

NAG Library

NAG C Library News, Mark 25

1 Introduction

At Mark 25 of the NAG C Library new functionality has been introduced in addition to improvements in existing areas. The Library now contains 1551 user-callable functions, all of which are documented, of which 58 are new at this mark.

Chapter d01 (Quadrature) has a function for high dimensional quadrature using sparse grids.

Chapter e01 (Interpolation) has a function for the triangulation of a two-dimensional scattered grid, and a function for the barycentric interpolation on function values on a triangulated scattered grid.

Chapter f01 (Matrix Operations, Including Inversion) has functions for converting between full, packed and rectangular full packed (RFP) matrix storage formats.

Chapter f02 (Eigenvalues and Eigenvectors) has a driver function for calculating selected eigenvalues/vectors of symmetric sparse matrices.

Chapter f07 (Linear Equations (LAPACK)) has functions for pivoted Cholesky factorization of positive semidefinite matrices and functions for the factorization, solution and inverse of positive definite matrices stored in rectangular full packed format.

Chapter f11 (Large Scale Linear Systems) has a function for the bandwidth reduction of a sparse symmetric matrix by reverse Cuthill–McKee reordering.

Chapter f16 (NAG Interface to BLAS) has linear algebra support functions for symmetric, Hermitian and triangular matrices stored in rectangular full packed format.

Chapter g01 (Simple Calculations on Statistical Data) has a function for computing probabilities for the Dickey–Fuller unit root test.

Chapter g02 (Correlation and Regression Analysis) has functions for performing Least Angle Regression (LARS), Least Absolute Shrinkage and Selection Operator (LASSO) and forward stagewise regression. There is also an additional nearest correlation matrix function that allows the leading principal submatrix to be preserved.

Chapter g05 (Random Number Generators) has functions for generating training and validation datasets suitable for use in cross-validation.

Chapter g13 (Time Series Analysis) has functions for computing: the Dickey–Fuller unit root test statistic; applying the unscented Kalman filter to a nonlinear state-space model with additive noise; and change point analysis using the PELT algorithm or using binary segmentation.

Chapter h (Operations Research) has a function for solving mixed integer nonlinear programming problems; optional settings for this are supplied and interrogated via two new option functions. Additionally, there is a function for approximating solutions to the classical travelling salesman problem.

Chapter x06 (OpenMP Utilities) is a new chapter of functions that provide utilities for controlling the OpenMP environment for your program.

2 New Functions

The 58 new user-callable functions included in the NAG C Library at Mark 25 are as follows.

Function Name	Purpose
d01esc	Multi-dimensional quadrature using sparse grids
e01eac	Triangulation of two-dimensional scattered grid, method of Renka and Cline

e01ebc	Barycentric interpolation on function values provided on a two-dimensional scattered grid
f01vac	Copies a real triangular matrix from full format to packed format
f01vbc	Copies a complex triangular matrix from full format to packed format
f01vcc	Copies a real triangular matrix from packed format to full format
f01vdc	Copies a complex triangular matrix from packed format to full format
f01vec	Copies a real triangular matrix from full format to Rectangular Full Packed format
f01vfc	Copies a complex triangular matrix from full format to Rectangular Full Packed format
f01vgc	Copies a real triangular matrix from Rectangular Full Packed format to full format
f01vhc	Copies a complex triangular matrix from Rectangular Full Packed format to full format
f01vjc	Copies a real triangular matrix from packed format to Rectangular Full Packed format
f01vkc	Copies a complex triangular matrix from packed format to Rectangular Full Packed format
f01vlc	Copies a real triangular matrix from Rectangular Full Packed format to packed format
f01vmc	Copies a complex triangular matrix from Rectangular Full Packed format to packed format
f02fkc	Selected eigenvalues and eigenvectors of a real symmetric sparse matrix
f07kdc	Cholesky factorization, with complete pivoting, of a real, symmetric, positive semidefinite matrix
f07krc	Cholesky factorization of complex Hermitian positive semidefinite matrix
f07wdc	Cholesky factorization of real symmetric positive definite matrix, Rectangular Full Packed format
f07wec	Solution of real symmetric positive definite system of linear equations, multiple right-hand sides, coefficient matrix already factorized by nag_dpftf (f07wdc), Rectangular Full Packed format
f07wjc	Inverse of real symmetric positive definite matrix, matrix already factorized by nag_dpftf (f07wdc), Rectangular Full Packed format
f07wkc	Inverse of real triangular matrix, Rectangular Full Packed format
f07wrc	Cholesky factorization of complex Hermitian positive definite matrix, Rectangular Full Packed format
f07wsc	Solution of complex Hermitian positive definite system of linear equations, multiple right-hand sides, coefficient matrix already factorized by nag_zpftf (f07wrc), Rectangular Full Packed format
f07wwc	Inverse of complex Hermitian positive definite matrix, matrix already factorized by nag_zpftf (f07wrc), Rectangular Full Packed format
f07wxc	Inverse of complex triangular matrix, Rectangular Full Packed format
f11yec	Reverse Cuthill–McKee reordering of a sparse symmetric matrix in CCS format
f16rkc	1-norm, ∞ -norm, Frobenius norm, largest absolute element, real symmetric matrix, Rectangular Full Packed format
f16ukc	1-norm, ∞ -norm, Frobenius norm, largest absolute element, complex Hermitian matrix, Rectangular Full Packed format
f16ylc	Solves a system of equations with multiple right-hand sides, real triangular coefficient matrix, Rectangular Full Packed format
f16yqc	Rank- k update of a real symmetric matrix, Rectangular Full Packed format

f16zlc	Solves system of equations with multiple right-hand sides, complex triangular coefficient matrix, Rectangular Full Packed format
f16zqc	Rank- k update of a complex Hermitian matrix, Rectangular Full Packed format
g01ewc	Computes probabilities for the Dickey–Fuller unit root test
g02anc	Computes a correlation matrix from an approximate matrix with fixed submatrix
g02mac	Least angle regression (LARS), least absolute shrinkage and selection operator (LASSO) and forward stagewise regression
g02mbc	Least Angle Regression (LARS), Least Absolute Shrinkage and Selection Operator (LASSO) and forward stagewise regression using the cross-products matrix
g02mcc	Additional parameter calculate following Least Angle Regression (LARS), Least Absolute Shrinkage and Selection Operator (LASSO) or forward stagewise regression
g05pvc	Permutates a matrix, vector, vector triplet into a form suitable for K -fold cross validation
g05pwc	Permutates a matrix, vector, vector triplet into a form suitable for random sub-sampling validation
g13awc	Computes (augmented) Dickey–Fuller unit root test statistic
g13ejc	Combined time and measurement update, one iteration of the Unscented Kalman Filter for a nonlinear state space model, with additive noise (reverse communication)
g13ekc	Combined time and measurement update, one iteration of the Unscented Kalman Filter for a nonlinear state space model, with additive noise
g13nac	Change point detection, using the PELT algorithm
g13nbc	Change points detection using the PELT algorithm, user supplied cost function
g13ndc	Change point detection, using binary segmentation
g13nec	Change point detection, using binary segmentation, user supplied cost function
h02dac	Mixed integer nonlinear programming
h02zkc	Option setting routine for nag_mip_sqp (h02dac)
h02zlc	Option getting routine for nag_mip_sqp (h02dac)
h03bbc	Travelling Salesman Problem, simulated annealing
x06aac	Sets the number of threads for OpenMP parallel regions
x06abc	The number of OpenMP threads in the current team
x06acc	An upper bound on the number of threads in the next parallel region
x06adc	The OpenMP thread number of the calling thread
x06afc	Tests for an active OpenMP parallel region
x06agc	Enables or disables nested OpenMP parallelism
x06ahc	Tests the status of nested OpenMP parallelism

3 Internal Changes Affecting Users

The following function has been significantly updated or enhanced at this mark.

nag_running_median_smoother (g10cac)

nag_running_median_smoother (g10cac) is a smoothing function with two possible smoothing methods. The function was previously using the incorrect method (i.e., if you asked for method A you would get method B, and vice versa).

4 Withdrawn Functions

The following functions have been withdrawn from the NAG C Library at Mark 25. Warning of their withdrawal was included in the NAG C Library Manual at Mark 24, together with advice on which functions to use instead. See the document ‘Advice on Replacement Calls for Withdrawn/Superseded Functions’ for more detailed guidance.

Withdrawn

Function	Replacement Function(s)
c05agc	nag_zero_cont_func_brent_binsrch (c05auc)
c05sdc	nag_zero_cont_func_brent (c05ayc)
c05ubc	nag_zero_nonlin_eqns_deriv_easy (c05rbc)
d01fcc	nag_multid_quad_adapt_1 (d01wcc)
d01gbc	nag_multid_quad_monte_carlo_1 (d01xbc)
f01bnc	nag_zpotrf (f07frc)
f01qcc	nag_dgeqrf (f08aec)
f01qdc	nag_dormqr (f08agc)
f01qec	nag_dorgqr (f08afc)
f01rcc	nag_zgeqrf (f08asc)
f01rdc	nag_zunmqr (f08auc)
f01rec	nag_zungqr (f08atc)
f03aec	nag_dpotrf (f07fdc) and nag_det_real_sym (f03bfc)
f03afc	nag_dgetrf (f07adc) and nag_det_real_gen (f03bac)
f03ahc	nag_zgetrf (f07arc) and nag_det_complex_gen (f03bnc)
f04adc	nag_complex_gen_lin_solve (f04cac)
f04agc	nag_dpotsr (f07fec)
f04ajc	nag_dgetrs (f07aec)
f04akc	nag_zgetrs (f07asc)
f04arc	nag_real_gen_lin_solve (f04bac)
f04awc	nag_zpotsr (f07fsc)
g02ewc	nag_full_step_regsn_monfun (g02efh) (see monfun in nag_full_step_regsn (g02efc))
x04aec	No replacement required.

5 Functions Scheduled for Withdrawal

The functions listed below are scheduled for withdrawal from the NAG C Library, because improved functions have now been included in the Library. You are advised to stop using functions which are scheduled for withdrawal and to use recommended replacement functions instead. See the document ‘Advice on Replacement Calls for Withdrawn/Superseded Functions’ for more detailed guidance, including advice on how to change a call to the old function into a call to its recommended replacement.

The following functions will be withdrawn at Mark 26.

**Functions
Scheduled
for
Withdrawal**

Replacement Function(s)

c06eac	nag_sum_fft_realherm_1d (c06pac)
c06ebc	nag_sum_fft_realherm_1d (c06pac)
c06ecc	nag_sum_fft_complex_1d (c06pcc)
c06ekc	nag_sum_convcorr_real (c06fkc)
c06frc	nag_sum_fft_complex_1d_multi (c06psc)
c06fuc	nag_sum_fft_complex_2d (c06puc)
c06gbc	No replacement required
c06gcc	No replacement required
c06hac	nag_sum_fft_sine (c06rec)
c06hbc	nag_sum_fft_cosine (c06rfc)
c06hcc	nag_sum_fft_qtrsine (c06rgc)
c06hdc	nag_sum_fft_qtrcosine (c06rhc)
d02pcc	nag_ode_ivp_rkts_range (d02pec) and associated d02p functions
d02pdc	nag_ode_ivp_rkts_onestep (d02pfc) and associated d02p functions
d02ppc	No replacement required
d02pvc	nag_ode_ivp_rkts_setup (d02pqc)
d02pwc	nag_ode_ivp_rkts_reset_tend (d02prc)
d02pxc	nag_ode_ivp_rkts_interp (d02psc)
d02pzc	nag_ode_ivp_rkts_errass (d02puc)
e04jbc	nag_opt_nlp (e04ucc)
f02aac	nag_dsyev (f08fac)
f02abc	nag_dsyev (f08fac)
f02adc	nag_dsygv (f08sac)
f02aec	nag_dsygv (f08sac)
f02afc	nag_dgeev (f08nac)
f02agc	nag_dgeev (f08nac)
f02awc	nag_zheev (f08fnc)
f02axc	nag_zheev (f08fnc)
f02bjc	nag_dggeev (f08wac)
f02wec	nag_dgesvd (f08kbc)
f02xec	nag_zgesvd (f08kpc)
g01aac	nag_summary_stats_onevar (g01atc)
g10bac	nag_kernel_density_gauss (g10bbc)

The following functions have been superseded, but will not be withdrawn from the Library until Mark 27 at the earliest.

Superseded

Function	Replacement Function(s)
d01tac	nag_quad_1d_gauss_vec (d01uac)
