NAG Library

Mark 26 NAG Fortran Library News

1 Introduction

At Mark 26 of the NAG Library new functionality has been introduced in addition to improvements in existing areas. The Library now contains 1875 user-callable routines, all of which are documented, of which 57 are new at this mark. Further new functionality has been introduced at Mark 26.1

Chapter C05 (Roots of One or More Transcendental Equations) has a new routine that finds a solution of a system of nonlinear equations using Anderson acceleration.

Chapter C06 (Summation of Series) has a new routine that calculates the fast Gauss transform approximation to the discrete Gauss transform.

Chapter D01 (Quadrature) has two new routines to calculate weights and abscissae for use in Gaussian quadrature and a new routine to solve a specific Gaussian quadrature problem.

Chapter D02 (Ordinary Differential Equations) has reverse communication versions of the Runge–Kutta step and interpolation routines. The interpolation routine has extended the functionality to include the high-order method.

Chapter E04 (Minimizing or Maximizing a Function) has a new suite of routines, 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.

At Mark 26.1, two new solvers are added to the NAG Modelling Optimization Suite. The first one is a derivative free solver for nonlinear least squares subject to bound constraints. It is aimed at small to medium sized data fitting or calibration problems (~100 variables) and is particularly suitable when the objective function is noisy or expensive to evaluate. The second one is a new interior point method for large scale linear programming problems (LP) that should offer significant speed-ups compared to the existing LP solvers in the NAG library.

Chapter F08 (Least Squares and Eigenvalue Problems (LAPACK)) has additional blocked (BLAS-3) variants of routines for computing the generalized SVD, or generalized eigenvalues of real or complex matrix pairs.

Chapter G02 (Correlation and Regression Analysis) has a new nearest correlation routine that, using a shrinking method, allows the fixing of arbitrary elements in the input matrix.

Chapter G04 (Analysis of Variance) has a new routine for calculating the intraclass correlation (ICC) for a number of different rater reliability study designs.

Chapter G22 (Linear Model Specification) contains utility routines for aiding in the construction of design matrices for use when fitting linear regression models.

Chapter S (Approximations of Special Functions) contains a new set of routines to evaluate Struve functions H_0, H_1, L_0 and L_1.

Chapter X06 (OpenMP Utilities) has a new routine to identify, at runtime, whether you are using a threaded Library or not.

At this release we have made a number of changes to the documentation and long names as follows.

The specification of routines in routine documents (see Section 2 in **d03pdf/d03pda**) now includes the C Header interface which can be used to call a NAG Library routine from C or C++; the name used for this interface is the Fortran Interface short name appended by an underscore (e.g., d03faf_ corresponds to d03faf). For routines with 'a' and 'f' versions, the same approach also applies to the 'a' version (e.g., d03pda_ corresponds to d03pda).

Some routine long names have been changed for the following reasons:

(a) to consistently use the Chapter identifying word (e.g., ‘opt’ for Chapter E04) as the second word in the long name.

(b) to avoid using a digit as the first character of the third word in the long name. This allows other environments to use the same long name: third and following words are used as a routine identifier inside a class name using the first two words.

(c) the word ‘withdrawn’ has been changed to ‘withdraw’ to be consistent with other routine long names using ‘withdraw’.

(d) ‘withdraw_’ has been removed from a few routines that are no longer to be withdrawn.

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.

We have also provided clarification of the term 'Direct and Reverse Communication Routines', see Section 3.3.3 in How to Use the NAG Library and its Documentation, and taken the decision to document a number of error conditions, i.e., Dynamic Memory Allocation, License Management and Unexpected Errors (see Sections 3.7, 3.8 and 3.9 in 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 Routines

2.1 New Routines at Mark 26.1

The 20 new user-callable routines included in the NAG Library at Mark 26.1 are as follows.

Routine Name	**Purpose**
c05mdf	Solution of a system of nonlinear equations using Anderson acceleration (reverse communication)
c06saf	Multidimensional fast Gauss transform
e04fff	Derivative free (DFO) solver for a nonlinear least squares objective function with bounded variables
e04mtf	Linear programming (LP), sparse, interior point method (IPM)
e04rmf	Define a nonlinear least squares objective function to a problem initialized by e04raf
e04rxf	Retrieve or write a piece of information in a problem handle initialized by e04raf
g04gaf	Intraclass correlation (ICC) for assessing rater reliability
g22yaf	Specify a linear model via a formula string
g22ybf	Describe a dataset
g22ycf	Construct a design matrix from a linear model specified using g22yaf
g22ydf	Construct a vector indicating which columns of a design matrix to include in a submodel specified using g22yaf
g22zaf	Destroy a G22 handle and deallocate all the memory used
g22zmf	Option setting routine for Chapter G22

g22znf	Option getting routine for Chapter G22
s17gaf	Struve function of order 0, $H_0(x)$
s17gbf	Struve function of order 1, $H_1(x)$
s18gaf	Modified Struve function of order 0, $L_0(x)$
s18gbf	Modified Struve function of order 1, $L_1(x)$
s18gcf	The function $I_0(x) - L_0(x)$, where $I_0(x)$ is a modified Bessel function and $L_0(x)$ is a Struve function
s18gdf	The function $I_1(x) - L_1(x)$, where $I_1(x)$ is a modified Bessel function and $L_1(x)$ is a Struve function

2.2 New Routines at Mark 26.0

The 37 new user-callable routines included in the NAG Library at Mark 26.0 are as follows.

Routine Name	**Purpose**
d01tdf	Calculation of weights and abscissae for Gaussian quadrature rules, method of Golub and Welsch
d01tef	Generates recursion coefficients needed by d01tdf to calculate a Gaussian quadrature rule
d01ubf	Non-automatic routine to evaluate $\int_0^\infty \exp(-x^2) f(x)\, dx$
d02pgf	Ordinary differential equations, initial value problem, Runge–Kutta method, integration by reverse communication
d02phf	Set up interpolant by reverse communication for solution and derivative evaluations at points within the range of the last integration step taken by d02pgf
d02pjf	Evaluate interpolant, set up using d02pqf, to approximate solution and/or solution derivatives at a point within the range of the last integration step taken by d02pgf
e04mwf	Write MPS data file defining LP, QP, MILP or MIQP problem
e04raf	Initialization of a handle for the NAG optimization modelling suite for problems, such as, linear programming (LP), quadratic programming (QP), nonlinear programming (NLP), least squares (LSQ) problems, linear semidefinite programming (SDP) or SDP with bilinear matrix inequalities (BMI-SDP)
e04rdf	A reader of sparse SDPA data files for linear SDP problems
e04ref	Define a linear objective function to a problem initialized by e04raf
e04rff	Define a linear or a quadratic objective function to a problem initialized by e04raf
e04rgf	Define a nonlinear objective function to a problem initialized by e04raf
e04rhf	Define bounds of variables of a problem initialized by e04raf
e04rjf	Define a block of linear constraints to a problem initialized by e04raf
e04rkf	Define a block of nonlinear constraints to a problem initialized by e04raf
e04rlf	Define a structure of Hessian of the objective, constraints or the Lagrangian to a problem initialized by e04raf
e04rnf	Add one or more linear matrix inequality constraints to a problem initialized by e04raf
e04rpf	Define bilinear matrix terms to a problem initialized by e04raf
e04ryf	Print information about a problem handle initialized by e04raf
e04rzf	Destroy the problem handle initialized by e04raf and deallocate all the memory used

e04stf	Run an interior point solver on a sparse nonlinear programming problem (NLP) initialized by e04raf and defined by other routines from the suite
e04svf	Run the Pennon solver on a compatible problem initialized by e04raf and defined by other routines from the suite, such as, semidefinite programming (SDP) and SDP with bilinear matrix inequalities (BMI)
e04zmf	Option setting routine for the solvers from the NAG optimization modelling suite
e04znf	Option getting routine for the solvers from the NAG optimization modelling suite
e04zpf	Option setting routine for the solvers from the NAG optimization modelling suite from external file
f08vcf	Computes, using BLAS-3, the generalized singular value decomposition of a real matrix pair
f08vgf	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
f08vqf	Computes, using BLAS-3, the generalized singular value decomposition of a complex matrix pair
f08vuf	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
f08wcf	Computes, for a real nonsymmetric matrix pair, using BLAS-3, the generalized eigenvalues, and optionally, the left and/or right generalized eigenvectors
f08wff	Performs, using BLAS-3, an orthogonal reduction of a pair of real general matrices to generalized upper Hessenberg form
f08wqf	Computes, for a complex nonsymmetric matrix pair, using BLAS-3, the generalized eigenvalues, and optionally, the left and/or right generalized eigenvectors
f08wtf	Performs, using BLAS-3, a unitary reduction of a pair of complex general matrices to generalized upper Hessenberg form
f08xcf	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
f08xqf	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
g02apf	Computes a correlation matrix from an approximate one using a specified target matrix
x06xaf	Tests whether a threaded NAG Library is being used

3 Internal Changes Affecting Users

The following routines have been significantly updated or enhanced at this mark and details are available in each routine document.

e01sgf

e01shf

e01tgf

e01thf

e01tkf

e01tlf

e01tmf

e01tnf

e01zmf

e01znf

e04rhf

e04stf

e04svf

For details of all known issues which have been reported for the NAG Library please refer to the Known Issues list available on the NAG Website.

4 Withdrawn Routines

The following routines have been withdrawn from the NAG Library at Mark 26. Warning of their withdrawal was included in the NAG Library Manual at Mark 25, together with advice on which routines to use instead. See the document 'Advice on Replacement Calls for Withdrawn/Superseded Routines' for more detailed guidance.

Withdrawn Routine	**Replacement Routine(s)**
c06eaf	c06paf
c06ebf	c06paf
c06ecf	c06pcf
c06ekf	c06fkf
c06frf	c06psf
c06fuf	c06puf
c06gbf	No replacement required
c06gcf	No replacement required
c06gqf	No replacement required
c06gsf	No replacement required
c06haf	c06ref
c06hbf	c06rff
c06hcf	c06rgf
c06hdf	c06rhf
d01baf	d01uaf
d01bbf	d01tbf
d02pcf	d02pef and associated D02P routines
d02pdf	d02pff or d02pgf and associated D02P routines
d02pvf	d02pqf
d02pwf	d02prf
d02pxf	d02psf
d02pyf	d02ptf
d02pzf	d02puf
f04ycf	f04ydf
f04zcf	f04zdf
g01aaf	g01atf

5 Routines Scheduled for Withdrawal

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

The following routines will be withdrawn at Mark 27.

Routines Scheduled for Withdrawal	**Replacement Routine(s)**
d02tkf	d02tlf
d03ryf	No replacement required
e02acf	e02alf
f02sdf	f12agf and f12fgf
f02wdf	f02wuf and f08aef (dgeqrf)
g01agf	No replacement required
g01ahf	No replacement required
g01ajf	No replacement required
g10baf	g10bbf

The following routines have been superseded, but will not be withdrawn from the Library until Mark 28 at the earliest.

Superseded Routine	**Replacement Routine(s)**
c06fpf	c06pqf
c06fqf	c06pqf
d01rbf	No replacement required
f04abf	f07fbf (dposvx)
f04aef	f07abf (dgesvx)
f04asf	f07fbf (dposvx)
f04atf	f07abf (dgesvx)