NAG Library

NAG C Library News, Mark 26

1 Introduction

At Mark 26 of the NAG C Library new functionality has been introduced in addition to improvements in existing areas. The Library now contains 1555 user-callable functions, all of which are documented, of which 37 are new at this mark.

Chapter d01 (Quadrature) has two new functions to calculate weights and abscissae for use in Gaussian quadrature and a new function to solve a specific Gaussian quadrature problem.

Chapter e04 (Minimizing or Maximizing a Function) has a new suite of functions, NAG Modelling Optimization Suite for quadratic programming (QP), linear semidefinite programming (SDP), semidefinite programming with bilinear matrix inequalities (BMI-SDP), and general nonlinear programming (NLP). This suite can, for example, solve the nearest correlation matrix problem with individually weighted elements or minimize the maximum eigenvalue of a matrix. The suite introduces a novel interface, allowing the gradual build up of a problem definition and avoiding the long parameter lists of earlier interfaces. The SDP solver is based upon a generalized augmented Lagrangian method and as such complements existing solvers in the optimization chapters. The QP/NLP solver of this suite is based upon IPOPT, an interior-point method optimization package, suitable for large-scale problems, that complements the active-set sequential quadratic programming (SQP) solvers already present.

Chapter f08 (Least Squares and Eigenvalue Problems (LAPACK)) has additional blocked (BLAS-3) variants of functions for computing the generalized SVD, or generalized eigenvalues of real or complex matrix pairs.

Chapter g02 (Correlation and Regression Analysis) has another nearest correlation function.

Chapter x06 (OpenMP Utilities has a new function to identify, at runtime, whether you are using a threaded Library or not.

At this release we have made changes to the introductory documentation supporting the Library. The document previously called the 'Essential Introduction' has been revised so that relevant information and advice on how to use the Library and its documentation can be found quickly. The document has been renamed to How to Use the NAG Library and its Documentation.

You will also notice that on every HTML page there is now a Keyword Search box.

2 New Functions

The 37 new user-callable functions included in the NAG C Library at Mark 26 are as follows.

Function Name	**Purpose**
d01tdc	Calculation of weights and abscissae for Gaussian quadrature rules, method of Golub and Welsch
d01tec	Generates recursion coefficients needed by nag_quad_1d_gauss_wrec (d01tdc) to calculate a Gaussian quadrature rule
d01ubc	Non-automatic function to evaluate $\int_0^\infty \exp(-x^2) f(x)\, dx$
d02pgc	Ordinary differential equations, initial value problem, Runge–Kutta method, integration by reverse communication
d02phc	Set up interpolant by reverse communication for solution and derivative evaluations at points within the range of the last integration step taken by nag_ode_ivp_rk_step_rev comm (d02pgc)

d02pjc	Evaluate interpolant, set up using nag_ode_ivp_rkts_setup (d02pqc), to approximate solution and/or solution derivatives at a point within the range of the last integration step taken by nag_ode_ivp_rk_step_revcomm (d02pgc)
e04mwc	Write MPS data file defining LP, QP, MILP or MIQP problem
e04rac	Initialization of a handle for the NAG optimization modelling suite for problems, such as, quadratic programming (QP), nonlinear programming (NLP), linear semidefinite programming (SDP) or SDP with bilinear matrix inequalities (BMI-SDP)
e04rdc	A reader of sparse SDPA data files for linear SDP problems
e04rec	Define a linear objective function to a problem initialized by nag_opt_handle_init (e04rac)
e04rfc	Define a linear or a quadratic objective function to a problem initialized by nag_opt_handle_init (e04rac)
e04rgc	Define a nonlinear objective function to a problem initialized by nag_opt_handle_init (e04rac)
e04rhc	Define bounds of variables of a problem initialized by nag_opt_handle_init (e04rac)
e04rjc	Define a block of linear constraints to a problem initialized by nag_opt_handle_init (e04rac)
e04rkc	Define a block of nonlinear constraints to a problem initialized by nag_opt_handle_init (e04rac)
e04rlc	Define a structure of Hessian of the objective, constraints or the Lagrangian to a problem initialized by nag_opt_handle_init (e04rac)
e04rnc	Add one or more linear matrix inequality constraints to a problem initialized by nag_opt_handle_init (e04rac)
e04rpc	Define bilinear matrix terms to a problem initialized by nag_opt_handle_init (e04rac)
e04ryc	Print information about a problem handle initialized by nag_opt_handle_init (e04rac)
e04rzc	Destroy the problem handle initialized by nag_opt_handle_init (e04rac) and deallocate all the memory used
e04stc	Run an interior point solver on a sparse nonlinear programming problem (NLP) initialized by nag_opt_handle_init (e04rac) and defined by other functions from the suite
e04svc	Run the Pennon solver on a compatible problem initialized by nag_opt_handle_init (e04rac) and defined by other functions from the suite, such as, semidefinite programming (SDP) and SDP with bilinear matrix inequalities (BMI)
e04zmc	Option setting routine for the solvers from the NAG optimization modelling suite
e04znc	Option getting routine for the solvers from the NAG optimization modelling suite
e04zpc	Option setting routine for the solvers from the NAG optimization modelling suite from external file
f08vcc	Computes, using BLAS-3, the generalized singular value decomposition of a real matrix pair
f08vgc	Produces orthogonal matrices, using BLAS-3, that simultaneously reduce the m by n matrix A and the p by n matrix B to upper triangular form
f08vqc	Computes, using BLAS-3, the generalized singular value decomposition of a complex matrix pair
f08vuc	Produces unitary matrices, using BLAS-3, that simultaneously reduce the complex, m by n, matrix A and the complex, p by n, matrix B to upper triangular form
f08wcc	Computes, for a real nonsymmetric matrix pair, using BLAS-3, the generalized eigenvalues, and optionally, the left and/or right generalized eigenvectors

f08wfc	Performs, using BLAS-3, an orthogonal reduction of a pair of real general matrices to generalized upper Hessenberg form
f08wqc	Computes, for a complex nonsymmetric matrix pair, using BLAS-3, the generalized eigenvalues, and optionally, the left and/or right generalized eigenvectors
f08wtc	Performs, using BLAS-3, a unitary reduction of a pair of complex general matrices to generalized upper Hessenberg form
f08xcc	Computes, for a real nonsymmetric matrix pair, using BLAS-3, the generalized eigenvalues, the generalized real Schur form and, optionally, the left and/or right matrices of Schur vectors
f08xqc	Computes, for a complex nonsymmetric matrix pair, using BLAS-3, the generalized eigenvalues, the generalized complex Schur form and, optionally, the left and/or right matrices of Schur vectors
g02apc	Computes a correlation matrix from an approximate one using a specified target matrix
x06xac	Tests whether a threaded NAG Library is being used

3 Internal Changes Affecting Users

There have been no internal changes at this mark.

4 Withdrawn Functions

The following functions have been withdrawn from the NAG C Library at Mark 26. Warning of their withdrawal was included in the NAG C Library Manual at Mark 25, 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)**
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_dggev (f08wac)
f02wec	nag_dgesvd (f08kbc)
f02xec	nag_zgesvd (f08kpc)
g01aac	nag_summary_stats_onevar (g01atc)
g10bac	nag_kernel_density_gauss (g10bbc)

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 27.

Functions Scheduled for Withdrawal	**Replacement Function(s)**
d01tac	nag_quad_1d_gauss_vec (d01uac)