the output of the [lu_factor](#) routine.

Parameters

in, out	<i>lu</i>	On input, the N-by-N matrix as output by lu_factor . On output, the N-by-N lower triangular matrix L.
out	<i>u</i>	An N-by-N matrix where the U matrix will be written.
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"> • LA_ARRAY_SIZE_ERROR: Occurs if any of the input array sizes are incorrect.

Definition at line 287 of file linalg_factor.f90.

4.6.2.5 subroutine linalg_factor::form_qr_no_pivot (real(dp), dimension(:, :), intent(inout) *r*, real(dp), dimension(:, :), intent(in) *tau*, real(dp), dimension(:, :), intent(out) *q*, real(dp), dimension(:), intent(out), optional, target *work*, integer(i32), intent(out), optional *olwork*, class(errors), intent(inout), optional, target *err*) [private]

Forms the full M-by-M orthogonal matrix Q from the elementary reflectors returned by the base QR factorization algorithm.

Parameters

in, out	<i>r</i>	On input, an M-by-N matrix where the elements below the diagonal contain the elementary reflectors generated from the QR factorization. On and above the diagonal, the matrix contains the matrix R. On output, the elements below the diagonal are zeroed such that the remaining matrix is simply the M-by-N matrix R.
in	<i>tau</i>	A MIN(M, N)-element array containing the scalar factors of each elementary reflector defined in <i>r</i> .
out	<i>q</i>	An M-by-M matrix where the full orthogonal matrix Q will be written. In the event that M > N, Q may be supplied as M-by-N, and therefore only return the useful submatrix Q1 (Q = [Q1, Q2]) as the factorization can be written as Q * R = [Q1, Q2] * [R1; 0].
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 <i>olwork</i> .

Parameters

out	<i>olwork</i>	An optional output used to determine workspace size. If supplied, the routine determines the optimal size for <code>work</code> , and returns without performing any actual calculations.
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>LA_ARRAY_SIZE_ERROR</code>: Occurs if any of the input arrays are not sized appropriately. • <code>LA_OUT_OF_MEMORY_ERROR</code>: Occurs if local memory must be allocated, and there is insufficient memory available.

Notes

This routine utilizes the LAPACK routine DORGQR.

Definition at line 693 of file `linalg_factor.f90`.

4.6.2.6 subroutine `linalg_factor::form_qr_pivot` (`real(dp)`, `dimension(:, :)`, `intent(inout)` *r*, `real(dp)`, `dimension(:, :)`, `intent(in)` *tau*, `integer(i32)`, `dimension(:, :)`, `intent(in)` *pvt*, `real(dp)`, `dimension(:, :)`, `intent(out)` *q*, `real(dp)`, `dimension(:, :)`, `intent(out)` *p*, `real(dp)`, `dimension(:, :)`, `intent(out)`, optional, `target` *work*, `integer(i32)`, `intent(out)`, optional *olwork*, `class(errors)`, `intent(inout)`, optional, `target` *err*) [`private`]

Forms the full M-by-M orthogonal matrix Q from the elementary reflectors returned by the base QR factorization algorithm.

Parameters

in, out	<i>r</i>	On input, an M-by-N matrix where the elements below the diagonal contain the elementary reflectors generated from the QR factorization. On and above the diagonal, the matrix contains the matrix R. On output, the elements below the diagonal are zeroed such that the remaining matrix is simply the M-by-N matrix R.
in	<i>tau</i>	A MIN(M, N)-element array containing the scalar factors of each elementary reflector defined in <code>r</code> .
in	<i>pvt</i>	An N-element column pivot array as returned by the QR factorization.
out	<i>q</i>	An M-by-M matrix where the full orthogonal matrix Q will be written. In the event that $M > N$, Q may be supplied as M-by-N, and therefore only return the useful submatrix Q1 ($Q = [Q1, Q2]$) as the factorization can be written as $Q * R = [Q1, Q2] * [R1; 0]$.
out	<i>p</i>	An N-by-N matrix where the pivot matrix will be written.
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> .
out	<i>olwork</i>	An optional output used to determine workspace size. If supplied, the routine determines the optimal size for <code>work</code> , and returns without performing any actual calculations.
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>LA_ARRAY_SIZE_ERROR</code>: Occurs if any of the input arrays are not sized appropriately. • <code>LA_OUT_OF_MEMORY_ERROR</code>: Occurs if local memory must be allocated, and there is insufficient memory available.

Notes

This routine utilizes the LAPACK routine DORGQR.

Definition at line 824 of file linalg_factor.f90.

4.6.2.7 subroutine, public linalg_factor::lu_factor (real(dp), dimension(:, :), intent(inout) *a*, integer(i32), dimension(:), intent(out) *ipvt*, class(errors), intent(inout), optional, target *err*)

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

Parameters

in, out	<i>a</i>	On input, the M-by-N matrix on which to operate. On output, the LU factored matrix in the form [L\U] where the unit diagonal elements of L are not stored.
out	<i>ipvt</i>	An MIN(M, N)-element array used to track row-pivot operations. The array stored pivot information such that row <i>I</i> is interchanged with row IPVT(<i>I</i>).
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"> LA_ARRAY_SIZE_ERROR: Occurs if <i>ipvt</i> is not sized appropriately. LA_SINGULAR_MATRIX_ERROR: Occurs as a warning if <i>a</i> is found to be singular.

Usage

To solve a system of N equations of N unknowns using LU factorization, the following code will suffice.

```
! Solve the system: A*X = B, where A is an N-by-N matrix, and B and X are
! N-by-NRHS in size.

! Variables
real(dp), dimension(n, n) :: a
real(dp), dimension(n, nrhs) :: b

! Define the array used to track row pivots.
integer(i32), dimension(n) :: pvt

! Initialize A and B...

! Compute the LU factorization of A. On output, A contains [L\U].
call lu_factor(a, pvt)

! Solve A*X = B for X - Note: X overwrites B.
call solve_lu(a, pvt, b)
```

Notes

This routine utilizes the LAPACK routine DGETRF.

See Also

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

Definition at line 126 of file linalg_factor.f90.

4.6.2.8 subroutine `linalg_factor::mult_qr_mtx` (logical, intent(in) *lside*, logical, intent(in) *trans*, real(dp), dimension(:,:), intent(inout) *a*, real(dp), dimension(:), intent(in) *tau*, real(dp), dimension(:,:), intent(inout) *c*, real(dp), dimension(:), intent(out), optional, target *work*, integer(i32), intent(out), optional *olwork*, class(errors), intent(inout), optional, target *err*) [private]

Multiplies a general matrix by the orthogonal matrix *Q* from a QR factorization such that: $C = \text{op}(Q) * C$, or $C = C * \text{op}(Q)$.

Parameters

in	<i>lside</i>	Set to true to apply <i>Q</i> or <i>Q**T</i> from the left; else, set to false to apply <i>Q</i> or <i>Q**T</i> from the right.
in	<i>trans</i>	Set to true to apply <i>Q**T</i> ; else, set to false.
in	<i>a</i>	On input, an LDA-by-K matrix containing the elementary reflectors output from the QR factorization. If <i>lside</i> is set to true, LDA = M, and $M \geq K \geq 0$; else, if <i>lside</i> is set to false, LDA = N, and $N \geq K \geq 0$. Notice, the contents of this matrix are restored on exit.
in	<i>tau</i>	A K-element array containing the scalar factors of each elementary reflector defined in <i>a</i> .
in, out	<i>c</i>	On input, the M-by-N matrix <i>C</i> . On output, the product of the orthogonal matrix <i>Q</i> and the original matrix <i>C</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 <i>olwork</i> .
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 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"> LA_ARRAY_SIZE_ERROR: Occurs if any of the input arrays are not sized appropriately. LA_OUT_OF_MEMORY_ERROR: Occurs if local memory must be allocated, and there is insufficient memory available.

Notes

This routine utilizes the LAPACK routine DORMQR.

Definition at line 926 of file `linalg_factor.f90`.

4.6.2.9 subroutine `linalg_factor::mult_qr_vec` (logical, intent(in) *trans*, real(dp), dimension(:,:), intent(inout) *a*, real(dp), dimension(:), intent(in) *tau*, real(dp), dimension(:), intent(inout) *c*, real(dp), dimension(:), intent(out), optional, target *work*, integer(i32), intent(out), optional *olwork*, class(errors), intent(inout), optional, target *err*) [private]

Multiplies a vector by the orthogonal matrix *Q* from a QR factorization such that: $C = \text{op}(Q) * C$.

Parameters

in	<i>trans</i>	Set to true to apply <i>Q**T</i> ; else, set to false.
in	<i>a</i>	On input, an M-by-K matrix containing the elementary reflectors output from the QR factorization. Notice, the contents of this matrix are restored on exit.

Parameters

in	<i>tau</i>	A K-element array containing the scalar factors of each elementary reflector defined in <i>a</i> .
in, out	<i>c</i>	On input, the M-element vector <i>C</i> . On output, the product of the orthogonal matrix <i>Q</i> and the original vector <i>C</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 <i>olwork</i> .
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 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"> LA_ARRAY_SIZE_ERROR: Occurs if any of the input arrays are not sized appropriately. LA_OUT_OF_MEMORY_ERROR: Occurs if local memory must be allocated, and there is insufficient memory available.

Notes

This routine is based upon the LAPACK routine DORM2R.

Definition at line 1053 of file linalg_factor.f90.

```
4.6.2.10 subroutine linalg_factor::mult_rz_mtx ( logical, intent(in) lside, logical, intent(in) trans, integer(i32), intent(in) l,
real(dp), dimension(:, :), intent(inout) a, real(dp), dimension(:), intent(in) tau, real(dp), dimension(:, :), intent(inout)
c, real(dp), dimension(:), intent(out), optional, target work, integer(i32), intent(out), optional olwork, class(errors),
intent(inout), optional, target err ) [private]
```

Multiplies a general matrix by the orthogonal matrix *Z* from an RZ factorization such that: $C = \text{op}(Z) * C$, or $C = C * \text{op}(Z)$.

Parameters

in	<i>lside</i>	Set to true to apply <i>Z</i> or <i>Z**T</i> from the left; else, set to false to apply <i>Z</i> or <i>Z**T</i> from the right.
in	<i>trans</i>	Set to true to apply <i>Z**T</i> ; else, set to false.
in	<i>l</i>	The number of columns in matrix <i>a</i> containing the meaningful part of the Householder vectors. If <i>lside</i> is true, $M \geq L \geq 0$; else, if <i>lside</i> is false, $N \geq L \geq 0$.
in, out	<i>a</i>	On input the K-by-LTA matrix <i>Z</i> , where LTA = <i>M</i> if <i>lside</i> is true; else, LTA = <i>N</i> if <i>lside</i> is false. The <i>l</i> -th row must contain the Householder vector in the last <i>k</i> rows. Notice, the contents of this matrix are restored on exit.
in	<i>tau</i>	A K-element array containing the scalar factors of the elementary reflectors, where $M \geq K \geq 0$ if <i>lside</i> is true; else, $N \geq K \geq 0$ if <i>lside</i> is false.
in, out	<i>c</i>	On input, the M-by-N matrix <i>C</i> . On output, the product of the orthogonal matrix <i>Z</i> and the original matrix <i>C</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 <i>olwork</i> .

Parameters

out	<i>olwork</i>	An optional output used to determine workspace size. If supplied, the routine determines the optimal size for <code>work</code> , and returns without performing any actual calculations.
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>LA_ARRAY_SIZE_ERROR</code>: Occurs if any of the input arrays are not sized appropriately. • <code>LA_OUT_OF_MEMORY_ERROR</code>: Occurs if local memory must be allocated, and there is insufficient memory available.

Notes

This routine utilizes the LAPACK routine DORMRZ.

Definition at line 1643 of file `linalg_factor.f90`.

```
4.6.2.11 subroutine linalg_factor::mult_rz_vec ( logical, intent(in) trans, integer(i32), intent(in) l, real(dp), dimension(:,:),
intent(inout) a, real(dp), dimension(:), intent(in) tau, real(dp), dimension(:), intent(inout) c, real(dp), dimension(:),
intent(out), optional, target work, integer(i32), intent(out), optional olwork, class(errors), intent(inout), optional, target
err ) [private]
```

Multiplies a vector by the orthogonal matrix Z from an RZ factorization such that: $C = \text{op}(Z) * C$.

Parameters

in	<i>trans</i>	Set to true to apply Z^{**T} ; else, set to false.
in	<i>l</i>	The number of columns in matrix <i>a</i> containing the meaningful part of the Householder vectors. If <code>lside</code> is true, $M \geq L \geq 0$; else, if <code>lside</code> is false, $N \geq L \geq 0$.
in, out	<i>a</i>	On input the K-by-LTA matrix Z , where $LTA = M$ if <code>lside</code> is true; else, $LTA = N$ if <code>lside</code> is false. The <i>l</i> -th row must contain the Householder vector in the last <i>k</i> rows. Notice, the contents of this matrix are restored on exit.
in	<i>tau</i>	A K-element array containing the scalar factors of the elementary reflectors, where $M \geq K \geq 0$ if <code>lside</code> is true; else, $N \geq K \geq 0$ if <code>lside</code> is false.
in, out	<i>c</i>	On input, the M-element array <i>C</i> . On output, the product of the orthogonal matrix Z and the original array <i>C</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> .
out	<i>olwork</i>	An optional output used to determine workspace size. If supplied, the routine determines the optimal size for <code>work</code> , and returns without performing any actual calculations.
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>LA_ARRAY_SIZE_ERROR</code>: Occurs if any of the input arrays are not sized appropriately. • <code>LA_OUT_OF_MEMORY_ERROR</code>: Occurs if local memory must be allocated, and there is insufficient memory available.

Notes

This routine utilizes the LAPACK routine DORMRZ.

Definition at line 1785 of file linalg_factor.f90.

4.6.2.12 `subroutine linalg_factor::qr_factor_no_pivot (real(dp), dimension(:, :), intent(inout) a, real(dp), dimension(:, :), intent(out) tau, real(dp), dimension(:, :), intent(out), optional, target work, integer(i32), intent(out), optional olwork, class(errors), intent(inout), optional, target err) [private]`

Computes the QR factorization of an M-by-N matrix without pivoting.

Parameters

in, out	<i>a</i>	On input, the M-by-N matrix to factor. On output, the elements on and above the diagonal contain the MIN(M, N)-by-N upper trapezoidal matrix R (R is upper triangular if M ≥ N). The elements below the diagonal, along with the array <i>tau</i> , represent the orthogonal matrix Q as a product of elementary reflectors.
out	<i>tau</i>	A MIN(M, N)-element array used to store the scalar factors of the elementary reflectors.
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 <i>olwork</i> .
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 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>LA_ARRAY_SIZE_ERROR</code>: Occurs if <i>tau</i> or <i>work</i> are not sized appropriately. • <code>LA_OUT_OF_MEMORY_ERROR</code>: Occurs if local memory must be allocated, and there is insufficient memory available.

Remarks

QR factorization without pivoting is best suited to solving an overdetermined system in least-squares terms, or to solve a normally defined system. To solve an underdetermined system, it is recommended to use either LQ factorization, or a column-pivoting based QR factorization.

Usage

To solve a system of M equations of N unknowns using QR factorization, the following code will suffice assuming M ≥ N.

```
! Solve the system: A*X = B in a least-squares sense, where A is an
! M-by-N matrix, B is an M-by-NRHS matrix, and X is an N-by-NRHS matrix.

! Variables
real(dp), dimension(m, n) :: a
real(dp), dimension(m, nrhs) :: b, qtb
real(dp), dimension(n, nrhs) :: x
real(dp), dimension(n) :: tau
real(dp), dimension(m, m) :: q

! Initialize A and B...

! Compute the QR factorization. We're intentionally not forming the full
! Q matrix, but instead storing it in terms of its elementary reflector
```

```

! components in the sub-diagonal portions of A, and the corresponding
! scalar factors in TAU.  Additionally, we'll let the algorithm allocate
! it's own workspace array; therefore, the call to factor A is:
call qr_factor(a, tau)

! Solve A*X = B for X.  The first N rows of B are used to store X.
call solve_qr(a, tau, b)

! Also note, we could form Q and R explicitly.  Then solution of the
! system of equations can be found.  First we form Q and R.
call form_qr(a, tau, q) ! Forms Q, and R is stored in A

! Since we now have Q and R, we seek a solution to the equation:
! Q*R*X = B, but Q is an orthogonal matrix (i.e. Q**T = inv(Q)).
! Then: R*X = Q**T * B, and R is upper triangular; therefore, back
! substitution will suffice for a solution procedure.
!
! Next, compute Q**T * B, and store in QTB.
call mtx_mult(.true., .false., 1.0d0, q, b, 0.0d0, qtb)

! Copy the first N rows of Q**T * B into X for the solution process.
! Notice, only the first N rows are needed as rows N+1:M are all zero in
! matrix R.
x = qtb(1:n,nrhs)

! Compute the solution and store in X
call solve_triangular_system(.true., .true., .false., .true., 1.0d0, &
a(1:n,1:n), x)

```

Notes

This routine utilizes the LAPACK routine DGEQRF.

Definition at line 424 of file linalg_factor.f90.

4.6.2.13 subroutine linalg_factor::qr_factor_pivot (real(dp), dimension(:,:), intent(inout) *a*, real(dp), dimension(:), intent(out) *tau*, integer(i32), dimension(:), intent(inout) *jpvt*, real(dp), dimension(:), intent(out), optional, target *work*, integer(i32), intent(out), optional *olwork*, class(errors), intent(inout), optional, target *err*) [private]

Computes the QR factorization of an M-by-N matrix with column pivoting such that $A * P = Q * R$.

Parameters

in, out	<i>a</i>	On input, the M-by-N matrix to factor. On output, the elements on and above the diagonal contain the MIN(M, N)-by-N upper trapezoidal matrix R (R is upper triangular if $M \geq N$). The elements below the diagonal, along with the array <i>tau</i> , represent the orthogonal matrix Q as a product of elementary reflectors.
out	<i>tau</i>	A MIN(M, N)-element array used to store the scalar factors of the elementary reflectors.
in, out	<i>jpvt</i>	On input, an N-element array that if JPVT(I) .ne. 0, the I-th column of A is permuted to the front of $A * P$; if JPVT(I) = 0, the I-th column of A is a free column. On output, if JPVT(I) = K, then the I-th column of $A * P$ was the K-th column of A.
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 <i>olwork</i> .
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 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"> LA_ARRAY_SIZE_ERROR: Occurs if any of the input arrays are not sized appropriately. LA_OUT_OF_MEMORY_ERROR: Occurs if local memory must be allocated, and there is insufficient memory available.

Usage

To solve a system of M equations of N unknowns using QR factorization, the following code will suffice for any M and N .

```
! Solve the least-squares ( $M \geq N$ ), or the underdetermined ( $M < N$ )
! problem  $A \cdot X = B$ , where  $A$  is an  $M$ -by- $N$  matrix,  $B$  is an  $M$ -by-NRHS matrix,
! and  $X$  is an  $N$ -by-NRHS matrix. In the underdetermined case, or the
! case where the rank of matrix  $A$  is less than  $N$ , the solution obtained
! contains the fewest possible non-zero entries.

! Variables
real(dp), dimension(m, n) :: a
real(dp), dimension(n, nrhs) :: b
real(dp), dimension(k) :: tau ! k = min(m, n)
real(dp), dimension(m, m) :: q
real(dp), dimension(n, n) :: p
integer(i32), dimension(n) :: pvt

! Initialize A and B...

! Allow all columns to be free.
pvt = 0

! Compute the QR factorization. We're intentionally not forming the full
! Q matrix, but instead storing it in terms of its elementary reflector
! components in the sub-diagonal portions of A, and the corresponding
! scalar factors in TAU. Additionally, we'll let the algorithm allocate
! it's own workspace array; therefore, the call to factor A is:
call qr_factor(a, tau, pvt)

! Solve  $A \cdot X = B$  for  $X$ . If  $M > N$ , the first  $N$  rows of  $B$  are used to store
!  $X$ . If  $M < N$ , the input matrix  $B$  must be  $N$ -by-NRHS, and only the first
!  $M$  rows are used for the actual matrix  $B$ . The remaining  $N-M$  rows
! can contain whatever as they are not referenced until they are
! overwritten by the  $N$ -by-NRHS solution matrix  $X$ .
call solve_qr(a, tau, pvt, b)

! Notice, if the explicit Q matrix from the factorization is desired,
! the form_qr routine works similarly as in the no-pivot case;
! however, the permutation matrix P is also constructed. The call would
! be as follows. Also, as with the no-pivot algorithm, the matrix R is
! stored in matrix A.
call form_qr(a, tau, pvt, q, p)

! Solution can proceed as per typical, but with a full Q matrix. Also
! note, the problem is of the form:  $A \cdot P = Q \cdot R$ . Solution is straight
! forward, as with the no-pivot case; however, if  $M < N$ , then  $R$  is upper
! trapezoidal, and must be appropriately partitioned to solve. The rank
! of matrix  $r$  should be considered when applying the partition.
```

Notes

This routine utilizes the LAPACK routine DGEQP3.

Definition at line 578 of file linalg_factor.f90.

4.6.2.14 subroutine, public linalg_factor::qr_rank1_update (real(dp), dimension(:, :), intent(inout) q , real(dp), dimension(:, :), intent(inout) r , real(dp), dimension(:, :), intent(inout) u , real(dp), dimension(:, :), intent(inout) v , real(dp), dimension(:, :), intent(out), optional, target $work$, class(errors), intent(inout), optional, target err)

Computes the rank 1 update to an M -by- N QR factored matrix A ($M \geq N$) where $A = Q \cdot R$, and $A1 = A + U \cdot V^{**T}$ such that $A1 = Q1 \cdot R1$.

Parameters

in, out	q	On input, the original M -by- K orthogonal matrix Q . On output, the updated matrix $Q1$.
in, out	r	On input, the M -by- N matrix R . On output, the updated matrix $R1$.
in, out	u	On input, the M -element U update vector. On output, the original content of the array is overwritten.
in, out	v	On input, the N -element V update vector. On output, the original content of the array is overwritten.

Parameters

out	<i>work</i>	An optional argument that if supplied prevents local memory allocation. If provided, the array must have at least 2*K elements.
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>LA_ARRAY_SIZE_ERROR</code>: Occurs if any of the input arrays are not sized appropriately. • <code>LA_OUT_OF_MEMORY_ERROR</code>: Occurs if local memory must be allocated, and there is insufficient memory available.

Remarks

Notice, K must either be equal to M , or to N . In the event that $K = N$, only the submatrix Qa is updated. This is appropriate as the QR factorization for an overdetermined system can be written as follows:

$$A = Q * R = \begin{bmatrix} Qa & Qb \end{bmatrix} * \begin{bmatrix} Ra \\ 0 \end{bmatrix}$$

Note: Ra is upper triangular of dimension N -by- N .

Notes

This routine utilizes the QRUPDATE routine DQR1UP.

See Also

[Source](#)

Definition at line 1179 of file `linalg_factor.f90`.

4.6.2.15 subroutine, public `linalg_factor::rz_factor` (`real(dp)`, `dimension(:, :)`, `intent(inout)` *a*, `real(dp)`, `dimension(:)`, `intent(out)` *tau*, `real(dp)`, `dimension(:)`, `intent(out)`, optional, target *work*, `integer(i32)`, `intent(out)`, optional *olwork*, `class(errors)`, `intent(inout)`, optional, target *err*)

Factors an upper trapezoidal matrix by means of orthogonal transformations such that $A = R * Z = (R \ 0) * Z$. Z is an orthogonal matrix of dimension N -by- N , and R is an M -by- M upper triangular matrix.

Parameters

in, out	<i>a</i>	On input, the M -by- N upper trapezoidal matrix to factor. On output, the leading M -by- M upper triangular part of the matrix contains the upper triangular matrix R , and elements $N-L+1$ to N of the first M rows of A , with the array <i>tau</i> , represent the orthogonal matrix Z as a product of M elementary reflectors.
out	<i>tau</i>	An M -element array used to store the scalar factors of the elementary reflectors.
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> .
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.

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>LA_ARRAY_SIZE_ERROR</code>: Occurs if any of the input arrays are not sized appropriately. • <code>LA_OUT_OF_MEMORY_ERROR</code>: Occurs if local memory must be allocated, and there is insufficient memory available.
-----	-----	--

Further Details

The factorization is obtained by Householder's method. The k th transformation matrix, $Z(k)$, which is used to introduce zeros into the $(m - k + 1)$ th row of A , is given in the form

$$Z(k) = \begin{pmatrix} I & 0 \\ 0 & T(k) \end{pmatrix},$$

where

$$T(k) = I - \tau u(k) u(k)^* T, \quad u(k) = \begin{pmatrix} 1 \\ 0 \\ z(k) \end{pmatrix},$$

τ is a scalar and $z(k)$ is an l element vector. τ and $z(k)$ are chosen to annihilate the elements of the k th row of A_2 .

The scalar τ is returned in the k th element of TAU and the vector $u(k)$ in the k th row of A_2 , such that the elements of $z(k)$ are in $a(k, l + 1)$, ..., $a(k, n)$. The elements of R are returned in the upper triangular part of A_1 .

Z is given by

$$Z = Z(1) * Z(2) * \dots * Z(m).$$

Notes

This routine is based upon the LAPACK routine DTZRZF.

See Also

- [LAPACK Users Manual](#)

Definition at line 1531 of file `linalg_factor.f90`.

4.6.2.16 `subroutine, public linalg_factor::svd (real(dp), dimension(:, :), intent(inout) a, real(dp), dimension(:), intent(out) s, real(dp), dimension(:, :), intent(out), optional u, real(dp), dimension(:, :), intent(out), optional vt, real(dp), dimension(:), intent(out), optional, target work, integer(i32), intent(out), optional olwork, class(errors), intent(inout), optional, target err)`

Computes the singular value decomposition of a matrix A . The SVD is defined as: $A = U * S * V^* T$, where U is an M -by- M orthogonal matrix, S is an M -by- N diagonal matrix, and V is an N -by- N orthogonal matrix.

Parameters

in, out	<i>a</i>	On input, the M-by-N matrix to factor. The matrix is overwritten on output.
out	<i>s</i>	A MIN(M, N)-element array containing the singular values of <i>a</i> sorted in descending order.
out	<i>u</i>	An optional argument, that if supplied, is used to contain the orthogonal matrix U from the decomposition. The matrix U contains the left singular vectors, and can be either M-by-M (all left singular vectors are computed), or M-by-MIN(M,N) (only the first MIN(M, N) left singular vectors are computed).
out	<i>vt</i>	An optional argument, that if supplied, is used to contain the transpose of the N-by-N orthogonal matrix V. The matrix V contains the right singular vectors.
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> .
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 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>LA_ARRAY_SIZE_ERROR</code>: Occurs if any of the input arrays are not sized appropriately. • <code>LA_OUT_OF_MEMORY_ERROR</code>: Occurs if local memory must be allocated, and there is insufficient memory available. • <code>LA_CONVERGENCE_ERROR</code>: Occurs as a warning if the QR iteration process could not converge to a zero value.

Usage

```

! Decompose matrix the M-by-N matrix A such that A = U * S * V**T with
! M >= N.

! Variables
real(dp), dimension(m, n) :: a
real(dp), dimension(m, m) :: u
real(dp), dimension(n, n) :: vt
real(dp), dimension(n) :: s

! Initialize A...

! Compute the SVD of A. On output, S contains the MIN(M,N) singular
! values of A in descending order, U contains the left singular vectors
! (one per column), and VT contains the right singular vectors (one per
! row).
call svd(a, s, u, vt)

! Note: If M > N, then we can make U M-by-N, and compute the N
! left singular vectors of A, as there are at most N singular values
! of A. Also, if M < N, then there are at most M singular values of A,
! and as such, the length of the array s should be m.

```

Notes

This routine utilizes the LAPACK routine DGESVD.

See Also

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

Definition at line 1944 of file `linalg_factor.f90`.

4.7 linalg_solve Module Reference

linalg_solve

Data Types

- interface [solve_cholesky](#)
Solves a system of Cholesky factored equations.
- interface [solve_least_squares](#)
Solves the overdetermined or underdetermined system ($A \cdot X = B$) of M equations of N unknowns.
- interface [solve_least_squares_full](#)
Solves the overdetermined or underdetermined system ($A \cdot X = B$) of M equations of N unknowns, but uses a full orthogonal factorization of the system.
- interface [solve_least_squares_svd](#)
Solves the overdetermined or underdetermined system ($A \cdot X = B$) of M equations of N unknowns using a singular value decomposition of matrix A .
- interface [solve_lu](#)
Solves a system of LU-factored equations.
- interface [solve_qr](#)
Solves a system of M QR-factored equations of N unknowns.
- interface [solve_triangular_system](#)
Solves a triangular system of equations.

Functions/Subroutines

- subroutine [solve_tri_mtx](#) (lside, upper, trans, nounit, alpha, a, b, err)
*Solves one of the matrix equations: $op(A) * X = alpha * B$, or $X * op(A) = alpha * B$, where A is a triangular matrix.*
- subroutine [solve_tri_vec](#) (upper, trans, nounit, a, x, err)
*Solves the system of equations: $op(A) * X = B$, where A is a triangular matrix.*
- subroutine [solve_lu_mtx](#) (a, ipvt, b, err)
Solves a system of LU-factored equations.
- subroutine [solve_lu_vec](#) (a, ipvt, b, err)
Solves a system of LU-factored equations.
- subroutine [solve_qr_no_pivot_mtx](#) (a, tau, b, work, olwork, err)
Solves a system of M QR-factored equations of N unknowns where $M \geq N$.
- subroutine [solve_qr_no_pivot_vec](#) (a, tau, b, work, olwork, err)
Solves a system of M QR-factored equations of N unknowns where $M \geq N$.
- subroutine [solve_qr_pivot_mtx](#) (a, tau, jpvt, b, work, olwork, err)
Solves a system of M QR-factored equations of N unknowns where the QR factorization made use of column pivoting.
- subroutine [solve_qr_pivot_vec](#) (a, tau, jpvt, b, work, olwork, err)
Solves a system of M QR-factored equations of N unknowns where the QR factorization made use of column pivoting.
- subroutine [solve_cholesky_mtx](#) (upper, a, b, err)
Solves a system of Cholesky factored equations.
- subroutine [solve_cholesky_vec](#) (upper, a, b, err)
Solves a system of Cholesky factored equations.
- subroutine, public [mtx_inverse](#) (a, iwork, work, olwork, err)
Computes the inverse of a square matrix.
- subroutine, public [mtx_pinverse](#) (a, ainvtol, work, olwork, err)

Computes the Moore-Penrose pseudo-inverse of a M -by- N matrix using the singular value decomposition of the matrix.

- subroutine `solve_least_squares_mtx` (`a`, `b`, `work`, `olwork`, `err`)
Solves the overdetermined or underdetermined system ($A \cdot X = B$) of M equations of N unknowns using a QR or LQ factorization of the matrix A . Notice, it is assumed that matrix A has full rank.
- subroutine `solve_least_squares_vec` (`a`, `b`, `work`, `olwork`, `err`)
Solves the overdetermined or underdetermined system ($A \cdot X = B$) of M equations of N unknowns using a QR or LQ factorization of the matrix A . Notice, it is assumed that matrix A has full rank.
- subroutine `solve_least_squares_mtx_pvt` (`a`, `b`, `ipvt`, `arnk`, `work`, `olwork`, `err`)
Solves the overdetermined or underdetermined system ($A \cdot X = B$) of M equations of N unknowns using a complete orthogonal factorization of matrix A .
- subroutine `solve_least_squares_vec_pvt` (`a`, `b`, `ipvt`, `arnk`, `work`, `olwork`, `err`)
Solves the overdetermined or underdetermined system ($A \cdot X = B$) of M equations of N unknowns using a complete orthogonal factorization of matrix A .
- subroutine `solve_least_squares_mtx_svd` (`a`, `b`, `arnk`, `s`, `work`, `olwork`, `err`)
Solves the overdetermined or underdetermined system ($A \cdot X = B$) of M equations of N unknowns using a singular value decomposition of matrix A .
- subroutine `solve_least_squares_vec_svd` (`a`, `b`, `arnk`, `s`, `work`, `olwork`, `err`)
Solves the overdetermined or underdetermined system ($A \cdot X = B$) of M equations of N unknowns using a singular value decomposition of matrix A .

4.7.1 Detailed Description

`linalg_solve`

Purpose

Provides a set of routines for solving systems of linear equations.

4.7.2 Function/Subroutine Documentation

4.7.2.1 subroutine, public `linalg_solve::mtx_inverse` (`real(dp)`, `dimension(:, :)`, `intent(inout)` `a`, `integer(i32)`, `dimension(:)`, `intent(out)`, optional, target `iwork`, `real(dp)`, `dimension(:)`, `intent(out)`, optional, target `work`, `integer(i32)`, `intent(out)`, optional `olwork`, `class(errors)`, `intent(inout)`, optional, target `err`)

Computes the inverse of a square matrix.

Parameters

in, out	<code>a</code>	On input, the N -by- N matrix to invert. On output, the inverted matrix.
out	<code>iwork</code>	An optional N -element integer workspace array.
out	<code>work</code>	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> .
out	<code>olwork</code>	An optional output used to determine workspace size. If supplied, the routine determines the optimal size for <code>work</code> , and returns without performing any actual calculations.

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>LA_ARRAY_SIZE_ERROR</code>: Occurs if <code>a</code> is not square. Will also occur if incorrectly sized workspace arrays are provided. • <code>LA_OUT_OF_MEMORY_ERROR</code>: Occurs if local memory must be allocated, and there is insufficient memory available. • <code>LA_SINGULAR_MATRIX_ERROR</code>: Occurs if the input matrix is singular.
-----	-----	---

Usage

```

! The following example illustrates how to solve a system of linear
! equations by matrix inversion. Notice, this is not a preferred
! solution technique (use LU factorization instead), but is merely a
! means of illustrating how to compute the inverse of a square matrix.

! Variables
real(dp), dimension(n, n) :: a
real(dp), dimension(n, nrhs) :: b, x

! Initialize A and B...

! Compute the inverse of A. The inverse will overwrite the original
! matrix.
call mtx_inverse(a)

! Solve A*X = B as X = inv(A) * B.
x = matmul(a, b)

```

Notes

This routine utilizes the LAPACK routines DGETRF to perform an LU factorization of the matrix, and DGETRI to invert the LU factored matrix.

See Also

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

Definition at line 1240 of file linalg_solve.f90.

4.7.2.2 subroutine, public linalg_solve::mtx_pinverse (real(dp), dimension(:, :), intent(inout) *a*, real(dp), dimension(:, :), intent(out) *ainv*, real(dp), intent(in), optional *tol*, real(dp), dimension(:, :), intent(out), optional, target *work*, integer(i32), intent(out), optional *olwork*, class(errors), intent(inout), optional, target *err*)

Computes the Moore-Penrose pseudo-inverse of a M-by-N matrix using the singular value decomposition of the matrix.

Parameters

in, out	<i>a</i>	On input, the M-by-N matrix to invert. The matrix is overwritten on output.
out	<i>ainv</i>	The N-by-M matrix where the pseudo-inverse of <i>a</i> will be written.

Parameters

in	<i>tol</i>	An optional input, that if supplied, overrides the default tolerance on singular values such that singular values less than this tolerance are forced to have a reciprocal of zero, as opposed to $1/S(I)$. The default tolerance is: $\text{MAX}(M, N) * \text{EPS} * \text{MAX}(S)$. If the supplied value is less than a value that causes an overflow, the tolerance reverts back to its default value, and the operation continues; however, a warning message is issued.
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> .
out	<i>olwork</i>	An optional output used to determine workspace size. If supplied, the routine determines the optimal size for <code>work</code> , and returns without performing any actual calculations.
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>LA_ARRAY_SIZE_ERROR</code>: Occurs if any of the input arrays are not sized appropriately. • <code>LA_OUT_OF_MEMORY_ERROR</code>: Occurs if local memory must be allocated, and there is insufficient memory available. • <code>LA_CONVERGENCE_ERROR</code>: Occurs as a warning if the QR iteration process could not converge to a zero value.

Usage

```

! Use the pseudo-inverse to obtain a least-squares solution to the
! overdetermined problem  $A \cdot X = B$ , where A is an M-by-N matrix ( $M \geq N$ ),
! B is an M-by-NRHS matrix, and X is an N-by-NRHS matrix.

! Variables
real(dp), dimension(m, n) :: a
real(dp), dimension(n, m) :: ainvs
real(dp), dimension(m, nrhs) :: b
real(dp), dimension(n, nrhs) :: x

! Initialize A, and B...

! Compute the pseudo-inverse of A. Let the subroutine allocate its
! own workspace array.
call mt_xpinverse(a, ainvs)

! Compute  $X = AINV * B$  to obtain the solution.
x = matmul(ainvs, b)

```

See Also

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

Definition at line 1400 of file `linalg_solve.f90`.

4.7.2.3 `subroutine linalg_solve::solve_cholesky_mtx (logical, intent(in) upper, real(dp), dimension(:, :), intent(in) a, real(dp), dimension(:, :), intent(inout) b, class(errors), intent(inout), optional, target err) [private]`

Solves a system of Cholesky factored equations.

Parameters

in	<i>upper</i>	Set to true if the original matrix A was factored such that $A = U^{**T} * U$; else, set to false if the factorization of A was $A = L^{**T} * L$.
in	<i>a</i>	The N-by-N Cholesky factored matrix.
in, out	<i>b</i>	On input, the N-by-NRHS right-hand-side matrix B. On output, the solution matrix X.
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"> LA_ARRAY_SIZE_ERROR: Occurs if any of the input array sizes are incorrect.

Notes

This routine utilizes the LAPACK routine DPOTRS.

Definition at line 1073 of file linalg_solve.f90.

```
4.7.2.4 subroutine linalg_solve::solve_cholesky_vec ( logical, intent(in) upper, real(dp), dimension(:,:), intent(in) a, real(dp),
dimension(:), intent(inout) b, class(errors), intent(inout), optional, target err ) [private]
```

Solves a system of Cholesky factored equations.

Parameters

in	<i>upper</i>	Set to true if the original matrix A was factored such that $A = U^{**T} * U$; else, set to false if the factorization of A was $A = L^{**T} * L$.
in	<i>a</i>	The N-by-N Cholesky factored matrix.
in, out	<i>b</i>	On input, the N-element right-hand-side vector B. On output, the solution vector X.
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"> LA_ARRAY_SIZE_ERROR: Occurs if any of the input array sizes are incorrect.

Notes

This routine utilizes the LAPACK routine DPOTRS.

Definition at line 1139 of file linalg_solve.f90.

```
4.7.2.5 subroutine linalg_solve::solve_least_squares_mtx ( real(dp), dimension(:,:), intent(inout) a, real(dp), dimension(:,:),
intent(inout) b, real(dp), dimension(:), intent(out), optional, target work, integer(i32), intent(out), optional olwork,
class(errors), intent(inout), optional, target err ) [private]
```

Solves the overdetermined or underdetermined system ($A * X = B$) of M equations of N unknowns using a QR or LQ factorization of the matrix A. Notice, it is assumed that matrix A has full rank.

Parameters

in, out	<i>a</i>	On input, the M-by-N matrix A. On output, if $M \geq N$, the QR factorization of A in the form as output by <code>qr_factor</code> ; else, if $M < N$, the LQ factorization of A.
in, out	<i>b</i>	If $M \geq N$, the M-by-NRHS matrix B. On output, the first N rows contain the N-by-NRHS solution matrix X. If $M < N$, an N-by-NRHS matrix with the first M rows containing the matrix B. On output, the N-by-NRHS solution matrix X.
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> .
out	<i>olwork</i>	An optional output used to determine workspace size. If supplied, the routine determines the optimal size for <code>work</code> , and returns without performing any actual calculations.
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>LA_ARRAY_SIZE_ERROR</code>: Occurs if any of the input arrays are not sized appropriately. • <code>LA_OUT_OF_MEMORY_ERROR</code>: Occurs if local memory must be allocated, and there is insufficient memory available. • <code>LA_INVALID_OPERATION_ERROR</code>: Occurs if <i>a</i> is not of full rank.

Notes

This routine utilizes the LAPACK routine DGELS.

Definition at line 1568 of file `linalg_solve.f90`.

```
4.7.2.6 subroutine linalg_solve::solve_least_squares_mtx_pvt ( real(dp), dimension(:, :), intent(inout) a, real(dp), dimension(:, :),
intent(inout) b, integer(i32), dimension(:), intent(inout), optional, target ipvt, integer(i32), intent(out), optional arnk,
real(dp), dimension(:), intent(out), optional, target work, integer(i32), intent(out), optional olwork, class(errors),
intent(inout), optional, target err ) [private]
```

Solves the overdetermined or underdetermined system ($A \cdot X = B$) of M equations of N unknowns using a complete orthogonal factorization of matrix A.

Parameters

in, out	<i>a</i>	On input, the M-by-N matrix A. On output, the matrix is overwritten by the details of its complete orthogonal factorization.
in, out	<i>b</i>	If $M \geq N$, the M-by-NRHS matrix B. On output, the first N rows contain the N-by-NRHS solution matrix X. If $M < N$, an N-by-NRHS matrix with the first M rows containing the matrix B. On output, the N-by-NRHS solution matrix X.
out	<i>ipvt</i>	An optional input that on input, an N-element array that if <code>IPVT(I) .ne. 0</code> , the I-th column of A is permuted to the front of $A \cdot P$; if <code>IPVT(I) = 0</code> , the I-th column of A is a free column. On output, if <code>IPVT(I) = K</code> , then the I-th column of $A \cdot P$ was the K-th column of A. If not supplied, memory is allocated internally, and IPVT is set to all zeros such that all columns are treated as free.
out	<i>arnk</i>	An optional output, that if provided, will return the rank of <i>a</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> .

Parameters

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>	<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"> • LA_ARRAY_SIZE_ERROR: Occurs if any of the input arrays are not sized appropriately. • LA_OUT_OF_MEMORY_ERROR: Occurs if local memory must be allocated, and there is insufficient memory available.

Notes

This routine utilizes the LAPACK routine DGELSY.

Definition at line 1786 of file linalg_solve.f90.

```
4.7.2.7 subroutine linalg_solve::solve_least_squares_mtx_svd ( real(dp), dimension(:,:), intent(inout) a, real(dp), dimension(:,:),
intent(inout) b, integer(i32), intent(out), optional arnk, real(dp), dimension(:), intent(out) s, real(dp), dimension(:),
intent(out), optional, target work, integer(i32), intent(out), optional olwork, class(errors), intent(inout), optional, target
err ) [private]
```

Solves the overdetermined or underdetermined system ($A \cdot X = B$) of M equations of N unknowns using a singular value decomposition of matrix A .

Parameters

in, out	<i>a</i>	On input, the M -by- N matrix A . On output, the matrix is overwritten by the details of its complete orthogonal factorization.
in, out	<i>b</i>	If $M \geq N$, the M -by- N -RHS matrix B . On output, the first N rows contain the N -by- N -RHS solution matrix X . If $M < N$, an N -by- N -RHS matrix with the first M rows containing the matrix B . On output, the N -by- N -RHS solution matrix X .
out	<i>arnk</i>	An optional output, that if provided, will return the rank of a .
out	<i>s</i>	A $\text{MIN}(M, N)$ -element array that on output contains the singular values of a in descending order. Notice, the condition number of a can be determined by $S(1) / S(\text{MIN}(M, N))$.
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 <i>olwork</i> .
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>	<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"> • LA_ARRAY_SIZE_ERROR: Occurs if any of the input arrays are not sized appropriately. • LA_OUT_OF_MEMORY_ERROR: Occurs if local memory must be allocated, and there is insufficient memory available. • LA_CONVERGENCE_ERROR: Occurs as a warning if the QR iteration process could not converge to a zero value.
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Notes

This routine utilizes the LAPACK routine DGELSS.

Definition at line 2076 of file linalg_solve.f90.

4.7.2.8 subroutine linalg_solve::solve_least_squares_vec (real(dp), dimension(:, :), intent(inout) *a*, real(dp), dimension(:), intent(inout) *b*, real(dp), dimension(:), intent(out), optional, target *work*, integer(i32), intent(out), optional *olwork*, class(errors), intent(inout), optional, target *err*) [private]

Solves the overdetermined or underdetermined system ($A \cdot X = B$) of M equations of N unknowns using a QR or LQ factorization of the matrix A . Notice, it is assumed that matrix A has full rank.

Parameters

in, out	<i>a</i>	On input, the M -by- N matrix A . On output, if $M \geq N$, the QR factorization of A in the form as output by <code>qr_factor</code> ; else, if $M < N$, the LQ factorization of A .
in, out	<i>b</i>	If $M \geq N$, the M -element array B . On output, the first N elements contain the N -element solution array X . If $M < N$, an N -element array with the first M elements containing the array B . On output, the N -element solution array X .
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> .
out	<i>olwork</i>	An optional output used to determine workspace size. If supplied, the routine determines the optimal size for <code>work</code> , and returns without performing any actual calculations.
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"> LA_ARRAY_SIZE_ERROR: Occurs if any of the input arrays are not sized appropriately. LA_OUT_OF_MEMORY_ERROR: Occurs if local memory must be allocated, and there is insufficient memory available. LA_INVALID_OPERATION_ERROR: Occurs if <i>a</i> is not of full rank.

Notes

This routine utilizes the LAPACK routine DGELS.

Definition at line 1674 of file linalg_solve.f90.

4.7.2.9 subroutine linalg_solve::solve_least_squares_vec_pvt (real(dp), dimension(:, :), intent(inout) *a*, real(dp), dimension(:), intent(inout) *b*, integer(i32), dimension(:), intent(inout), optional, target *ipvt*, integer(i32), intent(out), optional *arnk*, real(dp), dimension(:), intent(out), optional, target *work*, integer(i32), intent(out), optional *olwork*, class(errors), intent(inout), optional, target *err*) [private]

Solves the overdetermined or underdetermined system ($A \cdot X = B$) of M equations of N unknowns using a complete orthogonal factorization of matrix A .

Parameters

in, out	<i>a</i>	On input, the M-by-N matrix A. On output, the matrix is overwritten by the details of its complete orthogonal factorization.
in, out	<i>b</i>	If $M \geq N$, the M-element array B. On output, the first N elements contain the N-element solution array X. If $M < N$, an N-element array with the first M elements containing the array B. On output, the N-element solution array X.
out	<i>ipvt</i>	An optional input that on input, an N-element array that if $IPVT(l) \neq 0$, the l-th column of A is permuted to the front of $A * P$; if $IPVT(l) = 0$, the l-th column of A is a free column. On output, if $IPVT(l) = K$, then the l-th column of $A * P$ was the K-th column of A. If not supplied, memory is allocated internally, and IPVT is set to all zeros such that all columns are treated as free.
out	<i>arnk</i>	An optional output, that if provided, will return the rank of <i>a</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 <i>olwork</i> .
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 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"> • LA_ARRAY_SIZE_ERROR: Occurs if any of the input arrays are not sized appropriately. • LA_OUT_OF_MEMORY_ERROR: Occurs if local memory must be allocated, and there is insufficient memory available.

Notes

This routine utilizes the LAPACK routine DGELSY.

Definition at line 1932 of file linalg_solve.f90.

4.7.2.10 `subroutine linalg_solve::solve_least_squares_vec_svd (real(dp), dimension(:,:), intent(inout) a, real(dp), dimension(:), intent(inout) b, integer(i32), intent(out), optional arnk, real(dp), dimension(:), intent(out) s, real(dp), dimension(:), intent(out), optional, target work, integer(i32), intent(out), optional olwork, class(errors), intent(inout), optional, target err) [private]`

Solves the overdetermined or underdetermined system ($A * X = B$) of M equations of N unknowns using a singular value decomposition of matrix A.

Parameters

in, out	<i>a</i>	On input, the M-by-N matrix A. On output, the matrix is overwritten by the details of its complete orthogonal factorization.
in, out	<i>b</i>	If $M \geq N$, the M-by-NRHS matrix B. On output, the first N rows contain the N-by-NRHS solution matrix X. If $M < N$, an N-by-NRHS matrix with the first M rows containing the matrix B. On output, the N-by-NRHS solution matrix X.
out	<i>arnk</i>	An optional output, that if provided, will return the rank of <i>a</i> .
out	<i>s</i>	A $\min(M, N)$ -element array that on output contains the singular values of <i>a</i> in descending order. Notice, the condition number of <i>a</i> can be determined by $S(1) / S(\min(M, N))$.

Parameters

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> .
out	<i>olwork</i>	An optional output used to determine workspace size. If supplied, the routine determines the optimal size for <code>work</code> , and returns without performing any actual calculations.
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>LA_ARRAY_SIZE_ERROR</code>: Occurs if any of the input arrays are not sized appropriately. • <code>LA_OUT_OF_MEMORY_ERROR</code>: Occurs if local memory must be allocated, and there is insufficient memory available. • <code>LA_CONVERGENCE_ERROR</code>: Occurs as a warning if the QR iteration process could not converge to a zero value.

Notes

This routine utilizes the LAPACK routine DGEELSS.

Definition at line 2204 of file `linalg_solve.f90`.

4.7.2.11 `subroutine linalg_solve::solve_lu_mtx (real(dp), dimension(:, :), intent(in) a, integer(i32), dimension(:), intent(in) ipvt, real(dp), dimension(:, :), intent(inout) b, class(errors), intent(inout), optional, target err) [private]`

Solves a system of LU-factored equations.

Parameters

in	<i>a</i>	The N-by-N LU factored matrix as output by <code>lu_factor</code> .
in	<i>ipvt</i>	The N-element pivot array as output by <code>lu_factor</code> .
in, out	<i>b</i>	On input, the N-by-NRHS right-hand-side matrix. On output, the N-by-NRHS solution matrix.
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>LA_ARRAY_SIZE_ERROR</code>: Occurs if any of the input array sizes are incorrect.

Notes

The routine is based upon the LAPACK routine DGETRS.

Definition at line 351 of file `linalg_solve.f90`.

4.7.2.12 subroutine `linalg_solve::solve_lu_vec` (`real(dp)`, `dimension(:, :)`, `intent(in)` *a*, `integer(i32)`, `dimension(:)`, `intent(in)` *ipvt*, `real(dp)`, `dimension(:)`, `intent(inout)` *b*, `class(errors)`, `intent(inout)`, optional, `target err`) [`private`]

Solves a system of LU-factored equations.

Parameters

in	<i>a</i>	The N-by-N LU factored matrix as output by <code>lu_factor</code> .
in	<i>ipvt</i>	The N-element pivot array as output by <code>lu_factor</code> .
in, out	<i>b</i>	On input, the N-element right-hand-side array. On output, the N-element solution array.
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>LA_ARRAY_SIZE_ERROR</code>: Occurs if any of the input array sizes are incorrect.

Notes

The routine is based upon the LAPACK routine DGETRS.

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

4.7.2.13 subroutine `linalg_solve::solve_qr_no_pivot_mtx` (`real(dp)`, `dimension(:, :)`, `intent(inout)` *a*, `real(dp)`, `dimension(:)`, `intent(in)` *tau*, `real(dp)`, `dimension(:, :)`, `intent(inout)` *b*, `real(dp)`, `dimension(:)`, `intent(out)`, optional, `target work`, `integer(i32)`, `intent(out)`, optional *olwork*, `class(errors)`, `intent(inout)`, optional, `target err`) [`private`]

Solves a system of M QR-factored equations of N unknowns where $M \geq N$.

Parameters

in	<i>a</i>	On input, the M-by-N QR factored matrix as returned by <code>qr_factor</code> . On output, the contents of this matrix are restored. Notice, M must be greater than or equal to N.
in	<i>tau</i>	A MIN(M, N)-element array containing the scalar factors of the elementary reflectors as returned by <code>qr_factor</code> .
in	<i>b</i>	On input, the M-by-NRHS right-hand-side matrix. On output, the first N columns are overwritten by the solution matrix X.
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> .
out	<i>olwork</i>	An optional output used to determine workspace size. If supplied, the routine determines the optimal size for <code>work</code> , and returns without performing any actual calculations.
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>LA_ARRAY_SIZE_ERROR</code>: Occurs if any of the input arrays are not sized appropriately. • <code>LA_OUT_OF_MEMORY_ERROR</code>: Occurs if local memory must be allocated, and there is insufficient memory available.

Notes

This routine is based upon a subset of the LAPACK routine DGELS.

Definition at line 487 of file linalg_solve.f90.

4.7.2.14 `subroutine linalg_solve::solve_qr_no_pivot_vec (real(dp), dimension(:, :), intent(inout) a, real(dp), dimension(:), intent(in) tau, real(dp), dimension(:), intent(inout) b, real(dp), dimension(:), intent(out), optional, target work, integer(i32), intent(out), optional olwork, class(errors), intent(inout), optional, target err) [private]`

Solves a system of M QR-factored equations of N unknowns where $M \geq N$.

Parameters

in	<i>a</i>	On input, the M -by- N QR factored matrix as returned by <code>qr_factor</code> . On output, the contents of this matrix are restored. Notice, M must be greater than or equal to N .
in	<i>tau</i>	A $\min(M, N)$ -element array containing the scalar factors of the elementary reflectors as returned by <code>qr_factor</code> .
in	<i>b</i>	On input, the M -element right-hand-side vector. On output, the first N elements are overwritten by the solution vector X .
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> .
out	<i>olwork</i>	An optional output used to determine workspace size. If supplied, the routine determines the optimal size for <code>work</code> , and returns without performing any actual calculations.
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"> LA_ARRAY_SIZE_ERROR: Occurs if any of the input arrays are not sized appropriately. LA_OUT_OF_MEMORY_ERROR: Occurs if local memory must be allocated, and there is insufficient memory available.

Notes

This routine is based upon a subset of the LAPACK routine DGELS.

Definition at line 602 of file linalg_solve.f90.

4.7.2.15 `subroutine linalg_solve::solve_qr_pivot_mtx (real(dp), dimension(:, :), intent(inout) a, real(dp), dimension(:), intent(in) tau, integer(i32), dimension(:), intent(in) jpvt, real(dp), dimension(:, :), intent(inout) b, real(dp), dimension(:), intent(out), optional, target work, integer(i32), intent(out), optional olwork, class(errors), intent(inout), optional, target err) [private]`

Solves a system of M QR-factored equations of N unknowns where the QR factorization made use of column pivoting.

Parameters

in	<i>a</i>	On input, the M-by-N QR factored matrix as returned by <code>qr_factor</code> . On output, the contents of this matrix are altered.
in	<i>tau</i>	A MIN(M, N)-element array containing the scalar factors of the elementary reflectors as returned by <code>qr_factor</code> .
in	<i>jpvt</i>	An N-element array, as output by <code>qr_factor</code> , used to track the column pivots.
in	<i>b</i>	On input, the MAX(M, N)-by-NRHS matrix where the first M rows contain the right-hand-side matrix B. On output, the first N rows are overwritten by the solution matrix X.
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> .
out	<i>olwork</i>	An optional output used to determine workspace size. If supplied, the routine determines the optimal size for <code>work</code> , and returns without performing any actual calculations.
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>LA_ARRAY_SIZE_ERROR</code>: Occurs if any of the input arrays are not sized appropriately. • <code>LA_OUT_OF_MEMORY_ERROR</code>: Occurs if local memory must be allocated, and there is insufficient memory available.

Notes

This routine is based upon a subset of the LAPACK routine DGELSY.

Definition at line 715 of file `linalg_solve.f90`.

4.7.2.16 `subroutine linalg_solve::solve_qr_pivot_vec (real(dp), dimension(:, :), intent(inout) a, real(dp), dimension(:), intent(in) tau, integer(i32), dimension(:), intent(in) jpvt, real(dp), dimension(:), intent(inout) b, real(dp), dimension(:), intent(out), optional, target work, integer(i32), intent(out), optional olwork, class(errors), intent(inout), optional, target err)`
`[private]`

Solves a system of M QR-factored equations of N unknowns where the QR factorization made use of column pivoting.

Parameters

in	<i>a</i>	On input, the M-by-N QR factored matrix as returned by <code>qr_factor</code> . On output, the contents of this matrix are altered.
in	<i>tau</i>	A MIN(M, N)-element array containing the scalar factors of the elementary reflectors as returned by <code>qr_factor</code> .
in	<i>jpvt</i>	An N-element array, as output by <code>qr_factor</code> , used to track the column pivots.
in	<i>b</i>	On input, the MAX(M, N)-element array where the first M elements contain the right-hand-side vector B. On output, the first N elements are overwritten by the solution vector X.
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> .
out	<i>olwork</i>	An optional output used to determine workspace size. If supplied, the routine determines the optimal size for <code>work</code> , and returns without performing any actual calculations.

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"> LA_ARRAY_SIZE_ERROR: Occurs if any of the input arrays are not sized appropriately. LA_OUT_OF_MEMORY_ERROR: Occurs if local memory must be allocated, and there is insufficient memory available.
-----	-----	--

Notes

This routine is based upon a subset of the LAPACK routine DGELSY.

Definition at line 902 of file linalg_solve.f90.

4.7.2.17 subroutine linalg_solve::solve_tri_mtx (logical, intent(in) *lside*, logical, intent(in) *upper*, logical, intent(in) *trans*, logical, intent(in) *nounit*, real(dp), intent(in) *alpha*, real(dp), dimension(:,:), intent(in) *a*, real(dp), dimension(:,:), intent(inout) *b*, class(errors), intent(inout), optional, target *err*) [private]

Solves one of the matrix equations: $\text{op}(A) * X = \alpha * B$, or $X * \text{op}(A) = \alpha * B$, where A is a triangular matrix.

Parameters

in	<i>lside</i>	Set to true to solve $\text{op}(A) * X = \alpha * B$; else, set to false to solve $X * \text{op}(A) = \alpha * B$.
in	<i>upper</i>	Set to true if A is an upper triangular matrix; else, set to false if A is a lower triangular matrix.
in	<i>trans</i>	Set to true if $\text{op}(A) = A^{**T}$; else, set to false if $\text{op}(A) = A$.
in	<i>nounit</i>	Set to true if A is not a unit-diagonal matrix (ones on every diagonal element); else, set to false if A is a unit-diagonal matrix.
in	<i>alpha</i>	The scalar multiplier to B .
in	<i>a</i>	If <i>lside</i> is true, the M -by- M triangular matrix on which to operate; else, if <i>lside</i> is false, the N -by- N triangular matrix on which to operate.
in, out	<i>b</i>	On input, the M -by- N right-hand-side. On output, the M -by- N solution.
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"> LA_ARRAY_SIZE_ERROR: Occurs if <i>a</i> is not square, or if the sizes of <i>a</i> and <i>b</i> are not compatible.

Usage

To solve a triangular system of N equations of N unknowns $A * X = B$, where A is an N -by- N upper triangular matrix, and B and X are N -by- N matrices, the following code will suffice.

```
! Solve the system: A*X = B, where A is an upper triangular N-by-N
```

```

! matrix, and B and X are N-by-NRHS in size.

! Variables
integer(i32) :: info
real(dp), dimension(n, n) :: a
real(dp), dimension(n, nrhs) :: b

! Initialize A and B...

! Solve A*X = B for X - Note: X overwrites B.
call solve_triangular_system(.true., .true., .false., .true., &
    1.0d0, a, b)

```

Notes

This routine is based upon the BLAS routine DTRSM.

Definition at line 169 of file linalg_solve.f90.

4.7.2.18 subroutine linalg_solve::solve_tri_vec (logical, intent(in) *upper*, logical, intent(in) *trans*, logical, intent(in) *nounit*, real(dp), dimension(:,:), intent(in) *a*, real(dp), dimension(:), intent(inout) *x*, class(errors), intent(inout), optional, target *err*) [private]

Solves the system of equations: $\text{op}(A) * X = B$, where A is a triangular matrix.

Parameters

in	<i>upper</i>	Set to true if A is an upper triangular matrix; else, set to false if A is a lower triangular matrix.
in	<i>trans</i>	Set to true if $\text{op}(A) = A^{**T}$; else, set to false if $\text{op}(A) = A$.
in	<i>nounit</i>	Set to true if A is not a unit-diagonal matrix (ones on every diagonal element); else, set to false if A is a unit-diagonal matrix.
in	<i>a</i>	The N-by-N triangular matrix.
in, out	<i>x</i>	On input, the N-element right-hand-side array. On output, the N-element solution array.
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"> LA_ARRAY_SIZE_ERROR: Occurs if a is not square, or if the sizes of a and b are not compatible.

Usage

To solve a triangular system of N equations of N unknowns $A * X = B$, where A is an N-by-N upper triangular matrix, and B and X are N-element arrays, the following code will suffice.

```

! Solve the system: A*X = B, where A is an upper triangular N-by-N
! matrix, and B and X are N-elements in size.

! Variables
integer(i32) :: info
real(dp), dimension(n, n) :: a
real(dp), dimension(n) :: b

! Initialize A and B...

! Solve A*X = B for X - Note: X overwrites B.
call solve_triangular_system(.true., .false., a, b)

```

Notes

This routine is based upon the BLAS routine DTRSV.

Definition at line 275 of file linalg_solve.f90.

Chapter 5

Data Type Documentation

5.1 linalg_core::diag_mtx_mult Interface Reference

Multiplies a diagonal matrix with another matrix or array.

Private Member Functions

- subroutine [diag_mtx_mult_mtx](#) (lside, trans, alpha, a, b, beta, c, err)
*Computes the matrix operation: $C = \alpha * A * op(B) + \beta * C$, or $C = \alpha * op(B) * A + \beta * C$.*
- subroutine [diag_mtx_mult_mtx2](#) (lside, alpha, a, b, err)
*Computes the matrix operation: $B = \alpha * A * op(B)$, or $B = \alpha * op(B) * A$.*
- subroutine [diag_mtx_mult_mtx3](#) (lside, trans, alpha, a, b, beta, c, err)
*Computes the matrix operation: $C = \alpha * A * op(B) + \beta * C$, or $C = \alpha * op(B) * A + \beta * C$, where A and C are complex-valued.*
- subroutine [diag_mtx_mult_mtx4](#) (lside, trans, alpha, a, b, beta, c, err)
*Computes the matrix operation: $C = \alpha * A * op(B) + \beta * C$, or $C = \alpha * op(B) * A + \beta * C$, where A , B , and C are complex-valued.*

5.1.1 Detailed Description

Multiplies a diagonal matrix with another matrix or array.

Definition at line 45 of file linalg_core.f90.

5.1.2 Member Function/Subroutine Documentation

5.1.2.1 subroutine linalg_core::diag_mtx_mult::diag_mtx_mult_mtx (logical, intent(in) lside, logical, intent(in) trans, real(dp) alpha, real(dp), dimension(:), intent(in) a, real(dp), dimension(:, :), intent(in) b, real(dp) beta, real(dp), dimension(:, :), intent(inout) c, class(errors), intent(inout), optional, target err) [private]

Computes the matrix operation: $C = \alpha * A * op(B) + \beta * C$, or $C = \alpha * op(B) * A + \beta * C$.

Parameters

in	<i>lside</i>	Set to true to apply matrix A from the left; else, set to false to apply matrix A from the left.
in	<i>trans</i>	Set to true if $\text{op}(B) == B^{**T}$; else, set to false if $\text{op}(B) == B$.
in	<i>alpha</i>	A scalar multiplier.
in	<i>a</i>	A K-element array containing the diagonal elements of A where $K = \text{MIN}(M,P)$ if <i>lside</i> is true; else, if <i>lside</i> is false, $K = \text{MIN}(N,P)$.
in	<i>b</i>	The LDB-by-TDB matrix B where (LDB = leading dimension of B, and TDB = trailing dimension of B): <ul style="list-style-type: none"> <code>lside == true & trans == true</code>: LDB = N, TDB = P <code>lside == true & trans == false</code>: LDB = P, TDB = N <code>lside == false & trans == true</code>: LDB = P, TDB = M <code>lside == false & trans == false</code>: LDB = M, TDB = P
in	<i>beta</i>	A scalar multiplier.
in, out	<i>c</i>	On input, the M-by-N matrix C. On output, the resulting M-by-N matrix.
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>LA_ARRAY_SIZE_ERROR</code>: Occurs if any of the input array sizes are incorrect.

Definition at line 326 of file `linalg_core.f90`.

5.1.2.2 subroutine `linalg_core::diag_mtx_mult::diag_mtx_mult_mtx2` (`logical`, `intent(in) lside`, `real(dp)`, `intent(in) alpha`, `real(dp)`, `dimension(:)`, `intent(in) a`, `real(dp)`, `dimension(:, :)`, `intent(inout) b`, `class(errors)`, `intent(inout)`, optional, `target err`) [private]

Computes the matrix operation: $B = \alpha * A * \text{op}(B)$, or $B = \alpha * \text{op}(B) * A$.

Parameters

in	<i>lside</i>	Set to true to apply matrix A from the left; else, set to false to apply matrix A from the left.
in	<i>alpha</i>	A scalar multiplier.
in	<i>a</i>	A K-element array containing the diagonal elements of A where $K = \text{MIN}(M,P)$ if <i>lside</i> is true; else, if <i>lside</i> is false, $K = \text{MIN}(N,P)$.
in	<i>b</i>	On input, the M-by-N matrix B. On output, the resulting M-by-N matrix.
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>LA_ARRAY_SIZE_ERROR</code>: Occurs if any of the input array sizes are incorrect.

Definition at line 493 of file `linalg_core.f90`.

5.1.2.3 subroutine `linalg_core::diag_mtx_mult::diag_mtx_mult_mtx3` (`logical, intent(in) lside`, `logical, intent(in) trans`, `real(dp) alpha`, `complex(dp), dimension(:), intent(in) a`, `real(dp), dimension(:, :), intent(in) b`, `real(dp) beta`, `complex(dp), dimension(:, :), intent(inout) c`, `class(errors), intent(inout), optional, target err`) [private]

Computes the matrix operation: $C = \alpha * A * \text{op}(B) + \beta * C$, or $C = \alpha * \text{op}(B) * A + \beta * C$, where A and C are complex-valued.

Parameters

in	<i>lside</i>	Set to true to apply matrix A from the left; else, set to false to apply matrix A from the left.
in	<i>trans</i>	Set to true if $\text{op}(B) == B^{**T}$; else, set to false if $\text{op}(B) == B$.
in	<i>alpha</i>	A scalar multiplier.
in	<i>a</i>	A K -element array containing the diagonal elements of A where $K = \text{MIN}(M, P)$ if <i>lside</i> is true; else, if <i>lside</i> is false, $K = \text{MIN}(N, P)$.
in	<i>b</i>	The LDB-by-TDB matrix B where (LDB = leading dimension of B , and TDB = trailing dimension of B): <ul style="list-style-type: none"> <i>lside</i> == true & <i>trans</i> == true: LDB = N, TDB = P <i>lside</i> == true & <i>trans</i> == false: LDB = P, TDB = N <i>lside</i> == false & <i>trans</i> == true: LDB = P, TDB = M <i>lside</i> == false & <i>trans</i> == false: LDB = M, TDB = P
in	<i>beta</i>	A scalar multiplier.
in, out	<i>c</i>	On input, the M -by- N matrix C . On output, the resulting M -by- N matrix.
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"> LA_ARRAY_SIZE_ERROR: Occurs if any of the input array sizes are incorrect.

Definition at line 576 of file `linalg_core.f90`.

5.1.2.4 subroutine `linalg_core::diag_mtx_mult::diag_mtx_mult_mtx4` (`logical, intent(in) lside`, `logical, intent(in) trans`, `real(dp) alpha`, `complex(dp), dimension(:), intent(in) a`, `complex(dp), dimension(:, :), intent(in) b`, `real(dp) beta`, `complex(dp), dimension(:, :), intent(inout) c`, `class(errors), intent(inout), optional, target err`) [private]

Computes the matrix operation: $C = \alpha * A * \text{op}(B) + \beta * C$, or $C = \alpha * \text{op}(B) * A + \beta * C$, where A , B , and C are complex-valued.

Parameters

in	<i>lside</i>	Set to true to apply matrix A from the left; else, set to false to apply matrix A from the left.
in	<i>trans</i>	Set to true if $\text{op}(B) == B^{**T}$; else, set to false if $\text{op}(B) == B$.
in	<i>alpha</i>	A scalar multiplier.
in	<i>a</i>	A K -element array containing the diagonal elements of A where $K = \text{MIN}(M, P)$ if <i>lside</i> is true; else, if <i>lside</i> is false, $K = \text{MIN}(N, P)$.

Parameters

in	<i>b</i>	<p>The LDB-by-TDB matrix B where:</p> <ul style="list-style-type: none"> • <code>lside == true & trans == true</code>: LDA = N, TDB = P • <code>lside == true & trans == false</code>: LDA = P, TDB = N • <code>lside == false & trans == true</code>: LDA = P, TDB = M • <code>lside == false & trans == false</code>: LDA = M, TDB = P
in	<i>beta</i>	A scalar multiplier.
in, out	<i>c</i>	On input, the M-by-N matrix C. On output, the resulting M-by-N matrix.
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>LA_ARRAY_SIZE_ERROR</code>: Occurs if any of the input array sizes are incorrect.

Definition at line 752 of file `linalg_core.f90`.

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

- `/home/jason/Documents/Code/linalg/src/linalg_core.f90`

5.2 lapack::DLAMCH Interface Reference

Public Member Functions

- `real(dp)` function **dlamch** (cmach)

5.2.1 Detailed Description

Definition at line 14 of file `lapack.f90`.

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

- `/home/jason/Documents/Code/linalg/src/lapack.f90`

5.3 linalg_eigen::eigen Interface Reference

Computes the eigenvalues, and optionally the eigenvectors, of a matrix.

Private Member Functions

- subroutine [eigen_symm](#) (vecs, a, vals, work, olwork, err)
Computes the eigenvalues, and optionally the eigenvectors of a real, symmetric matrix.
- subroutine [eigen_asymm](#) (a, vals, vecs, work, olwork, err)
Computes the eigenvalues, and optionally the right eigenvectors of a square matrix.
- subroutine [eigen_gen](#) (a, b, alpha, beta, vecs, work, olwork, err)
*Computes the eigenvalues, and optionally the right eigenvectors of a square matrix assuming the structure of the eigenvalue problem is $A*X = \lambda*B*X$.*

5.3.1 Detailed Description

Computes the eigenvalues, and optionally the eigenvectors, of a matrix.

See Also

- [Wikipedia](#)
- [Wolfram MathWorld](#)
- [LAPACK Users Manual](#)

Definition at line 24 of file linalg_eigen.f90.

5.3.2 Member Function/Subroutine Documentation

5.3.2.1 subroutine linalg_eigen::eigen::eigen_asymm (real(dp), dimension(:, :), intent(inout) a, complex(dp), dimension(:), intent(out) vals, complex(dp), dimension(:, :), intent(out), optional vecs, real(dp), dimension(:), intent(out), optional, pointer work, integer(i32), intent(out), optional olwork, class(errors), intent(inout), optional, target err) [private]

Computes the eigenvalues, and optionally the right eigenvectors of a square matrix.

Parameters

in, out	a	On input, the N-by-N matrix on which to operate. On output, the contents of this matrix are overwritten.
out	vals	An N-element array containing the eigenvalues of the matrix. The eigenvalues are not sorted.
out	vecs	An optional N-by-N matrix, that if supplied, signals to compute the right eigenvectors (one per column). If not provided, only the eigenvalues will be computed.
out	work	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 olwork.
out	olwork	An optional output used to determine workspace size. If supplied, the routine determines the optimal size for work, and returns without performing any actual calculations.
out	err	An optional errors-based object that if provided can be used to retrieve information relating to any errors encountered during execution. If not provided, a default implementation of the errors class is used internally to provide error handling. Possible errors and warning messages that may be encountered are as follows. <ul style="list-style-type: none"> • LA_ARRAY_SIZE_ERROR: Occurs if any of the input arrays are not sized appropriately. • LA_OUT_OF_MEMORY_ERROR: Occurs if local memory must be allocated, and there is insufficient memory available.
Generated by Doxygen		<ul style="list-style-type: none"> • LA_CONVERGENCE_ERROR: Occurs if the algorithm failed to converge.

Notes

This routine utilizes the LAPACK routine DGEEV.

Definition at line 185 of file linalg_eigen.f90.

```
5.3.2.2 subroutine linalg_eigen::eigen::eigen_gen ( real(dp), dimension(:,:), intent(inout) a, real(dp), dimension(:,:), intent(inout)
b, complex(dp), dimension(:,:), intent(out) alpha, real(dp), dimension(:,:), intent(out), optional beta, complex(dp),
dimension(:,:), intent(out), optional vecs, real(dp), dimension(:,:), intent(out), optional, pointer work, integer(i32),
intent(out), optional olwork, class(errors), intent(inout), optional, target err ) [private]
```

Computes the eigenvalues, and optionally the right eigenvectors of a square matrix assuming the structure of the eigenvalue problem is $A \cdot X = \lambda B \cdot X$.

Parameters

in, out	<i>a</i>	On input, the N-by-N matrix A. On output, the contents of this matrix are overwritten.
in, out	<i>b</i>	On input, the N-by-N matrix B. On output, the contents of this matrix are overwritten.
out	<i>alpha</i>	An N-element array that, if <i>beta</i> is not supplied, contains the eigenvalues. If <i>beta</i> is supplied however, the eigenvalues must be computed as ALPHA / BETA. This however, is not as trivial as it seems as it is entirely possible, and likely, that ALPHA / BETA can overflow or underflow. With that said, the values in ALPHA will always be less than and usually comparable with the NORM(A).
out	<i>beta</i>	An optional N-element array that if provided forces <i>alpha</i> to return the numerator, and this array contains the denominator used to determine the eigenvalues as ALPHA / BETA. If used, the values in this array will always be less than and usually comparable with the NORM(B).
out	<i>vecs</i>	An optional N-by-N matrix, that if supplied, signals to compute the right eigenvectors (one per column). If not provided, only the eigenvalues will be computed.
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 <i>olwork</i> .
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 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"> LA_ARRAY_SIZE_ERROR: Occurs if any of the input arrays are not sized appropriately. 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.

Usage

As an example, consider the eigenvalue problem arising from a mechanical system of masses and springs such that the masses are described by a mass matrix *M*, and the arrangement of springs are described by a stiffness matrix *K*.

```
! Parameters
real(dp), parameter :: pi = 3.141592653589793d0
```

```

! Variables
real(dp), dimension(n, n) :: m, k
complex(dp), dimension(n, n) :: mode_shapes
complex(dp), dimension(n) :: vals
real(dp), dimension(n) :: nat_freq

! Initialize the mass matrix (m) and the stiffness matrix (k)...

! Solve the eigenvalue problem. The eigenvectors define the mode shapes
! for the system (each eigenvector defines a different mode shape, and
! are stored one per column).
call eigen(k, m, vals, vecs = mode_shapes)

! The eigenvalues represent the square of the system natural frequencies.
! Also, a properly constrained mechanical system will exhibit only real
! eigenvalues; therefore, the following relationship will return the
! natural frequencies with units of Hz.
nat_freq = sqrt(real(vals, dp)) / (2.0d0 * pi)

```

Notes

This routine utilizes the LAPACK routine DGGEV.

Definition at line 426 of file linalg_eigen.f90.

5.3.2.3 subroutine linalg_eigen::eigen::eigen_symm (logical, intent(in) *vecs*, real(dp), dimension(:, :), intent(inout) *a*, real(dp), dimension(:, :), intent(out) *vals*, real(dp), dimension(:, :), intent(out), optional, pointer *work*, integer(i32), intent(out), optional *olwork*, class(errors), intent(inout), optional, target *err*) [private]

Computes the eigenvalues, and optionally the eigenvectors of a real, symmetric matrix.

Parameters

in	<i>vecs</i>	Set to true to compute the eigenvectors as well as the eigenvalues; else, set to false to just compute the eigenvalues.
in, out	<i>a</i>	On input, the N-by-N symmetric matrix on which to operate. On output, and if <i>vecs</i> is set to true, the matrix will contain the eigenvectors (one per column) corresponding to each eigenvalue in <i>vals</i> . If <i>vecs</i> is set to false, the lower triangular portion of the matrix is overwritten.
out	<i>vals</i>	An N-element array that will contain the eigenvalues sorted into ascending order.
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 <i>olwork</i> .
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 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"> LA_ARRAY_SIZE_ERROR: Occurs if any of the input arrays are not sized appropriately. 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.

Notes

This routine utilizes the LAPACK routine DSYEV.

Definition at line 68 of file linalg_eigen.f90.

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

- /home/jason/Documents/Code/linalg/src/linalg_eigen.f90

5.4 linalg_factor::form_lu Interface Reference

Extracts the L and U matrices from the condensed [L\U] storage format used by the [lu_factor](#).

Private Member Functions

- subroutine [form_lu_all](#) (lu, ipvt, u, p, err)
Extracts the L, U, and P matrices from the output of the [lu_factor](#) routine.
- subroutine [form_lu_only](#) (lu, u, err)
Extracts the L, and U matrices from the output of the [lu_factor](#) routine.

5.4.1 Detailed Description

Extracts the L and U matrices from the condensed [L\U] storage format used by the [lu_factor](#).

Definition at line 30 of file linalg_factor.f90.

5.4.2 Member Function/Subroutine Documentation

5.4.2.1 subroutine linalg_factor::form_lu::form_lu_all (real(dp), dimension(:,:), intent(inout) *lu*, integer(i32), dimension(:), intent(in) *ipvt*, real(dp), dimension(:,:), intent(out) *u*, real(dp), dimension(:,:), intent(out) *p*, class(errors), intent(inout), optional, target *err*) [private]

Extracts the L, U, and P matrices from the output of the [lu_factor](#) routine.

Parameters

in, out	<i>lu</i>	On input, the N-by-N matrix as output by lu_factor . On output, the N-by-N lower triangular matrix L.
in	<i>ipvt</i>	The N-element pivot array as output by lu_factor .
out	<i>u</i>	An N-by-N matrix where the U matrix will be written.
out	<i>p</i>	An N-by-N matrix where the row permutation matrix will be written.
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"> • LA_ARRAY_SIZE_ERROR: Occurs if any of the input array sizes are incorrect.

Remarks

This routine allows extraction of the actual "L", "U", and "P" matrices of the decomposition. To use these matrices to solve the system $A \cdot X = B$, the following approach is used.

1. First, solve the linear system: $L \cdot Y = P \cdot B$ for Y .
2. Second, solve the linear system: $U \cdot X = Y$ for X .

Notice, as both L and U are triangular in structure, the above equations can be solved by forward and backward substitution.

See Also

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

Definition at line 210 of file linalg_factor.f90.

```
5.4.2.2 subroutine linalg_factor::form_lu::form_lu_only ( real(dp), dimension(:, :), intent(inout) lu, real(dp), dimension(:, :),
               intent(out) u, class(errors), intent(inout), optional, target err ) [private]
```

Extracts the L , and U matrices from the output of the [lu_factor](#) routine.

Parameters

in, out	<i>lu</i>	On input, the N-by-N matrix as output by lu_factor . On output, the N-by-N lower triangular matrix L .
out	<i>u</i>	An N-by-N matrix where the U matrix will be written.
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"> • LA_ARRAY_SIZE_ERROR: Occurs if any of the input array sizes are incorrect.

Definition at line 287 of file linalg_factor.f90.

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

- /home/jason/Documents/Code/linalg/src/linalg_factor.f90

5.5 linalg_factor::form_qr Interface Reference

Forms the full M-by-M orthogonal matrix Q from the elementary reflectors returned by the base QR factorization algorithm.

Private Member Functions

- subroutine `form_qr_no_pivot` (*r*, *tau*, *q*, *work*, *olwork*, *err*)
Forms the full *M*-by-*M* orthogonal matrix *Q* from the elementary reflectors returned by the base QR factorization algorithm.
- subroutine `form_qr_pivot` (*r*, *tau*, *pvt*, *q*, *p*, *work*, *olwork*, *err*)
Forms the full *M*-by-*M* orthogonal matrix *Q* from the elementary reflectors returned by the base QR factorization algorithm.

5.5.1 Detailed Description

Forms the full *M*-by-*M* orthogonal matrix *Q* from the elementary reflectors returned by the base QR factorization algorithm.

See Also

- [Wikipedia](#)
- [LAPACK Users Manual](#)

Definition at line 54 of file `linalg_factor.f90`.

5.5.2 Member Function/Subroutine Documentation

5.5.2.1 subroutine `linalg_factor::form_qr::form_qr_no_pivot` (*real*(*dp*), *dimension*(:,:), *intent*(*inout*) *r*, *real*(*dp*), *dimension*(:), *intent*(*in*) *tau*, *real*(*dp*), *dimension*(:,:), *intent*(*out*) *q*, *real*(*dp*), *dimension*(:), *intent*(*out*), optional, target *work*, *integer*(*i32*), *intent*(*out*), optional *olwork*, *class*(*errors*), *intent*(*inout*), optional, target *err*) [*private*]

Forms the full *M*-by-*M* orthogonal matrix *Q* from the elementary reflectors returned by the base QR factorization algorithm.

Parameters

<i>in, out</i>	<i>r</i>	On input, an <i>M</i> -by- <i>N</i> matrix where the elements below the diagonal contain the elementary reflectors generated from the QR factorization. On and above the diagonal, the matrix contains the matrix <i>R</i> . On output, the elements below the diagonal are zeroed such that the remaining matrix is simply the <i>M</i> -by- <i>N</i> matrix <i>R</i> .
<i>in</i>	<i>tau</i>	A MIN(<i>M</i> , <i>N</i>)-element array containing the scalar factors of each elementary reflector defined in <i>r</i> .
<i>out</i>	<i>q</i>	An <i>M</i> -by- <i>M</i> matrix where the full orthogonal matrix <i>Q</i> will be written. In the event that <i>M</i> > <i>N</i> , <i>Q</i> may be supplied as <i>M</i> -by- <i>N</i> , and therefore only return the useful submatrix <i>Q1</i> (<i>Q</i> = [<i>Q1</i> , <i>Q2</i>]) as the factorization can be written as <i>Q</i> * <i>R</i> = [<i>Q1</i> , <i>Q2</i>] * [<i>R1</i> ; 0].
<i>out</i>	<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 <i>olwork</i> .
<i>out</i>	<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.
<i>out</i>	<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>LA_ARRAY_SIZE_ERROR</code>: Occurs if any of the input arrays are not sized appropriately.
		<div>Generated by Doxygen</div> <ul style="list-style-type: none"> • <code>LA_OUT_OF_MEMORY_ERROR</code>: Occurs if local memory must be allocated, and there is insufficient memory available.

Notes

This routine utilizes the LAPACK routine DORGQR.

Definition at line 693 of file linalg_factor.f90.

5.5.2.2 subroutine linalg_factor::form_qr::form_qr_pivot (real(dp), dimension(:,:), intent(inout) *r*, real(dp), dimension(:), intent(in) *tau*, integer(i32), dimension(:), intent(in) *pvt*, real(dp), dimension(:,:), intent(out) *q*, real(dp), dimension(:,:), intent(out) *p*, real(dp), dimension(:), intent(out), optional, target *work*, integer(i32), intent(out), optional *olwork*, class(errors), intent(inout), optional, target *err*) [private]

Forms the full M-by-M orthogonal matrix Q from the elementary reflectors returned by the base QR factorization algorithm.

Parameters

in, out	<i>r</i>	On input, an M-by-N matrix where the elements below the diagonal contain the elementary reflectors generated from the QR factorization. On and above the diagonal, the matrix contains the matrix R. On output, the elements below the diagonal are zeroed such that the remaining matrix is simply the M-by-N matrix R.
in	<i>tau</i>	A MIN(M, N)-element array containing the scalar factors of each elementary reflector defined in <i>r</i> .
in	<i>pvt</i>	An N-element column pivot array as returned by the QR factorization.
out	<i>q</i>	An M-by-M matrix where the full orthogonal matrix Q will be written. In the event that $M > N$, Q may be supplied as M-by-N, and therefore only return the useful submatrix Q1 ($Q = [Q1, Q2]$) as the factorization can be written as $Q * R = [Q1, Q2] * [R1; 0]$.
out	<i>p</i>	An N-by-N matrix where the pivot matrix will be written.
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 <i>olwork</i> .
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 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"> LA_ARRAY_SIZE_ERROR: Occurs if any of the input arrays are not sized appropriately. LA_OUT_OF_MEMORY_ERROR: Occurs if local memory must be allocated, and there is insufficient memory available.

Notes

This routine utilizes the LAPACK routine DORGQR.

Definition at line 824 of file linalg_factor.f90.

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

- /home/jason/Documents/Code/linalg/src/linalg_factor.f90

5.6 linalg_core::mtx_mult Interface Reference

Performs the matrix operation: $C = \alpha * \text{op}(A) * \text{op}(B) + \beta * C$.

Private Member Functions

- subroutine `mtx_mult_mtx` (`transa`, `transb`, `alpha`, `a`, `b`, `beta`, `c`, `err`)
*Performs the matrix operation: $C = \alpha * \text{op}(A) * \text{op}(B) + \beta * C$.*
- subroutine `mtx_mult_vec` (`trans`, `alpha`, `a`, `b`, `beta`, `c`, `err`)
*Performs the matrix-vector operation: $c = \alpha * \text{op}(A) * b + \beta * c$.*

5.6.1 Detailed Description

Performs the matrix operation: $C = \alpha * \text{op}(A) * \text{op}(B) + \beta * C$.

Definition at line 38 of file `linalg_core.f90`.

5.6.2 Member Function/Subroutine Documentation

5.6.2.1 subroutine `linalg_core::mtx_mult::mtx_mult_mtx` (`logical`, intent(in) `transa`, `logical`, intent(in) `transb`, `real(dp)`, intent(in) `alpha`, `real(dp)`, dimension(:,:), intent(in) `a`, `real(dp)`, dimension(:,:), intent(in) `b`, `real(dp)`, intent(in) `beta`, `real(dp)`, dimension(:,:), intent(inout) `c`, `class(errors)`, intent(inout), optional, target `err`) [private]

Performs the matrix operation: $C = \alpha * \text{op}(A) * \text{op}(B) + \beta * C$.

Parameters

in	<code>transa</code>	Set to true if $\text{op}(A) = A^{**T}$; else, set to false for $\text{op}(A) = A$.
in	<code>transb</code>	Set to true if $\text{op}(B) = B^{**T}$; else, set to false for $\text{op}(B) = B$.
in	<code>alpha</code>	A scalar multiplier.
in	<code>a</code>	If <code>transa</code> is set to true, an K-by-M matrix; else, if <code>transa</code> is set to false, an M-by-K matrix.
in	<code>b</code>	If <code>transb</code> is set to true, an N-by-K matrix; else, if <code>transb</code> is set to false, a K-by-N matrix.
in	<code>beta</code>	A scalar multiplier.
in, out	<code>c</code>	On input, the M-by-N matrix C. On output, the M-by-N result.
out	<code>err</code>	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>LA_ARRAY_SIZE_ERROR</code>: Occurs if any of the input array sizes are incorrect.

Notes

This routine utilizes the BLAS routine DGEMM.

Definition at line 82 of file `linalg_core.f90`.

5.6.2.2 subroutine `linalg_core::mtx_mult::mtx_mult_vec` (`logical`, `intent(in)` *trans*, `real(dp)`, `intent(in)` *alpha*, `real(dp)`, `dimension(:, :)`, `intent(in)` *a*, `real(dp)`, `dimension(:)`, `intent(in)` *b*, `real(dp)`, `intent(in)` *beta*, `real(dp)`, `dimension(:)`, `intent(inout)` *c*, `class(errors)`, `intent(inout)`, `optional`, `target` *err*) [private]

Performs the matrix-vector operation: $c = \alpha * \text{op}(A) * b + \beta * c$.

Parameters

in	<i>trans</i>	Set to true if $\text{op}(A) = A^{**T}$; else, set to false for $\text{op}(A) = A$.
in	<i>alpha</i>	A scalar multiplier.
in	<i>a</i>	The M-by-N matrix A.
in	<i>b</i>	If <i>trans</i> is set to true, an M-element array; else, if <i>trans</i> is set to false, an N-element array.
in	<i>beta</i>	A scalar multiplier.
in, out	<i>c</i>	On input, if <i>trans</i> is set to true, an N-element array; else, if <i>trans</i> is set to false, an M-element array. On output, the results of the operation.
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"> LA_ARRAY_SIZE_ERROR: Occurs if any of the input array sizes are incorrect.

Notes

This routine utilizes the BLAS routine DGEMV.

Definition at line 176 of file `linalg_core.f90`.

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

- `/home/jason/Documents/Code/linalg/src/linalg_core.f90`

5.7 linalg_factor::mult_qr Interface Reference

Multiplies a general matrix by the orthogonal matrix Q from a QR factorization.

Private Member Functions

- subroutine `mult_qr_mtx` (*lside*, *trans*, *a*, *tau*, *c*, *work*, *olwork*, *err*)
*Multiplies a general matrix by the orthogonal matrix Q from a QR factorization such that: $C = \text{op}(Q) * C$, or $C = C * \text{op}(Q)$.*
- subroutine `mult_qr_vec` (*trans*, *a*, *tau*, *c*, *work*, *olwork*, *err*)
*Multiplies a vector by the orthogonal matrix Q from a QR factorization such that: $C = \text{op}(Q) * C$.*

5.7.1 Detailed Description

Multiplies a general matrix by the orthogonal matrix Q from a QR factorization.

Definition at line 62 of file `linalg_factor.f90`.

5.7.2 Member Function/Subroutine Documentation

5.7.2.1 subroutine `linalg_factor::mult_qr::mult_qr_mtx` (`logical`, intent(in) *lside*, `logical`, intent(in) *trans*, `real(dp)`, dimension(:,:), intent(inout) *a*, `real(dp)`, dimension(:), intent(in) *tau*, `real(dp)`, dimension(:,:), intent(inout) *c*, `real(dp)`, dimension(:), intent(out), optional, target *work*, `integer(i32)`, intent(out), optional *olwork*, `class(errors)`, intent(inout), optional, target *err*) [`private`]

Multiplies a general matrix by the orthogonal matrix Q from a QR factorization such that: $C = \text{op}(Q) * C$, or $C = C * \text{op}(Q)$.

Parameters

in	<i>lside</i>	Set to true to apply Q or Q**T from the left; else, set to false to apply Q or Q**T from the right.
in	<i>trans</i>	Set to true to apply Q**T; else, set to false.
in	<i>a</i>	On input, an LDA-by-K matrix containing the elementary reflectors output from the QR factorization. If <i>lside</i> is set to true, LDA = M, and $M \geq K \geq 0$; else, if <i>lside</i> is set to false, LDA = N, and $N \geq K \geq 0$. Notice, the contents of this matrix are restored on exit.
in	<i>tau</i>	A K-element array containing the scalar factors of each elementary reflector defined in <i>a</i> .
in, out	<i>c</i>	On input, the M-by-N matrix C. On output, the product of the orthogonal matrix Q and the original matrix C.
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 <i>olwork</i> .
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 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"> LA_ARRAY_SIZE_ERROR: Occurs if any of the input arrays are not sized appropriately. LA_OUT_OF_MEMORY_ERROR: Occurs if local memory must be allocated, and there is insufficient memory available.

Notes

This routine utilizes the LAPACK routine DORMQR.

Definition at line 926 of file `linalg_factor.f90`.

5.7.2.2 subroutine `linalg_factor::mult_qr::mult_qr_vec` (`logical`, intent(in) *trans*, `real(dp)`, dimension(:,:), intent(inout) *a*, `real(dp)`, dimension(:), intent(in) *tau*, `real(dp)`, dimension(:), intent(inout) *c*, `real(dp)`, dimension(:), intent(out), optional, target *work*, `integer(i32)`, intent(out), optional *olwork*, `class(errors)`, intent(inout), optional, target *err*) [`private`]

Multiplies a vector by the orthogonal matrix Q from a QR factorization such that: $C = \text{op}(Q) * C$.

Parameters

in	<i>trans</i>	Set to true to apply Q**T; else, set to false.
----	--------------	--

Parameters

in	<i>a</i>	On input, an M-by-K matrix containing the elementary reflectors output from the QR factorization. Notice, the contents of this matrix are restored on exit.
in	<i>tau</i>	A K-element array containing the scalar factors of each elementary reflector defined in <i>a</i> .
in, out	<i>c</i>	On input, the M-element vector C. On output, the product of the orthogonal matrix Q and the original vector C.
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> .
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 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"> LA_ARRAY_SIZE_ERROR: Occurs if any of the input arrays are not sized appropriately. LA_OUT_OF_MEMORY_ERROR: Occurs if local memory must be allocated, and there is insufficient memory available.

Notes

This routine is based upon the LAPACK routine DORM2R.

Definition at line 1053 of file `linalg_factor.f90`.

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

- `/home/jason/Documents/Code/linalg/src/linalg_factor.f90`

5.8 linalg_factor::mult_rz Interface Reference

Multiplies a general matrix by the orthogonal matrix Z from an RZ factorization.

Private Member Functions

- subroutine `mult_rz_mtx` (lside, trans, l, a, tau, c, work, olwork, err)
*Multiplies a general matrix by the orthogonal matrix Z from an RZ factorization such that: $C = op(Z) * C$, or $C = C * op(Z)$.*
- subroutine `mult_rz_vec` (trans, l, a, tau, c, work, olwork, err)
*Multiplies a vector by the orthogonal matrix Z from an RZ factorization such that: $C = op(Z) * C$.*

5.8.1 Detailed Description

Multiplies a general matrix by the orthogonal matrix Z from an RZ factorization.

Definition at line 70 of file `linalg_factor.f90`.

5.8.2 Member Function/Subroutine Documentation

5.8.2.1 subroutine `linalg_factor::mult_rz::mult_rz_mtx` (logical, intent(in) *lside*, logical, intent(in) *trans*, integer(i32), intent(in) *l*, real(dp), dimension(:,:), intent(inout) *a*, real(dp), dimension(:), intent(in) *tau*, real(dp), dimension(:,:), intent(inout) *c*, real(dp), dimension(:), intent(out), optional, target *work*, integer(i32), intent(out), optional *olwork*, class(errors), intent(inout), optional, target *err*) [private]

Multiplies a general matrix by the orthogonal matrix Z from an RZ factorization such that: $C = \text{op}(Z) * C$, or $C = C * \text{op}(Z)$.

Parameters

in	<i>lside</i>	Set to true to apply Z or Z**T from the left; else, set to false to apply Z or Z**T from the right.
in	<i>trans</i>	Set to true to apply Z**T; else, set to false.
in	<i>l</i>	The number of columns in matrix a containing the meaningful part of the Householder vectors. If <i>lside</i> is true, $M \geq L \geq 0$; else, if <i>lside</i> is false, $N \geq L \geq 0$.
in, out	<i>a</i>	On input the K-by-LTA matrix Z, where LTA = M if <i>lside</i> is true; else, LTA = N if <i>lside</i> is false. The l-th row must contain the Householder vector in the last k rows. Notice, the contents of this matrix are restored on exit.
in	<i>tau</i>	A K-element array containing the scalar factors of the elementary reflectors, where $M \geq K \geq 0$ if <i>lside</i> is true; else, $N \geq K \geq 0$ if <i>lside</i> is false.
in, out	<i>c</i>	On input, the M-by-N matrix C. On output, the product of the orthogonal matrix Z and the original matrix C.
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 <i>olwork</i> .
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 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"> LA_ARRAY_SIZE_ERROR: Occurs if any of the input arrays are not sized appropriately. LA_OUT_OF_MEMORY_ERROR: Occurs if local memory must be allocated, and there is insufficient memory available.

Notes

This routine utilizes the LAPACK routine DORMRZ.

Definition at line 1643 of file `linalg_factor.f90`.

5.8.2.2 subroutine `linalg_factor::mult_rz::mult_rz_vec` (logical, intent(in) *trans*, integer(i32), intent(in) *l*, real(dp), dimension(:,:), intent(inout) *a*, real(dp), dimension(:), intent(in) *tau*, real(dp), dimension(:), intent(inout) *c*, real(dp), dimension(:), intent(out), optional, target *work*, integer(i32), intent(out), optional *olwork*, class(errors), intent(inout), optional, target *err*) [private]

Multiplies a vector by the orthogonal matrix Z from an RZ factorization such that: $C = \text{op}(Z) * C$.

Parameters

in	<i>trans</i>	Set to true to apply Z^{**T} ; else, set to false.
in	<i>l</i>	The number of columns in matrix <i>a</i> containing the meaningful part of the Householder vectors. If <i>lside</i> is true, $M \geq L \geq 0$; else, if <i>lside</i> is false, $N \geq L \geq 0$.
in, out	<i>a</i>	On input the K-by-LTA matrix <i>Z</i> , where LTA = <i>M</i> if <i>lside</i> is true; else, LTA = <i>N</i> if <i>lside</i> is false. The <i>l</i> -th row must contain the Householder vector in the last <i>k</i> rows. Notice, the contents of this matrix are restored on exit.
in	<i>tau</i>	A K-element array containing the scalar factors of the elementary reflectors, where $M \geq K \geq 0$ if <i>lside</i> is true; else, $N \geq K \geq 0$ if <i>lside</i> is false.
in, out	<i>c</i>	On input, the M-element array <i>C</i> . On output, the product of the orthogonal matrix <i>Z</i> and the original array <i>C</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 <i>olwork</i> .
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 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>LA_ARRAY_SIZE_ERROR</code>: Occurs if any of the input arrays are not sized appropriately. • <code>LA_OUT_OF_MEMORY_ERROR</code>: Occurs if local memory must be allocated, and there is insufficient memory available.

Notes

This routine utilizes the LAPACK routine DORMRZ.

Definition at line 1785 of file `linalg_factor.f90`.

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

- `/home/jason/Documents/Code/linalg/src/linalg_factor.f90`

5.9 linalg_factor::qr_factor Interface Reference

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

Private Member Functions

- subroutine `qr_factor_no_pivot` (*a*, *tau*, *work*, *olwork*, *err*)
Computes the QR factorization of an M-by-N matrix without pivoting.
- subroutine `qr_factor_pivot` (*a*, *tau*, *jpvt*, *work*, *olwork*, *err*)
*Computes the QR factorization of an M-by-N matrix with column pivoting such that $A * P = Q * R$.*

5.9.1 Detailed Description

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

See Also

- [Wikipedia](#)
- [Wolfram MathWorld](#)
- [LAPACK Users Manual](#)

Definition at line 42 of file `linalg_factor.f90`.

5.9.2 Member Function/Subroutine Documentation

5.9.2.1 `subroutine linalg_factor::qr_factor::qr_factor_no_pivot (real(dp), dimension(:, :), intent(inout) a, real(dp), dimension(:, :), intent(out) tau, real(dp), dimension(:, :), intent(out), optional, target work, integer(i32), intent(out), optional olwork, class(errors), intent(inout), optional, target err) [private]`

Computes the QR factorization of an M-by-N matrix without pivoting.

Parameters

in, out	<i>a</i>	On input, the M-by-N matrix to factor. On output, the elements on and above the diagonal contain the MIN(M, N)-by-N upper trapezoidal matrix R (R is upper triangular if M ≥ N). The elements below the diagonal, along with the array <i>tau</i> , represent the orthogonal matrix Q as a product of elementary reflectors.
out	<i>tau</i>	A MIN(M, N)-element array used to store the scalar factors of the elementary reflectors.
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 <i>olwork</i> .
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 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>LA_ARRAY_SIZE_ERROR</code>: Occurs if <i>tau</i> or <i>work</i> are not sized appropriately. • <code>LA_OUT_OF_MEMORY_ERROR</code>: Occurs if local memory must be allocated, and there is insufficient memory available.

Remarks

QR factorization without pivoting is best suited to solving an overdetermined system in least-squares terms, or to solve a normally defined system. To solve an underdetermined system, it is recommended to use either LQ factorization, or a column-pivoting based QR factorization.

Usage

To solve a system of M equations of N unknowns using QR factorization, the following code will suffice assuming M ≥ N.

```

! Solve the system: A*X = B in a least-squares sense, where A is an
! M-by-N matrix, B is an M-by-NRHS matrix, and X is an N-by-NRHS matrix.

! Variables
real(dp), dimension(m, n) :: a
real(dp), dimension(m, nrhs) :: b, qtb
real(dp), dimension(n, nrhs) :: x
real(dp), dimension(n) :: tau
real(dp), dimension(m, m) :: q

! Initialize A and B...

! Compute the QR factorization. We're intentionally not forming the full
! Q matrix, but instead storing it in terms of its elementary reflector
! components in the sub-diagonal portions of A, and the corresponding
! scalar factors in TAU. Additionally, we'll let the algorithm allocate
! it's own workspace array; therefore, the call to factor A is:
call qr_factor(a, tau)

! Solve A*X = B for X. The first N rows of B are used to store X.
call solve_qr(a, tau, b)

! Also note, we could form Q and R explicitly. Then solution of the
! system of equations can be found. First we form Q and R.
call form_qr(a, tau, q) ! Forms Q, and R is stored in A

! Since we now have Q and R, we seek a solution to the equation:
! Q*R*X = B, but Q is an orthogonal matrix (i.e. Q**T = inv(Q)).
! Then: R*X = Q**T * B, and R is upper triangular; therefore, back
! substitution will suffice for a solution procedure.
!
! Next, compute Q**T * B, and store in QTB.
call mtx_mult(.true., .false., 1.0d0, q, b, 0.0d0, qtb)

! Copy the first N rows of Q**T * B into X for the solution process.
! Notice, only the first N rows are needed as rows N+1:M are all zero in
! matrix R.
x = qtb(1:n,nrhs)

! Compute the solution and store in X
call solve_triangular_system(.true., .true., .false., .true., 1.0d0, &
a(1:n,1:n), x)

```

Notes

This routine utilizes the LAPACK routine DGEQRF.

Definition at line 424 of file linalg_factor.f90.

5.9.2.2 subroutine linalg_factor::qr_factor::qr_factor_pivot (real(dp), dimension(:, :), intent(inout) *a*, real(dp), dimension(:), intent(out) *tau*, integer(i32), dimension(:), intent(inout) *jpvt*, real(dp), dimension(:), intent(out), optional, target *work*, integer(i32), intent(out), optional *olwork*, class(errors), intent(inout), optional, target *err*) [private]

Computes the QR factorization of an M-by-N matrix with column pivoting such that $A * P = Q * R$.

Parameters

in, out	<i>a</i>	On input, the M-by-N matrix to factor. On output, the elements on and above the diagonal contain the MIN(M, N)-by-N upper trapezoidal matrix R (R is upper triangular if $M \geq N$). The elements below the diagonal, along with the array <i>tau</i> , represent the orthogonal matrix Q as a product of elementary reflectors.
out	<i>tau</i>	A MIN(M, N)-element array used to store the scalar factors of the elementary reflectors.
in, out	<i>jpvt</i>	On input, an N-element array that if JPVT(I) .ne. 0, the I-th column of A is permuted to the front of $A * P$; if JPVT(I) = 0, the I-th column of A is a free column. On output, if JPVT(I) = K, then the I-th column of $A * P$ was the K-th column of A.
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 <i>olwork</i> .

Parameters

out	<i>olwork</i>	An optional output used to determine workspace size. If supplied, the routine determines the optimal size for <code>work</code> , and returns without performing any actual calculations.
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>LA_ARRAY_SIZE_ERROR</code>: Occurs if any of the input arrays are not sized appropriately. • <code>LA_OUT_OF_MEMORY_ERROR</code>: Occurs if local memory must be allocated, and there is insufficient memory available.

Usage

To solve a system of M equations of N unknowns using QR factorization, the following code will suffice for any M and N .

```
! Solve the least-squares (M >= N), or the underdetermined (M < N)
! problem A*X = B, where A is an M-by-N matrix, B is an M-by-NRHS matrix,
! and X is an N-by-NRHS matrix. In the underdetermined case, or the
! case where the rank of matrix A is less than N, the solution obtained
! contains the fewest possible non-zero entries.

! Variables
real(dp), dimension(m, n) :: a
real(dp), dimension(n, nrhs) :: b
real(dp), dimension(k) :: tau ! k = min(m, n)
real(dp), dimension(m, m) :: q
real(dp), dimension(n, n) :: p
integer(i32), dimension(n) :: pvt

! Initialize A and B...

! Allow all columns to be free.
pvt = 0

! Compute the QR factorization. We're intentionally not forming the full
! Q matrix, but instead storing it in terms of its elementary reflector
! components in the sub-diagonal portions of A, and the corresponding
! scalar factors in TAU. Additionally, we'll let the algorithm allocate
! it's own workspace array; therefore, the call to factor A is:
call qr_factor(a, tau, pvt)

! Solve A*X = B for X. If M > N, the first N rows of B are used to store
! X. If M < N, the input matrix B must be N-by-NRHS, and only the first
! M rows are used for the actual matrix B. The remaining N-M rows
! can contain whatever as they are not referenced until they are
! overwritten by the N-by-NRHS solution matrix X.
call solve_qr(a, tau, pvt, b)

! Notice, if the explicit Q matrix from the factorization is desired,
! the form_qr routine works similarly as in the no-pivot case;
! however, the permutation matrix P is also constructed. The call would
! be as follows. Also, as with the no-pivot algorithm, the matrix R is
! stored in matrix A.
call form_qr(a, tau, pvt, q, p)

! Solution can proceed as per typical, but with a full Q matrix. Also
! note, the problem is of the form: A*P = Q*R. Solution is straight
! forward, as with the no-pivot case; however, if M < N, then R is upper
! trapezoidal, and must be appropriately partitioned to solve. The rank
! of matrix r should be considered when applying the partition.
```

Notes

This routine utilizes the LAPACK routine DGEQP3.

Definition at line 578 of file `linalg_factor.f90`.

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

- `/home/jason/Documents/Code/linalg/src/linalg_factor.f90`

5.10 linalg_solve::solve_cholesky Interface Reference

Solves a system of Cholesky factored equations.

Private Member Functions

- subroutine [solve_cholesky_mtx](#) (upper, a, b, err)
Solves a system of Cholesky factored equations.
- subroutine [solve_cholesky_vec](#) (upper, a, b, err)
Solves a system of Cholesky factored equations.

5.10.1 Detailed Description

Solves a system of Cholesky factored equations.

Definition at line 83 of file linalg_solve.f90.

5.10.2 Member Function/Subroutine Documentation

5.10.2.1 subroutine linalg_solve::solve_cholesky::solve_cholesky_mtx (logical, intent(in) *upper*, real(dp), dimension(:,:), intent(in) *a*, real(dp), dimension(:,:), intent(inout) *b*, class(errors), intent(inout), optional, target *err*) [private]

Solves a system of Cholesky factored equations.

Parameters

in	<i>upper</i>	Set to true if the original matrix A was factored such that $A = U^{**T} * U$; else, set to false if the factorization of A was $A = L^{**T} * L$.
in	<i>a</i>	The N-by-N Cholesky factored matrix.
in, out	<i>b</i>	On input, the N-by-NRHS right-hand-side matrix B. On output, the solution matrix X.
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"> • LA_ARRAY_SIZE_ERROR: Occurs if any of the input array sizes are incorrect.

Notes

This routine utilizes the LAPACK routine DPOTRS.

Definition at line 1073 of file linalg_solve.f90.

5.10.2.2 subroutine linalg_solve::solve_cholesky::solve_cholesky_vec (logical, intent(in) *upper*, real(dp), dimension(:,:), intent(in) *a*, real(dp), dimension(:,:), intent(inout) *b*, class(errors), intent(inout), optional, target *err*) [private]

Solves a system of Cholesky factored equations.

Parameters

in	<i>upper</i>	Set to true if the original matrix A was factored such that $A = U^{**T} * U$; else, set to false if the factorization of A was $A = L^{**T} * L$.
in	<i>a</i>	The N-by-N Cholesky factored matrix.
in, out	<i>b</i>	On input, the N-element right-hand-side vector B. On output, the solution vector X.
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"> LA_ARRAY_SIZE_ERROR: Occurs if any of the input array sizes are incorrect.

Notes

This routine utilizes the LAPACK routine DPOTRS.

Definition at line 1139 of file linalg_solve.f90.

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

- /home/jason/Documents/Code/linalg/src/linalg_solve.f90

5.11 linalg_solve::solve_least_squares Interface Reference

Solves the overdetermined or underdetermined system ($A * X = B$) of M equations of N unknowns.

Private Member Functions

- subroutine [solve_least_squares_mtx](#) (a, b, work, olwork, err)
*Solves the overdetermined or underdetermined system ($A * X = B$) of M equations of N unknowns using a QR or LQ factorization of the matrix A. Notice, it is assumed that matrix A has full rank.*
- subroutine [solve_least_squares_vec](#) (a, b, work, olwork, err)
*Solves the overdetermined or underdetermined system ($A * X = B$) of M equations of N unknowns using a QR or LQ factorization of the matrix A. Notice, it is assumed that matrix A has full rank.*

5.11.1 Detailed Description

Solves the overdetermined or underdetermined system ($A * X = B$) of M equations of N unknowns.

Definition at line 91 of file linalg_solve.f90.

5.11.2 Member Function/Subroutine Documentation

5.11.2.1 subroutine linalg_solve::solve_least_squares::solve_least_squares_mtx (real(dp), dimension(:, :), intent(inout) a, real(dp), dimension(:, :), intent(inout) b, real(dp), dimension(:), intent(out), optional, target work, integer(i32), intent(out), optional olwork, class(errors), intent(inout), optional, target err) [private]

Solves the overdetermined or underdetermined system ($A * X = B$) of M equations of N unknowns using a QR or LQ factorization of the matrix A. Notice, it is assumed that matrix A has full rank.

Parameters

in, out	<i>a</i>	On input, the M-by-N matrix A. On output, if $M \geq N$, the QR factorization of A in the form as output by <code>qr_factor</code> ; else, if $M < N$, the LQ factorization of A.
in, out	<i>b</i>	If $M \geq N$, the M-by-NRHS matrix B. On output, the first N rows contain the N-by-NRHS solution matrix X. If $M < N$, an N-by-NRHS matrix with the first M rows containing the matrix B. On output, the N-by-NRHS solution matrix X.
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> .
out	<i>olwork</i>	An optional output used to determine workspace size. If supplied, the routine determines the optimal size for <code>work</code> , and returns without performing any actual calculations.
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>LA_ARRAY_SIZE_ERROR</code>: Occurs if any of the input arrays are not sized appropriately. • <code>LA_OUT_OF_MEMORY_ERROR</code>: Occurs if local memory must be allocated, and there is insufficient memory available. • <code>LA_INVALID_OPERATION_ERROR</code>: Occurs if <i>a</i> is not of full rank.

Notes

This routine utilizes the LAPACK routine DGELS.

Definition at line 1568 of file `linalg_solve.f90`.

5.11.2.2 `subroutine linalg_solve::solve_least_squares::solve_least_squares_vec (real(dp), dimension(:, :), intent(inout) a, real(dp), dimension(:), intent(inout) b, real(dp), dimension(:), intent(out), optional, target work, integer(i32), intent(out), optional olwork, class(errors), intent(inout), optional, target err) [private]`

Solves the overdetermined or underdetermined system ($A \cdot X = B$) of M equations of N unknowns using a QR or LQ factorization of the matrix A. Notice, it is assumed that matrix A has full rank.

Parameters

in, out	<i>a</i>	On input, the M-by-N matrix A. On output, if $M \geq N$, the QR factorization of A in the form as output by <code>qr_factor</code> ; else, if $M < N$, the LQ factorization of A.
in, out	<i>b</i>	If $M \geq N$, the M-element array B. On output, the first N elements contain the N-element solution array X. If $M < N$, an N-element array with the first M elements containing the array B. On output, the N-element solution array X.
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> .
out	<i>olwork</i>	An optional output used to determine workspace size. If supplied, the routine determines the optimal size for <code>work</code> , and returns without performing any actual calculations.

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>LA_ARRAY_SIZE_ERROR</code>: Occurs if any of the input arrays are not sized appropriately. • <code>LA_OUT_OF_MEMORY_ERROR</code>: Occurs if local memory must be allocated, and there is insufficient memory available. • <code>LA_INVALID_OPERATION_ERROR</code>: Occurs if <code>a</code> is not of full rank.
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Notes

This routine utilizes the LAPACK routine DGELS.

Definition at line 1674 of file `linalg_solve.f90`.

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

- `/home/jason/Documents/Code/linalg/src/linalg_solve.f90`

5.12 linalg_solve::solve_least_squares_full Interface Reference

Solves the overdetermined or underdetermined system ($A \cdot X = B$) of M equations of N unknowns, but uses a full orthogonal factorization of the system.

Private Member Functions

- subroutine `solve_least_squares_mtx_pvt` (`a`, `b`, `ipvt`, `arnk`, `work`, `olwork`, `err`)
Solves the overdetermined or underdetermined system ($A \cdot X = B$) of M equations of N unknowns using a complete orthogonal factorization of matrix A .
- subroutine `solve_least_squares_vec_pvt` (`a`, `b`, `ipvt`, `arnk`, `work`, `olwork`, `err`)
Solves the overdetermined or underdetermined system ($A \cdot X = B$) of M equations of N unknowns using a complete orthogonal factorization of matrix A .

5.12.1 Detailed Description

Solves the overdetermined or underdetermined system ($A \cdot X = B$) of M equations of N unknowns, but uses a full orthogonal factorization of the system.

Definition at line 100 of file `linalg_solve.f90`.

5.12.2 Member Function/Subroutine Documentation

- 5.12.2.1 subroutine `linalg_solve::solve_least_squares_full::solve_least_squares_mtx_pvt` (`real(dp)`, `dimension(:, :)`, `intent(inout)` `a`, `real(dp)`, `dimension(:, :)`, `intent(inout)` `b`, `integer(i32)`, `dimension(:)`, `intent(inout)`, optional, target `ipvt`, `integer(i32)`, `intent(out)`, optional `arnk`, `real(dp)`, `dimension(:)`, `intent(out)`, optional, target `work`, `integer(i32)`, `intent(out)`, optional `olwork`, `class(errors)`, `intent(inout)`, optional, target `err`) `[private]`

Solves the overdetermined or underdetermined system ($A \cdot X = B$) of M equations of N unknowns using a complete orthogonal factorization of matrix A .

Parameters

in, out	<i>a</i>	On input, the M-by-N matrix A. On output, the matrix is overwritten by the details of its complete orthogonal factorization.
in, out	<i>b</i>	If $M \geq N$, the M-by-NRHS matrix B. On output, the first N rows contain the N-by-NRHS solution matrix X. If $M < N$, an N-by-NRHS matrix with the first M rows containing the matrix B. On output, the N-by-NRHS solution matrix X.
out	<i>ipvt</i>	An optional input that on input, an N-element array that if $IPVT(l) \neq 0$, the l-th column of A is permuted to the front of $A * P$; if $IPVT(l) = 0$, the l-th column of A is a free column. On output, if $IPVT(l) = K$, then the l-th column of $A * P$ was the K-th column of A. If not supplied, memory is allocated internally, and IPVT is set to all zeros such that all columns are treated as free.
out	<i>arnk</i>	An optional output, that if provided, will return the rank of <i>a</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 <i>olwork</i> .
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 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"> • LA_ARRAY_SIZE_ERROR: Occurs if any of the input arrays are not sized appropriately. • LA_OUT_OF_MEMORY_ERROR: Occurs if local memory must be allocated, and there is insufficient memory available.

Notes

This routine utilizes the LAPACK routine DGELSY.

Definition at line 1786 of file linalg_solve.f90.

```
5.12.2.2 subroutine linalg_solve::solve_least_squares_full::solve_least_squares_vec_pvt ( real(dp), dimension(:, :), intent(inout)
a, real(dp), dimension(:), intent(inout) b, integer(i32), dimension(:), intent(inout), optional, target ipvt, integer(i32),
intent(out), optional arnk, real(dp), dimension(:), intent(out), optional, target work, integer(i32), intent(out), optional
olwork, class(errors), intent(inout), optional, target err ) [private]
```

Solves the overdetermined or underdetermined system ($A * X = B$) of M equations of N unknowns using a complete orthogonal factorization of matrix A.

Parameters

in, out	<i>a</i>	On input, the M-by-N matrix A. On output, the matrix is overwritten by the details of its complete orthogonal factorization.
in, out	<i>b</i>	If $M \geq N$, the M-element array B. On output, the first N elements contain the N-element solution array X. If $M < N$, an N-element array with the first M elements containing the array B. On output, the N-element solution array X.
out	<i>ipvt</i>	An optional input that on input, an N-element array that if $IPVT(l) \neq 0$, the l-th column of A is permuted to the front of $A * P$; if $IPVT(l) = 0$, the l-th column of A is a free column. On output, if $IPVT(l) = K$, then the l-th column of $A * P$ was the K-th column of A. If not supplied, memory is allocated internally, and IPVT is set to all zeros such that all columns are treated as free.

Parameters

out	<i>arnk</i>	An optional output, that if provided, will return the rank of <i>a</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> .
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>	<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>LA_ARRAY_SIZE_ERROR</code>: Occurs if any of the input arrays are not sized appropriately. • <code>LA_OUT_OF_MEMORY_ERROR</code>: Occurs if local memory must be allocated, and there is insufficient memory available.

Notes

This routine utilizes the LAPACK routine DGELSY.

Definition at line 1932 of file `linalg_solve.f90`.

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

- `/home/jason/Documents/Code/linalg/src/linalg_solve.f90`

5.13 linalg_solve::solve_least_squares_svd Interface Reference

Solves the overdetermined or underdetermined system ($A \cdot X = B$) of M equations of N unknowns using a singular value decomposition of matrix A .

Private Member Functions

- subroutine `solve_least_squares_mtx_svd` (*a*, *b*, *arnk*, *s*, *work*, *olwork*, *err*)
Solves the overdetermined or underdetermined system ($A \cdot X = B$) of M equations of N unknowns using a singular value decomposition of matrix A .
- subroutine `solve_least_squares_vec_svd` (*a*, *b*, *arnk*, *s*, *work*, *olwork*, *err*)
Solves the overdetermined or underdetermined system ($A \cdot X = B$) of M equations of N unknowns using a singular value decomposition of matrix A .

5.13.1 Detailed Description

Solves the overdetermined or underdetermined system ($A \cdot X = B$) of M equations of N unknowns using a singular value decomposition of matrix A .

Definition at line 109 of file `linalg_solve.f90`.

5.13.2 Member Function/Subroutine Documentation

5.13.2.1 subroutine `linalg_solve::solve_least_squares_svd::solve_least_squares_mtx_svd` (`real(dp)`, `dimension(:, :)`,
`intent(inout) a`, `real(dp)`, `dimension(:, :)`, `intent(inout) b`, `integer(i32)`, `intent(out)`, optional `arnk`, `real(dp)`, `dimension(:, :)`,
`intent(out) s`, `real(dp)`, `dimension(:, :)`, `intent(out)`, optional, target `work`, `integer(i32)`, `intent(out)`, optional `olwork`,
`class(errors)`, `intent(inout)`, optional, target `err`) [`private`]

Solves the overdetermined or underdetermined system ($A \cdot X = B$) of M equations of N unknowns using a singular value decomposition of matrix A .

Parameters

<code>in, out</code>	<code>a</code>	On input, the M -by- N matrix A . On output, the matrix is overwritten by the details of its complete orthogonal factorization.
<code>in, out</code>	<code>b</code>	If $M \geq N$, the M -by- N -RHS matrix B . On output, the first N rows contain the N -by- N -RHS solution matrix X . If $M < N$, an N -by- N -RHS matrix with the first M rows containing the matrix B . On output, the N -by- N -RHS solution matrix X .
<code>out</code>	<code>arnk</code>	An optional output, that if provided, will return the rank of a .
<code>out</code>	<code>s</code>	A $\min(M, N)$ -element array that on output contains the singular values of a in descending order. Notice, the condition number of a can be determined by $S(1) / S(\min(M, N))$.
<code>out</code>	<code>work</code>	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> .
<code>out</code>	<code>olwork</code>	An optional output used to determine workspace size. If supplied, the routine determines the optimal size for <code>work</code> , and returns without performing any actual calculations.
<code>out</code>	<code>err</code>	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>LA_ARRAY_SIZE_ERROR</code>: Occurs if any of the input arrays are not sized appropriately. • <code>LA_OUT_OF_MEMORY_ERROR</code>: Occurs if local memory must be allocated, and there is insufficient memory available. • <code>LA_CONVERGENCE_ERROR</code>: Occurs as a warning if the QR iteration process could not converge to a zero value.

Notes

This routine utilizes the LAPACK routine DGELSS.

Definition at line 2076 of file `linalg_solve.f90`.

5.13.2.2 subroutine `linalg_solve::solve_least_squares_svd::solve_least_squares_vec_svd` (`real(dp)`, `dimension(:, :)`,
`intent(inout) a`, `real(dp)`, `dimension(:, :)`, `intent(inout) b`, `integer(i32)`, `intent(out)`, optional `arnk`, `real(dp)`, `dimension(:, :)`,
`intent(out) s`, `real(dp)`, `dimension(:, :)`, `intent(out)`, optional, target `work`, `integer(i32)`, `intent(out)`, optional `olwork`,
`class(errors)`, `intent(inout)`, optional, target `err`) [`private`]

Solves the overdetermined or underdetermined system ($A \cdot X = B$) of M equations of N unknowns using a singular value decomposition of matrix A .

Parameters

in, out	<i>a</i>	On input, the M-by-N matrix A. On output, the matrix is overwritten by the details of its complete orthogonal factorization.
in, out	<i>b</i>	If $M \geq N$, the M-by-NRHS matrix B. On output, the first N rows contain the N-by-NRHS solution matrix X. If $M < N$, an N-by-NRHS matrix with the first M rows containing the matrix B. On output, the N-by-NRHS solution matrix X.
out	<i>arnk</i>	An optional output, that if provided, will return the rank of <i>a</i> .
out	<i>s</i>	A MIN(M, N)-element array that on output contains the singular values of <i>a</i> in descending order. Notice, the condition number of <i>a</i> can be determined by $S(1) / S(\text{MIN}(M, N))$.
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> .
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 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>LA_ARRAY_SIZE_ERROR</code>: Occurs if any of the input arrays are not sized appropriately. • <code>LA_OUT_OF_MEMORY_ERROR</code>: Occurs if local memory must be allocated, and there is insufficient memory available. • <code>LA_CONVERGENCE_ERROR</code>: Occurs as a warning if the QR iteration process could not converge to a zero value.

Notes

This routine utilizes the LAPACK routine DGELSS.

Definition at line 2204 of file `linalg_solve.f90`.

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

- `/home/jason/Documents/Code/linalg/src/linalg_solve.f90`

5.14 linalg_solve::solve_lu Interface Reference

Solves a system of LU-factored equations.

Private Member Functions

- subroutine `solve_lu_mtx` (*a*, *ipvt*, *b*, *err*)
Solves a system of LU-factored equations.
- subroutine `solve_lu_vec` (*a*, *ipvt*, *b*, *err*)
Solves a system of LU-factored equations.

5.14.1 Detailed Description

Solves a system of LU-factored equations.

Usage

To solve a system of N equations of N unknowns using LU factorization, the following code will suffice.

```
! Solve the system: A*X = B, where A is an N-by-N matrix, and B and X are
! N-by-NRHS in size.

! Variables
real(dp), dimension(n, n) :: a
real(dp), dimension(n, nrhs) :: b

! Define the array used to track row pivots.
integer(i32), dimension(n) :: pvt

! Initialize A and B...

! Compute the LU factorization of A. On output, A contains [L\U].
call lu_factor(a, pvt)

! Solve A*X = B for X - Note: X overwrites B.
call solve_lu(a, pvt, b)
```

See Also

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

Definition at line 63 of file linalg_solve.f90.

5.14.2 Member Function/Subroutine Documentation

5.14.2.1 subroutine linalg_solve::solve_lu::solve_lu_mtx (real(dp), dimension(:,:), intent(in) *a*, integer(i32), dimension(:), intent(in) *ipvt*, real(dp), dimension(:,:), intent(inout) *b*, class(errors), intent(inout), optional, target *err*)
[private]

Solves a system of LU-factored equations.

Parameters

in	<i>a</i>	The N-by-N LU factored matrix as output by lu_factor.
in	<i>ipvt</i>	The N-element pivot array as output by lu_factor.
in, out	<i>b</i>	On input, the N-by-NRHS right-hand-side matrix. On output, the N-by-NRHS solution matrix.
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"> • LA_ARRAY_SIZE_ERROR: Occurs if any of the input array sizes are incorrect.

Notes

The routine is based upon the LAPACK routine DGETRS.

Definition at line 351 of file linalg_solve.f90.

5.14.2.2 subroutine `linalg_solve::solve_lu::solve_lu_vec` (`real(dp)`, `dimension(:, :)`, `intent(in)` `a`, `integer(i32)`, `dimension(:)`, `intent(in)` `ipvt`, `real(dp)`, `dimension(:)`, `intent(inout)` `b`, `class(errors)`, `intent(inout)`, `optional`, `target` `err`) `[private]`

Solves a system of LU-factored equations.

Parameters

<code>in</code>	<code>a</code>	The N-by-N LU factored matrix as output by <code>lu_factor</code> .
<code>in</code>	<code>ipvt</code>	The N-element pivot array as output by <code>lu_factor</code> .
<code>in, out</code>	<code>b</code>	On input, the N-element right-hand-side array. On output, the N-element solution array.
<code>out</code>	<code>err</code>	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>LA_ARRAY_SIZE_ERROR</code>: Occurs if any of the input array sizes are incorrect.

Notes

The routine is based upon the LAPACK routine DGETRS.

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

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

- `/home/jason/Documents/Code/linalg/src/linalg_solve.f90`

5.15 linalg_solve::solve_qr Interface Reference

Solves a system of M QR-factored equations of N unknowns.

Private Member Functions

- subroutine `solve_qr_no_pivot_mtx` (`a`, `tau`, `b`, `work`, `olwork`, `err`)
Solves a system of M QR-factored equations of N unknowns where $M \geq N$.
- subroutine `solve_qr_no_pivot_vec` (`a`, `tau`, `b`, `work`, `olwork`, `err`)
Solves a system of M QR-factored equations of N unknowns where $M \geq N$.
- subroutine `solve_qr_pivot_mtx` (`a`, `tau`, `jpvt`, `b`, `work`, `olwork`, `err`)
Solves a system of M QR-factored equations of N unknowns where the QR factorization made use of column pivoting.
- subroutine `solve_qr_pivot_vec` (`a`, `tau`, `jpvt`, `b`, `work`, `olwork`, `err`)
Solves a system of M QR-factored equations of N unknowns where the QR factorization made use of column pivoting.

5.15.1 Detailed Description

Solves a system of M QR-factored equations of N unknowns.

See Also

- [Wikipedia](#)
- [LAPACK Users Manual](#)

Definition at line 74 of file `linalg_solve.f90`.

5.15.2 Member Function/Subroutine Documentation

5.15.2.1 subroutine `linalg_solve::solve_qr::solve_qr_no_pivot_mtx` (`real(dp)`, `dimension(:, :)`, `intent(inout)` *a*, `real(dp)`, `dimension(:, :)`, `intent(in)` *tau*, `real(dp)`, `dimension(:, :)`, `intent(inout)` *b*, `real(dp)`, `dimension(:, :)`, `intent(out)`, optional, target *work*, `integer(i32)`, `intent(out)`, optional *olwork*, `class(errors)`, `intent(inout)`, optional, target *err*) [`private`]

Solves a system of M QR-factored equations of N unknowns where $M \geq N$.

Parameters

in	<i>a</i>	On input, the M-by-N QR factored matrix as returned by <code>qr_factor</code> . On output, the contents of this matrix are restored. Notice, M must be greater than or equal to N.
in	<i>tau</i>	A MIN(M, N)-element array containing the scalar factors of the elementary reflectors as returned by <code>qr_factor</code> .
in	<i>b</i>	On input, the M-by-NRHS right-hand-side matrix. On output, the first N columns are overwritten by the solution matrix X.
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> .
out	<i>olwork</i>	An optional output used to determine workspace size. If supplied, the routine determines the optimal size for <code>work</code> , and returns without performing any actual calculations.
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"> LA_ARRAY_SIZE_ERROR: Occurs if any of the input arrays are not sized appropriately. LA_OUT_OF_MEMORY_ERROR: Occurs if local memory must be allocated, and there is insufficient memory available.

Notes

This routine is based upon a subset of the LAPACK routine DGELS.

Definition at line 487 of file `linalg_solve.f90`.

5.15.2.2 subroutine `linalg_solve::solve_qr::solve_qr_no_pivot_vec` (`real(dp)`, `dimension(:, :)`, `intent(inout)` *a*, `real(dp)`, `dimension(:, :)`, `intent(in)` *tau*, `real(dp)`, `dimension(:, :)`, `intent(inout)` *b*, `real(dp)`, `dimension(:, :)`, `intent(out)`, optional, target *work*, `integer(i32)`, `intent(out)`, optional *olwork*, `class(errors)`, `intent(inout)`, optional, target *err*) [`private`]

Solves a system of M QR-factored equations of N unknowns where $M \geq N$.

Parameters

in	<i>a</i>	On input, the M-by-N QR factored matrix as returned by <code>qr_factor</code> . On output, the contents of this matrix are restored. Notice, M must be greater than or equal to N.
in	<i>tau</i>	A MIN(M, N)-element array containing the scalar factors of the elementary reflectors as returned by <code>qr_factor</code> .
in	<i>b</i>	On input, the M-element right-hand-side vector. On output, the first N elements are overwritten by the solution vector X.

Parameters

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 <i>olwork</i> .
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 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"> LA_ARRAY_SIZE_ERROR: Occurs if any of the input arrays are not sized appropriately. LA_OUT_OF_MEMORY_ERROR: Occurs if local memory must be allocated, and there is insufficient memory available.

Notes

This routine is based upon a subset of the LAPACK routine DGELS.

Definition at line 602 of file linalg_solve.f90.

5.15.2.3 `subroutine linalg_solve::solve_qr::solve_qr_pivot_mtx (real(dp), dimension(:, :), intent(inout) a, real(dp), dimension(:), intent(in) tau, integer(i32), dimension(:), intent(in) jpvt, real(dp), dimension(:, :), intent(inout) b, real(dp), dimension(:), intent(out), optional, target work, integer(i32), intent(out), optional olwork, class(errors), intent(inout), optional, target err) [private]`

Solves a system of M QR-factored equations of N unknowns where the QR factorization made use of column pivoting.

Parameters

in	<i>a</i>	On input, the M-by-N QR factored matrix as returned by <i>qr_factor</i> . On output, the contents of this matrix are altered.
in	<i>tau</i>	A MIN(M, N)-element array containing the scalar factors of the elementary reflectors as returned by <i>qr_factor</i> .
in	<i>jpvt</i>	An N-element array, as output by <i>qr_factor</i> , used to track the column pivots.
in	<i>b</i>	On input, the MAX(M, N)-by-NRHS matrix where the first M rows contain the right-hand-side matrix B. On output, the first N rows are overwritten by the solution matrix X.
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 <i>olwork</i> .
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 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"> LA_ARRAY_SIZE_ERROR: Occurs if any of the input arrays are not sized appropriately. LA_OUT_OF_MEMORY_ERROR: Occurs if local memory must be allocated, and there is insufficient memory available.
		Generated by Doxygen

Notes

This routine is based upon a subset of the LAPACK routine DGELSY.

Definition at line 715 of file linalg_solve.f90.

5.15.2.4 subroutine linalg_solve::solve_qr::solve_qr_pivot_vec (real(dp), dimension(:,:), intent(inout) *a*, real(dp), dimension(:), intent(in) *tau*, integer(i32), dimension(:), intent(in) *jpvt*, real(dp), dimension(:), intent(inout) *b*, real(dp), dimension(:), intent(out), optional, target *work*, integer(i32), intent(out), optional *olwork*, class(errors), intent(inout), optional, target *err*) [private]

Solves a system of *M* QR-factored equations of *N* unknowns where the QR factorization made use of column pivoting.

Parameters

in	<i>a</i>	On input, the <i>M</i> -by- <i>N</i> QR factored matrix as returned by <i>qr_factor</i> . On output, the contents of this matrix are altered.
in	<i>tau</i>	A MIN(<i>M</i> , <i>N</i>)-element array containing the scalar factors of the elementary reflectors as returned by <i>qr_factor</i> .
in	<i>jpvt</i>	An <i>N</i> -element array, as output by <i>qr_factor</i> , used to track the column pivots.
in	<i>b</i>	On input, the MAX(<i>M</i> , <i>N</i>)-element array where the first <i>M</i> elements contain the right-hand-side vector <i>B</i> . On output, the first <i>N</i> elements are overwritten by the solution vector <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 <i>olwork</i> .
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 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"> LA_ARRAY_SIZE_ERROR: Occurs if any of the input arrays are not sized appropriately. LA_OUT_OF_MEMORY_ERROR: Occurs if local memory must be allocated, and there is insufficient memory available.

Notes

This routine is based upon a subset of the LAPACK routine DGELSY.

Definition at line 902 of file linalg_solve.f90.

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

- /home/jason/Documents/Code/linalg/src/linalg_solve.f90

5.16 linalg_solve::solve_triangular_system Interface Reference

Solves a triangular system of equations.

Private Member Functions

- subroutine `solve_tri_mtx` (`lside`, `upper`, `trans`, `nounit`, `alpha`, `a`, `b`, `err`)
Solves one of the matrix equations: $op(A) * X = alpha * B$, or $X * op(A) = alpha * B$, where A is a triangular matrix.
- subroutine `solve_tri_vec` (`upper`, `trans`, `nounit`, `a`, `x`, `err`)
Solves the system of equations: $op(A) * X = B$, where A is a triangular matrix.

5.16.1 Detailed Description

Solves a triangular system of equations.

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

5.16.2 Member Function/Subroutine Documentation

5.16.2.1 subroutine `linalg_solve::solve_triangular_system::solve_tri_mtx` (`logical`, intent(in) `lside`, `logical`, intent(in) `upper`, `logical`, intent(in) `trans`, `logical`, intent(in) `nounit`, `real(dp)`, intent(in) `alpha`, `real(dp)`, dimension(:,:), intent(in) `a`, `real(dp)`, dimension(:,:), intent(inout) `b`, `class(errors)`, intent(inout), optional, target `err`) [private]

Solves one of the matrix equations: $op(A) * X = alpha * B$, or $X * op(A) = alpha * B$, where A is a triangular matrix.

Parameters

in	<code>lside</code>	Set to true to solve $op(A) * X = alpha * B$; else, set to false to solve $X * op(A) = alpha * B$.
in	<code>upper</code>	Set to true if A is an upper triangular matrix; else, set to false if A is a lower triangular matrix.
in	<code>trans</code>	Set to true if $op(A) = A^{**T}$; else, set to false if $op(A) = A$.
in	<code>nounit</code>	Set to true if A is not a unit-diagonal matrix (ones on every diagonal element); else, set to false if A is a unit-diagonal matrix.
in	<code>alpha</code>	The scalar multiplier to B .
in	<code>a</code>	If <code>lside</code> is true, the M-by-M triangular matrix on which to operate; else, if <code>lside</code> is false, the N-by-N triangular matrix on which to operate.
in, out	<code>b</code>	On input, the M-by-N right-hand-side. On output, the M-by-N solution.
out	<code>err</code>	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>LA_ARRAY_SIZE_ERROR</code>: Occurs if <code>a</code> is not square, or if the sizes of <code>a</code> and <code>b</code> are not compatible.

Usage

To solve a triangular system of N equations of N unknowns $A * X = B$, where A is an N -by- N upper triangular matrix, and B and X are N -by- N matrices, the following code will suffice.

```
! Solve the system: A*X = B, where A is an upper triangular N-by-N
! matrix, and B and X are N-by-NRHS in size.

! Variables
```

```

integer(i32) :: info
real(dp), dimension(n, n) :: a
real(dp), dimension(n, nrhs) :: b

! Initialize A and B...

! Solve A*X = B for X - Note: X overwrites B.
call solve_triangular_system(.true., .true., .false., .true., &
    1.0d0, a, b)

```

Notes

This routine is based upon the BLAS routine DTRSM.

Definition at line 169 of file linalg_solve.f90.

5.16.2.2 subroutine linalg_solve::solve_triangular_system::solve_tri_vec (logical, intent(in) *upper*, logical, intent(in) *trans*, logical, intent(in) *nounit*, real(dp), dimension(:, :), intent(in) *a*, real(dp), dimension(:), intent(inout) *x*, class(errors), intent(inout), optional, target *err*) [private]

Solves the system of equations: $\text{op}(A) * X = B$, where A is a triangular matrix.

Parameters

in	<i>upper</i>	Set to true if A is an upper triangular matrix; else, set to false if A is a lower triangular matrix.
in	<i>trans</i>	Set to true if $\text{op}(A) = A^{**T}$; else, set to false if $\text{op}(A) = A$.
in	<i>nounit</i>	Set to true if A is not a unit-diagonal matrix (ones on every diagonal element); else, set to false if A is a unit-diagonal matrix.
in	<i>a</i>	The N-by-N triangular matrix.
in, out	<i>x</i>	On input, the N-element right-hand-side array. On output, the N-element solution array.
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"> LA_ARRAY_SIZE_ERROR: Occurs if a is not square, or if the sizes of a and b are not compatible.

Usage

To solve a triangular system of N equations of N unknowns $A * X = B$, where A is an N-by-N upper triangular matrix, and B and X are N-element arrays, the following code will suffice.

```

! Solve the system: A*X = B, where A is an upper triangular N-by-N
! matrix, and B and X are N-elements in size.

! Variables
integer(i32) :: info
real(dp), dimension(n, n) :: a
real(dp), dimension(n) :: b

! Initialize A and B...

! Solve A*X = B for X - Note: X overwrites B.
call solve_triangular_system(.true., .false., a, b)

```

Notes

This routine is based upon the BLAS routine DTRSV.

Definition at line 275 of file linalg_solve.f90.

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

- /home/jason/Documents/Code/linalg/src/linalg_solve.f90

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