SUBJECT WISE LIST OF FORTRAN SUBPROGRAMS

Chapter 2 Roundoff Error

CASSUM	Cascade sum of a finite series using a function to calculate the terms
$CASSUM_A$	Cascade sum of a finite series using an array to supply the terms
ROUND	Rounding a floating-point number to a specified number of digits

Chapter 3 Linear Algebraic Equations

GAUELM	Solve a system	of linear	equations	using	Gaussian	elimination
OTICELLI		or micar	Cquadions	using	Caussian	CIIIIIIIIIIIIIIIIIIIIIIIIIIIIIIIIIIIIII

GAUELM_C Solve a system of linear equations using Gaussian elimination (complex version)

MATINV	Calculate inverse of a square matrix using Gaussian elimination
CROUT	Solve a system of linear equations using Crout's algorithm

CROUT_C Solve a system of linear equations using Crout's algorithm (complex version)

CROUTH Iterative refinement of solution of a system of linear equations

CHOLSK Solve a system of linear equations with symmetric positive definite matrix using Cholesky's decomposition

GAUBND Solve a system of linear equations with a band matrix using Gaussian elimination with partial pivoting

GAUBND_C Solve a system of linear equations with a band matrix using Gaussian elimination with partial pivoting (complex version)

SVD Singular value decomposition of a matrix

SVDEVL Solve a system of linear equations using singular value decomposition

Chapter 4 Interpolation

DIVDIF	Calculate interpolation and its derivatives using divided difference formula
DIVDIF0	Divided difference interpolation formula (no derivatives version)
NEARST	Find nearest point in an ordered table using bisection
SPLINE	Calculate coefficients of interpolating cubic spline
SPLEVL	Evaluate the cubic spline and its derivatives at a specified point
SMOOTH	Draw a smooth curve through a set of points using cubic spline
BSPLIN	Calculate B-spline basis functions on a set of knots
BSPINT	Calculate coefficients of B-spline interpolation
BSPEVL	Evaluate function value and its derivatives using B-spline expansion

2 Subject Wise List of Fortran Subprograms

RATNAL Calculate rational function interpolation POLY2 Calculate polynomial interpolation in two dimensions LINRN Calculate linear interpolation in n dimensions LOCATE Find the bracketing subinterval in an ordered table BSPINT2 Calculate coefficients of B-spline interpolation in two dimensions BSPEV2 Evaluate function value and derivatives using B-spline expansion in two dimensions **BSPINTN** Calculate coefficients of B-spline interpolation in n dimensions **BSPEVN** Evaluate function value using B-spline expansion in n dimensions BSPEVN1 Evaluate function value and first derivative using B-spline expansion in ndimensions BSPEVN2Evaluate function value and first and second derivatives using B-spline expansion in n dimensions Chapter 5 Differentiation DRVT Differentiation using $h \to 0$ extrapolation Chapter 6 Integration **SIMSON** Integration using Simpson's 1/3 rule SPLINT Integrate a tabulated function using cubic spline **BSPQD** Integrate a B-spline expansion ROMBRG Romberg integration **EPSILN** Integration using ϵ -algorithm GAUSS Integration using Gauss-Legendre formula GAUCBY Integration using Gauss-Chebyshev formula with weight function, $w(x) = 1/\sqrt{(x-A)(B-x)}$ GAUCB1 Integration using Gauss-Chebyshev formula with weight function, $w(x) = \sqrt{(x-A)/(B-x)}$ GAUCB2 Integration using Gauss-Chebyshev formula with weight function, $w(x) = \sqrt{(x-A)(B-x)}$ Integration over (0, A] with square root singularity using a combination of GAUSQ2 Gaussian formulae GAUSQ Integration over (0, A] using Gaussian formula with weight function, $w(x) = 1/\sqrt{x}$ **GAULAG** Integration over $[A, \infty)$ using a combination of Gaussian formulae LAGURE Integration over $[A, \infty)$ using Gauss-Laguerre formula HERMIT Integration over $(-\infty, \infty)$ using Gauss-Hermite formula GAULG2 Integration over (0, A] with logarithmic singularity using a combination of Gaussian formulae GAULOG Integration over (0, A] using Gaussian formula with weight function, $w(x) = \ln(A/x)$ GAUSRC Calculate weights and abscissas of Gaussian formula using recurrence relation of orthogonal polynomials **GAULEG** Calculate weights and abscissas of Gauss-Legendre quadrature formulae

	Subject Wise List of Fortran Subprograms 3
GAUJAC	Calculate weights and abscissas of Gauss-Jacobi quadrature formulae
LAGURW	Calculate weights and abscissas of Gauss-Laguerre quadrature formulae
GAUHER	Calculate weights and abscissas of Gauss-Hermite quadrature formulae
GAUSWT	Calculate weights and abscissas of Gaussian formula using moments of weight function
FILON	Integration of an oscillatory function using Filon's formula
ADPINT	Adaptive integration over a finite interval
KRONRD	Integration using Gauss-Kronrod formula for use with ADPINT
GAUS16	Integration using 16 point Gauss-Legendre formula for use with ADPINT
CAUCHY	Calculate Cauchy principal value of an integral
EULER	Summation of alternating series using Euler transformation
BSPQD2	Integrate a B-spline expansion in two dimensions
BSPQDN	Integrate a B-spline expansion in n dimensions
MULINT	Multiple integration using product Gauss rule with varying number of points
NGAUSS	Multiple integration using a specified product Gauss rule
SPHND	To convert from hyper-spherical coordinates to Cartesian coordinates
STRINT	Multiple integration using monomial rules with varying number of points
STROUD	Multiple integration using a specified monomial rule
MCARLO	Multiple integration using Monte Carlo method
RAN1	Generate a sequence of random numbers with uniform distribution
RANF	Generate a sequence of random numbers with uniform distribution
EQUIDS	Multiple integration using equidistributed sequences
	Chapter 7 Nonlinear Algebraic Equations
BISECT	Solve a nonlinear equation using bisection
SECANT	Solve a nonlinear equation using secant iteration
${ m SECAN}_{-2}$	Solve a nonlinear equation using secant iteration with function in scaled form
	$(f(x) = F(x)2^{i(x)})$
SECANC	Complex roots of a nonlinear equation using secant iteration
SECANC_2	Complex roots of a nonlinear equation using secant iteration with function in scaled form $(f(x) = F(x)2^{i(x)})$
SECANI	Solve a nonlinear equation using secant iteration (with reverse communication)
NEWRAP	Solve a nonlinear equation using Newton-Raphson method
BRENT	Solve a nonlinear equation using Brent's method
Q = 4 = Q = =	

Locate complex zeros by looking for sign changes

Complex root using Muller's method

form, $f(x) \times 2^{i(x)}$

 $f(x) \times 2^{i(x)}$

Complex roots of a nonlinear equation with deflation

Contour integration over a circular contour for DELVES

Complex roots of a nonlinear equation with deflation, function value in scaled

Complex root using Muller's method with function value in a scaled form,

Complex zeros of an analytic function using quadrature based method

SEARCH

ZROOT

ZROOT2

MULLER

MULER2

DELVES

CONTUR

Subject Wise List of Fortran Subprograms

NEWRAC Complex root of a nonlinear equation using Newton-Raphson method **POLYR** All roots of a polynomial with real coefficients LAGITR One root of a polynomial with real coefficients using Laguerre's method **POLYC** All roots of a polynomial with complex coefficients LAGITC One root of a polynomial with complex coefficients using Laguerre's method **DAVIDN** Solve a system of nonlinear equations using Davidenko's method coupled with Newton's method DAVIDN_B Solve a system of nonlinear equations using Davidenko's method coupled

with Broyden's method **NEWTON** Solve a system of nonlinear equations using Newton's method

BROYDN Solve a system of nonlinear equations using Broyden's method

Chapter 8 Optimisation

BRACKM Bracketing a minimum in one dimension GOLDEN Minimisation in one dimension using golden section search **BRENTM** Minimisation in one dimension using Brent's method

DAVIDM Minimisation in one dimension using cubic Hermite interpolation

BFGS Minimisation in n dimensions using quasi-Newton method with BFGS for-

mula

LINMIN Line search for quasi-Newton method

FLNM Calculate the function value for line search for quasi-Newton method

NMINF Minimisation in n dimensions using direction set method

LINMNF Line search for direction set method

FLN Calculate the function value for line search for direction set method

SIMPLX Solving a linear programming problem using simplex method

SIMPX Simplex method for a linear programming problem in the standard form

Statistical Inferences Chapter 9

SHSORT Sorting an array in ascending order using shell sort algorithm

GAMMAP Calculate incomplete Gamma function BETAP Calculate incomplete Beta function

BETSER Calculate incomplete Beta function using a power series approximation BETCON1 Calculate incomplete Beta function using a continued fraction approximation **BETCON** Calculate incomplete Beta function using an alternative continued fraction

approximation

BETAI Calculate incomplete Beta function by directly evaluating the integral

FBETA Calculate the integrand for BETAI

RANGAU Generate a sequence of random numbers with Gaussian distribution Generate a sequence of random numbers with binomial distribution **IRANBIN IRANPOI** Generate a sequence of random numbers with Poisson distribution

PCOR Calculate the probability that two uncorrelated sequences will give a corre-

lation coefficient exceeding a given value

Chapter 10 **Functional Approximations POLFIT** Least squares polynomial fit using orthogonal polynomials POLEVL Evaluate the fitted polynomial and its derivatives at a specified point POLFIT1 Least squares polynomial fit using orthogonal polynomials, simplified version for multiple data sets **POLORT** Evaluate the orthogonal polynomial basis functions at a given point POLFIT2 Least squares polynomial fit using orthogonal polynomials in two dimensions POLEV2 Evaluate the fitted polynomial and its derivatives at a specified point in two dimensions **POLFITN** Least squares polynomial fit using orthogonal polynomials in n dimensions **POLEVN** Evaluate the fitted polynomial at a specified point in n dimensions POLEVN1 Evaluate the fitted polynomial and first derivative at a specified point in ndimensions POLEVN2Evaluate the fitted polynomial and first and second derivatives at a specified point in n dimensions LLSQ Linear least squares fit in n dimensions to a user defined set of basis functions **BSPFIT** Least squares fit to B-spline basis functions in one dimension BSPFIT2 Least squares fit to B-spline basis in two dimensions with equal weights BSPFITW2 Least squares fit to B-spline basis in two dimensions with arbitrary weights **BSPFITN** Least squares fit to B-spline basis in n dimensions with equal weights BSPFITWN Least squares fit to B-spline basis in n dimensions with arbitrary weights LINFITXY Least squares straight line fit when there are errors in both x and y values NLLSQ Calculate the Chi square function for a nonlinear least squares fit using quasi Newton method (BFGS) NLLSQ_F Calculate the Chi square function for a nonlinear least squares fit using direction set method (NMINF) DFT Discrete Fourier transform of complex data with arbitrary number of points FFT Fast Fourier transform of complex data FFTR Fast Fourier transform of real data FFTN Fast Fourier transform of complex data in n dimensions LAPINV Inverse Laplace transform POLD Evaluate a polynomial and its derivative at any point RMK Evaluate a rational function at any point RMK1 Evaluate a rational function at any point (constant term in denominator 1) RMKD Evaluate a rational function and its derivative at any point RMKD1 Evaluate a rational function and its derivative at any point (constant term in denominator 1) PADE Calculate coefficients of Padé approximations **CHEBCF** Convert from power series to Chebyshev expansion and vice versa

CHEBEX Calculate the coefficients of Chebyshev expansion

CHEBAP Rational function approximation using Chebyshev polynomials

REMES Minimax approximation to mathematical functions using Remes algorithm FM Calculate error in rational function approximation for use with REMES

GAMMA Calculate Gamma function at real x, $\Gamma(x)$

Calculate natural logarithm of Gamma function at real x, $\ln |\Gamma(x)|$ GAMMAL Calculate Error function at real xERF **ERFC** Calculate complementary Error function at real x BJ0Calculate Bessel function of first kind of order zero, $J_0(x)$ BJ1 Calculate Bessel function of first kind of order one, $J_1(x)$ BJNCalculate Bessel function of first kind of integral order, $J_n(x)$ BY0Calculate Bessel function of second kind of order zero, $Y_0(x)$ BJY0 Calculate Bessel function of first and second kind of order zero BY1 Calculate Bessel function of second kind of order one, $Y_1(x)$ BJY1 Calculate Bessel function of first and second kind of order one BYN Calculate Bessel function of second kind of integral order, $Y_n(x)$ SPHBJN Calculate spherical Bessel function of integral order, $j_n(x)$ Calculate modified Bessel function of first kind of order zero, $I_0(x)$ BI0BI1 Calculate modified Bessel function of first kind of order one, $I_1(x)$ BINCalculate modified Bessel function of first kind of integral order, $I_n(x)$ BK0Calculate modified Bessel function of second kind of order zero, $K_0(x)$ Calculate modified Bessel function of second kind of order one, $K_1(x)$ BK1Calculate modified Bessel function of second kind of integral order, $K_n(x)$ BKNDAWSON Calculate the value of Dawson's integral FERMM05 Calculate the Fermi integrals for k = -1/2FERM05 Calculate the Fermi integrals for k = 1/2Calculate the Fermi integrals for k = 3/2FERM15 FERM25 Calculate the Fermi integrals for k = 5/2PLEG Calculate the Legendre polynomial, $P_{\ell}(x)$ PLM Calculate the associated Legendre function, $P_{\ell}^{m}(x)$ YLM Calculate the spherical harmonic, $Y_{\ell}^{m}(\theta,\phi)$ Calculate the spherical harmonic, $Y_{\ell}^{m}(\cos\theta,\phi)$ YLM_X **MINMAX** Rational function minimax approximation to discrete data POLYL1 Polynomial L_1 -approximation to discrete data LINL1 Linear L_1 -approximation to discrete data for arbitrary basis functions SIMPL1 Modified simplex method for LP problems in L_1 -approximation Chapter 11 Algebraic Eigenvalue Problem **INVIT** Real eigenvalue and eigenvector of a real matrix using inverse iteration

INVIT L
Real eigenvalue and eigenvector of a real matrix using inverse iteration
Real eigenvalue and left-eigenvector of a real matrix using inverse iteration
INVIT_CL
Complex eigenvalue and eigenvector of a real matrix using inverse iteration
Complex eigenvalue and left-eigenvector of a real matrix using inverse iteration
INVIT_CC
Complex eigenvalue and eigenvector of a complex matrix using inverse iteration

INVIT_CC Complex eigenvalue and eigenvector of a complex matrix using inverse iteration

TRED2 Reduction of a real symmetric matrix to symmetric tridiagonal form using Householder transformations

TRBAK Back-transform eigenvectors of tridiagonal matrix to original matrix

TQL2 Eigenvalue problem for a symmetric tridiagonal matrix using QL-algorithm

TRIDIA Specified eigenvalues and eigenvectors of a symmetric tridiagonal matrix using Sturm sequence and inverse iteration **STURM** Locate eigenvalues of a symmetric tridiagonal matrix using Sturm sequence TINVIT Eigenvalue and eigenvector of a symmetric tridiagonal matrix using inverse **HEREVP** Eigenvalue problem for a complex Hermitian matrix BALANC Balancing a general real matrix BALBAK Back-transform eigenvectors of balanced matrix to original matrix BALBAK_L Back-transform left-eigenvectors of balanced matrix to original matrix **ELMHES** Reduce a real matrix to Hessenberg form using Gaussian elimination HQR Eigenvalues of a Hessenberg matrix using QR-algorithm **Ordinary Differential Equations** Chapter 12 RKMInitial value problem using fourth-order Runge-Kutta method with adaptive

step size RKM_{-2} Initial value problem using second-order Runge-Kutta method with adaptive step size RK4

One step of integration using fourth-order Runge-Kutta method One step of integration using second-order Runge-Kutta method

MSTEP Initial value problem using predictor-corrector method with adaptive step

ADAMS One step of integration using fourth-order Adams method STRT4 Starting values for multistep method using Runge-Kutta method GEAR One step of integration using fourth-order stiffly stable method EXTP Initial value problem using extrapolation method

RK2

FDM Two-point boundary value problem using finite difference method **GEVP** Eigenvalue problem in differential equations using finite differences

GEVP_C Eigenvalue problem in differential equations using finite differences (complex version)

GAUBLK Solve a system of linear equations involving finite difference matrix

GAUBLK_C Solve a system of linear equations involving finite difference matrix (complex version)

SETMAT Generate finite difference matrix for a system of differential equations

SETMAT_C Generate finite difference matrix for a system of differential equations (complex version)

BSPODE Two-point boundary value problem using expansion method with B-spline basis functions

Chapter 13 **Integral Equations**

FRED Solve a Fredholm equation using quadrature method **FREDCO** Solve a Fredholm equation using collocation method **FUNK** Integrand = $K(x,t)\phi_i(t)$, for evaluating integrals in collocation method RLS Solve a linear inversion problem using regularised least squares technique **FORW** Solve the forward problem

8 Subject Wise List of Fortran Subprograms

VOLT Solve a linear Volterra equation using trapezoidal rule

VOLT2 Solve a nonlinear Volterra equation of the second kind using Simpson's rule

Chapter 14 Partial Differential Equations

CRANK Linear second-order parabolic equation using Crank-Nicolson method

LINES Nonlinear parabolic equations using the method of lines

ADM Parabolic equation in two space variables using alternating direction method

LAX Nonlinear hyperbolic equations using the Lax-Wendroff method

SOR Linear second-order elliptic equations using the successive over-relaxation

(SOR) method

ADI Linear second-order elliptic equations using the alternating direction implicit

iterative (ADI) method

ALPHABETIC LIST OF FORTRAN SUBPROGRAMS

ADAMS One step of integration using fourth-order Adams method

ADI Linear second-order elliptic equations using the alternating direction implicit

iterative (ADI) method

ADM Parabolic equation in two space variables using alternating direction method

ADPINT Adaptive integration over a finite interval

BALANC Balancing a general real matrix

BALBAK Back-transform eigenvectors of balanced matrix to original matrix
BALBAK_L Back-transform left-eigenvectors of balanced matrix to original matrix
BETAI Calculate incomplete Beta function by directly evaluating the integral

BETAP Calculate incomplete Beta function

BETCON1 Calculate incomplete Beta function using a continued fraction approximation BETCON Calculate incomplete Beta function using an alternative continued fraction

approximation

BETSER Calculate incomplete Beta function using a power series approximation BFGS Minimisation in n dimensions using quasi-Newton method with BFGS for-

mula

BIO Calculate modified Bessel function of first kind of order zero, $I_0(x)$ BI1 Calculate modified Bessel function of first kind of order one, $I_1(x)$ BIN Calculate modified Bessel function of first kind of integral order, $I_n(x)$

BISECT Solve a nonlinear equation using bisection

BJ0 Calculate Bessel function of first kind of order zero, $J_0(x)$ BJ1 Calculate Bessel function of first kind of order one, $J_1(x)$ BJN Calculate Bessel function of first kind of integral order, $J_n(x)$ BJY0 Calculate Bessel function of first and second kind of order zero BJY1 Calculate Bessel function of first and second kind of order one

BK0 Calculate modified Bessel function of second kind of order zero, $K_0(x)$ BK1 Calculate modified Bessel function of second kind of order one, $K_1(x)$ BKN Calculate modified Bessel function of second kind of integral order, $K_n(x)$

BRACKM Bracketing a minimum in one dimension

BRENTM Minimisation in one dimension using Brent's method BRENT Solve a nonlinear equation using Brent's method

BROYDN Solve a system of nonlinear equations using Broyden's method

with Broyden's method

BSPEV2	Evaluate function value and derivatives using B-spline expansion in two dimensions
BSPEVL	Evaluate function value and its derivatives using B-spline expansion
BSPEVN	Evaluate function value using B-spline expansion in n dimensions
BSPEVN1	Evaluate function value and first derivative using B-spline expansion in n
2012 (111	dimensions
BSPEVN2	Evaluate function value and first and second derivatives using B-spline ex-
DCDEIT	pansion in n dimensions
BSPFIT	Least squares fit to B-spline basis functions in one dimension
BSPFIT2	Least squares fit to B-spline basis in two dimensions with equal weights
BSPFITN	Least squares fit to B-spline basis in n dimensions with equal weights
BSPFITW2	Least squares fit to B-spline basis in two dimensions with arbitrary weights
BSPFITWN	Least squares fit to B-spline basis in n dimensions with arbitrary weights
BSPINT	Calculate coefficients of B-spline interpolation
BSPINT2	Calculate coefficients of B-spline interpolation in two dimensions
BSPINTN	Calculate coefficients of B-spline interpolation in n dimensions
BSPLIN	Calculate B-spline basis functions on a set of knots
BSPODE	Two-point boundary value problem using expansion method with B-spline
	basis functions
BSPQD	Integrate a B-spline expansion
BSPQD2	Integrate a B-spline expansion in two dimensions
BSPQDN	Integrate a B-spline expansion in n dimensions
BY0	Calculate Bessel function of second kind of order zero, $Y_0(x)$
BY1	Calculate Bessel function of second kind of order one, $Y_1(x)$
BYN	Calculate Bessel function of second kind of integral order, $Y_n(x)$
CASSUM	Cascade sum of a finite series using a function to calculate the terms
$CASSUM_A$	Cascade sum of a finite series using an array to supply the terms
CAUCHY	Calculate Cauchy principal value of an integral
CHEBAP	Rational function approximation using Chebyshev polynomials
CHEBCF	Convert from power series to Chebyshev expansion and vice versa
CHEBEX	Calculate the coefficients of Chebyshev expansion
CHOLSK	Solve a system of linear equations with symmetric positive definite matrix
	using Cholesky's decomposition
CONTUR	Contour integration over a circular contour for DELVES
CRANK	Linear second-order parabolic equation using Crank-Nicolson method
CROUT	Solve a system of linear equations using Crout's algorithm
$CROUT_C$	Solve a system of linear equations using Crout's algorithm (complex version)
CROUTH	Iterative refinement of solution of a system of linear equations
DAVIDM	Minimisation in one dimension using cubic Hermite interpolation
DAVIDN	Solve a system of nonlinear equations using Davidenko's method coupled
	with Newton's method
DAVIDN_B	Solve a system of nonlinear equations using Davidenko's method coupled
	with Provider's method

DAWSON Calculate the value of Dawson's integral

DELVES Complex zeros of an analytic function using quadrature based method
DFT DIVDIF Calculate interpolation and its derivatives using divided difference formula

DIVDIF0 Divided difference interpolation formula (no derivatives version)

DRVT Differentiation using $h \to 0$ extrapolation

ELMHES Reduce a real matrix to Hessenberg form using Gaussian elimination

EPSILN Integration using ϵ -algorithm

EQUIDS Multiple integration using equidistributed sequences

ERF Calculate Error function at real x

ERFC Calculate complementary Error function at real x

EULER Summation of alternating series using Euler transformation

EXTP Initial value problem using extrapolation method

FBETA Calculate the integrand for BETAI

FDM Two-point boundary value problem using finite difference method

FERM05 Calculate the Fermi integrals for k = 1/2FERM15 Calculate the Fermi integrals for k = 3/2FERM25 Calculate the Fermi integrals for k = 5/2FERMM05 Calculate the Fermi integrals for k = -1/2FFT Fast Fourier transform of complex data

FFTN Fast Fourier transform of complex data in n dimensions

FFTR Fast Fourier transform of real data

FILON Integration of an oscillatory function using Filon's formula

FLN Calculate the function value for line search for direction set method
FLNM Calculate the function value for line search for quasi-Newton method
Calculate error in rational function approximation for use with REMES

FORW Solve the forward problem

FRED Solve a Fredholm equation using quadrature method FREDCO Solve a Fredholm equation using collocation method

FUNK Integrand = $K(x,t)\phi_i(t)$, for evaluating integrals in collocation method

GAMMAL Calculate natural logarithm of Gamma function at real x, $\ln |\Gamma(x)|$

GAMMA Calculate Gamma function at real x, $\Gamma(x)$ GAMMAP Calculate incomplete Gamma function

GAUBLK Solve a system of linear equations involving finite difference matrix

GAUBLK_C Solve a system of linear equations involving finite difference matrix (complex version)

GAUBND Solve a system of linear equations with a band matrix using Gaussian elimination with partial pivoting

GAUBND_C Solve a system of linear equations with a band matrix using Gaussian elimination with partial pivoting (complex version)

GAUCB1 Integration using Gauss-Chebyshev formula with weight function, $w(x) = \sqrt{(x-A)/(B-x)}$ GAUCB2 Integration using Gauss-Chebyshev formula with weight function, $w(x) = \sqrt{(x-A)(B-x)}$ GAUCBY Integration using Gauss-Chebyshev formula with weight function,

GAUCBY Integration using Gauss-Chebyshev formula with weight function $w(x) = 1/\sqrt{(x-A)(B-x)}$

GAUELM Solve a system of linear equations using Gaussian elimination

GAUELM_C Solve a system of linear equations using Gaussian elimination (complex version)

GAUHER Calculate weights and abscissas of Gauss-Hermite quadrature formulae GAUJAC Calculate weights and abscissas of Gauss-Jacobi quadrature formulae GAULAG Integration over $[A, \infty)$ using a combination of Gaussian formulae Calculate weights and abscissas of Gauss-Legendre quadrature formulae

GAULG2 Integration over (0, A] with logarithmic singularity using a combination of Gaussian formulae

GAULOG Integration over (0, A] using Gaussian formula with weight function, $w(x) = \ln(A/x)$

GAUS16 Integration using 16 point Gauss-Legendre formula for use with ADPINT GAUSQ Integration over (0, A] using Gaussian formula with weight function,

 $w(x) = 1/\sqrt{x}$ GAUSQ2 Integration over (0, A] with square root singularity using a combination of

GAUSRC Calculate weights and abscissas of Gaussian formula using recurrence relation of orthogonal polynomials

GAUSS Integration using Gauss-Legendre formula

Gaussian formulae

GAUSWT Calculate weights and abscissas of Gaussian formula using moments of weight function

GEAR One step of integration using fourth-order stiffly stable method GEVP Eigenvalue problem in differential equations using finite differences

GEVP_C Eigenvalue problem in differential equations using finite differences (complex version)

GOLDEN Minimisation in one dimension using golden section search

 $\begin{array}{ll} \text{HEREVP} & \text{Eigenvalue problem for a complex Hermitian matrix} \\ \text{HERMIT} & \text{Integration over } (-\infty, \infty) \text{ using Gauss-Hermite formula} \\ \text{HQR} & \text{Eigenvalues of a Hessenberg matrix using QR-algorithm} \end{array}$

INVIT Real eigenvalue and eigenvector of a real matrix using inverse iteration
INVIT_C Complex eigenvalue and eigenvector of a real matrix using inverse iteration
Complex eigenvalue and eigenvector of a complex matrix using inverse iteration
ation

 ${\small \textbf{INVIT_CL}} \quad \textbf{Complex eigenvalue and left-eigenvector of a real matrix using inverse iteration}$

INVIT_L Real eigenvalue and left-eigenvector of a real matrix using inverse iteration IRANBIN Generate a sequence of random numbers with binomial distribution Generate a sequence of random numbers with Poisson distribution

KRONRD Integration using Gauss-Kronrod formula for use with ADPINT

LAGITC One root of a polynomial with complex coefficients using Laguerre's method LAGITR One root of a polynomial with real coefficients using Laguerre's method

LAGURE Integration over $[A, \infty)$ using Gauss-Laguerre formula

LAGURW Calculate weights and abscissas of Gauss-Laguerre quadrature formulae

LAPINV Inverse Laplace transform

LAX Nonlinear hyperbolic equations using the Lax-Wendroff method

LINES Nonlinear parabolic equations using the method of lines

LINFITXY Least squares straight line fit when there are errors in both x and y values LINL1 Linear L_1 -approximation to discrete data for arbitrary basis functions

LINMIN Line search for quasi-Newton method LINMNF Line search for direction set method

LINRN Calculate linear interpolation in n dimensions

LLSQ Linear least squares fit in n dimensions to a user defined set of basis functions

LOCATE Find the bracketing subinterval in an ordered table

MATINV Calculate inverse of a square matrix using Gaussian elimination

MCARLO Multiple integration using Monte Carlo method

MINMAX Rational function minimax approximation to discrete data

MSTEP Initial value problem using predictor-corrector method with adaptive step

size

MULER2 Complex root using Muller's method with function value in a scaled form,

 $f(x) \times 2^{i(x)}$

MULINT Multiple integration using product Gauss rule with varying number of points

MULLER Complex root using Muller's method

NEARST Find nearest point in an ordered table using bisection

NEWRAC Complex root of a nonlinear equation using Newton-Raphson method

NEWRAP Solve a nonlinear equation using Newton-Raphson method NEWTON Solve a system of nonlinear equations using Newton's method NGAUSS Multiple integration using a specified product Gauss rule

NLLSQ Calculate the Chi square function for a nonlinear least squares fit using quasi

Newton method (BFGS)

NLLSQ_F Calculate the Chi square function for a nonlinear least squares fit using di-

rection set method (NMINF)

NMINF Minimisation in n dimensions using direction set method

PADE Calculate coefficients of Padé approximations

PCOR Calculate the probability that two uncorrelated sequences will give a corre-

lation coefficient exceeding a given value

PLEG Calculate the Legendre polynomial, $P_{\ell}(x)$

PLM Calculate the associated Legendre function, $P_{\ell}^{m}(x)$ POLD Evaluate a polynomial and its derivative at any point

14 Alphabetic List of Fortran Subprograms

POLEV2 Evaluate the fitted polynomial and its derivatives at a specified point in two dimensions POLEVL Evaluate the fitted polynomial and its derivatives at a specified point **POLEVN** Evaluate the fitted polynomial at a specified point in n dimensions POLEVN1 Evaluate the fitted polynomial and first derivative at a specified point in ndimensions POLEVN2 Evaluate the fitted polynomial and first and second derivatives at a specified point in n dimensions POLFIT Least squares polynomial fit using orthogonal polynomials POLFIT1 Least squares polynomial fit using orthogonal polynomials, simplified version for multiple data sets POLFIT2 Least squares polynomial fit using orthogonal polynomials in two dimensions **POLFITN** Least squares polynomial fit using orthogonal polynomials in n dimensions **POLORT** Evaluate the orthogonal polynomial basis functions at a given point POLY2 Calculate polynomial interpolation in two dimensions POLYC All roots of a polynomial with complex coefficients POLYL1 Polynomial L_1 -approximation to discrete data **POLYR** All roots of a polynomial with real coefficients RAN1 Generate a sequence of random numbers with uniform distribution RANF Generate a sequence of random numbers with uniform distribution RANGAU Generate a sequence of random numbers with Gaussian distribution Calculate rational function interpolation RATNAL REMES Minimax approximation to mathematical functions using Remes algorithm RK2One step of integration using second-order Runge-Kutta method RK4One step of integration using fourth-order Runge-Kutta method RKM Initial value problem using fourth-order Runge-Kutta method with adaptive step size RKM_{-2} Initial value problem using second-order Runge-Kutta method with adaptive step size RLS Solve a linear inversion problem using regularised least squares technique RMKEvaluate a rational function at any point RMK1Evaluate a rational function at any point (constant term in denominator 1) **RMKD** Evaluate a rational function and its derivative at any point RMKD1 Evaluate a rational function and its derivative at any point (constant term in denominator 1) ROMBRG Romberg integration ROUND Rounding a floating-point number to a specified number of digits SEARCH Locate complex zeros by looking for sign changes SECANC Complex roots of a nonlinear equation using secant iteration SECANC_2 Complex roots of a nonlinear equation using secant iteration with function in scaled form $(f(x) = F(x)2^{i(x)})$ **SECANI** Solve a nonlinear equation using secant iteration (with reverse communication)

SECANT Solve a nonlinear equation using secant iteration SECAN_2 Solve a nonlinear equation using secant iteration with function in scaled form $(f(x) = F(x)2^{i(x)})$ **SETMAT** Generate finite difference matrix for a system of differential equations SETMAT_C Generate finite difference matrix for a system of differential equations (complex version) SHSORT Sorting an array in ascending order using shell sort algorithm SIMPL1 Modified simplex method for LP problems in L_1 -approximation **SIMPLX** Solving a linear programming problem using simplex method SIMPX Simplex method for a linear programming problem in the standard form **SIMSON** Integration using Simpson's 1/3 rule **SMOOTH** Draw a smooth curve through a set of points using cubic spline SOR Linear second-order elliptic equations using the successive over-relaxation (SOR) method **SPHBJN** Calculate spherical Bessel function of integral order, $j_n(x)$ SPHND To convert from hyper-spherical coordinates to Cartesian coordinates SPLEVL Evaluate the cubic spline and its derivatives at a specified point SPLINE Calculate coefficients of interpolating cubic spline SPLINT Integrate a tabulated function using cubic spline **STRINT** Multiple integration using monomial rules with varying number of points STROUD Multiple integration using a specified monomial rule STRT4 Starting values for multistep method using Runge-Kutta method STURM Locate eigenvalues of a symmetric tridiagonal matrix using Sturm sequence SVDSingular value decomposition of a matrix SVDEVL Solve a system of linear equations using singular value decomposition TINVIT Eigenvalue and eigenvector of a symmetric tridiagonal matrix using inverse iteration TQL2Eigenvalue problem for a symmetric tridiagonal matrix using QL-algorithm TRBAK Back-transform eigenvectors of tridiagonal matrix to original matrix TRED2 Reduction of a real symmetric matrix to symmetric tridiagonal form using Householder transformations **TRIDIA** Specified eigenvalues and eigenvectors of a symmetric tridiagonal matrix using Sturm sequence and inverse iteration VOLT Solve a linear Volterra equation using trapezoidal rule VOLT2 Solve a nonlinear Volterra equation of the second kind using Simpson's rule YLM Calculate the spherical harmonic, $Y_{\ell}^{m}(\theta,\phi)$ YLM_X Calculate the spherical harmonic, $Y_{\ell}^{m}(\cos\theta,\phi)$

ZROOT Complex roots of a nonlinear equation with deflation

ZROOT2 Complex roots of a nonlinear equation with deflation, function value in scaled form, $f(x) \times 2^{i(x)}$