GenStat

Running the NAG Library from GenStat

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NAG Library

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- Collection of numerical and statistical algorithms
  - Supplied by Numerical Algorithms Group (NAG)
  - Available in Fortran and C
  - Website: www.nag.co.uk
- Routines include
  - Ordinary differential equations
  - Numerical integration and differentiation
  - Linear programming
  - Many standard statistical analysis

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NAG routines in GenStat

- Embedded Fortran library
- Complements facilities in GenStat
- NAG directive
- Available routines
  - `NAG [PRINT=algorithms]`
- Examples available via help menu
  - Help | Examples | Commands
- NAG algorithm documentation
  - View or Download from nag.co.uk or www.vsni.co.uk

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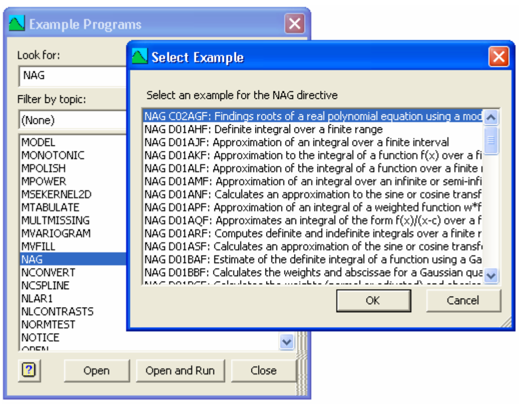
NAG Examples

Examples for each NAG function:



NAG directive

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- Option NAME
  - Name of routine in full, e.g. D02KDF
  - Note NAG routine names not distinct to first 4 characters
- Parameter ARGUMENTS
  - Arguments for call in a pointer
  - Elements in same order as for NAG routine
  - Input arguments must be defined, output arguments do not
  - Pointer to expressions can be used for NAG arguments that expect subroutines or functions
- Parameter RESULT

  Stores the return value of the NAG algorithm if it is a function

```
NAG   [NAME=C02AGF] !p(A,N,SCALE,Z,W,IFAIL)
```

NAG Documentation

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C02 – Zeros of Polynomials C02AGF

NAG Fortran Library Routine Document

C02AGF

1 Purpose

C02AGF finds all the roots of a real polynomial equation, using a variant of Laguerre's Method.

2 Specification

```
SUBROUTINE C02AGF(A, N, SCALE, Z, W, IFAIL)
INTEGER          N, IFAIL
real             A(N+1), Z(2,N), W(2*(N+1))
LOGICAL          SCALE
```

3 Description

The routine attempts to find all the roots of the nth degree real polynomial equation

$$P(z) = a_0 z^n + a_1 z^{n-1} + a_2 z^{n-2} + \ldots + a_{n-1} z + a_n = 0.$$

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Genstat Implementation

- Basic Rules:
  - Ignore distinction between **REAL** and **INTEGER**
  - 0 and 1 in GenStat correspond to **LOGICAL** values **.FALSE.** and **.TRUE.**

  - Scalar values are passed as **SCALAR**
  - 1-dimensional arrays are passed as **VARIATE**
  - 2-dimensional arrays are passed as **MATRIX**
- Working arrays just need to be declared of the correct size
- Output structures will be formed to suit the result, but if declared must be of the right type

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Setting Up the Call

```
INTEGER N                          - degree of polynomial
    SCALAR     N; 5

real A(N+1)                        - polynomial coefficients
    VARIATE    [N+1]   A; !(1...6)

LOGICAL SCALE
    SCALAR     SCALE; 0

real W(2*(N+1))                    – workspace
    VARIATE    [2*(N+1)]   W

real Z(2,N), INTEGER IFAIL         - outputs
    MATRIX     [2;N]   Z           (optional)
    SCALAR     IFAIL

                 SUBROUTINE C02AGF(A, N, SCALE, Z, W, IFAIL)
POINTER  ARGS; !p( A,N,SCALE, Z, W,IFAIL)
NAG      [NAME=C02AGF] ARGS
```

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Example Output

```
VARIATE     A; VALUES=!(1...6)
SCALAR      N; VALUE = NVAL(A) - 1
SCALAR      SCALE; VALUE = 0
VARIATE     [NVALUES = 2*(N+1)] W
POINTER     [VALUES=A,N,SCALE,\                        "entry arguments"
            Z,\                                        "exit  arguments"
            W,IFAIL] ARGS                              "entry arguments"
NAG         [NAME=C02AGF] ARGS

"The real and imaginary parts of the roots are stored in first and
 second rows of Z respectively."
PRINT       Z

               Z
                1          2          3          4          5

    1     -1.4918     0.5517     0.5517    -0.8058    -0.8058
    2      0.0000     1.2533    -1.2533     1.2229    -1.2229
```

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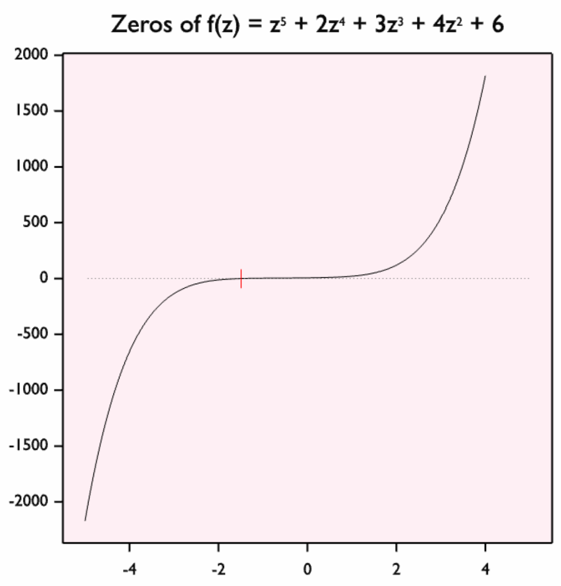

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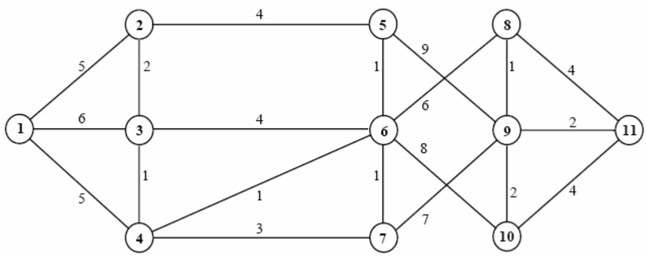
H03ADF - Shortest Path

Dijkstra’s algorithm to find the shortest path through a directed or undirected network:



Shortest path: 1 - 4 - 6 - 8 - 9 – 11

Length: 15

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H03ADF - Shortest Path

```
SCALAR     N, NS, NE, NNZ, DIRECT; \
            VALUE = 11,1,11,20,0
VARIATE    [NVALUES=NNZ]   D, IROW, ICOL
READ D, IROW, ICOL
6.0 6 8
1.0 8 9
2.0 9 11  .... Etc.

SCALAR                  SPLEN
VARIATE    [NVALUES=N]      PATH
VARIATE    [NVALUES=3*N+1] IWORK
VARIATE    [NVALUES=2*N]   WORK

POINTER    [VALUES=N, NS, NE, DIRECT, NNZ, \
              D, IROW, ICOL, SPLEN,            \
              PATH, IWORK, WORK, IFAIL] ARGS

NAG        [NAME=H03ADF] ARGS
```

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Passing Functions

Many NAG subroutines include a function as an argument. For example, D01AJF which calculates a definite integral for a supplied function.

$$\int_B^A \frac{x \sin(30x)}{\sqrt{1-(x/2\pi)^2}}\,\mathrm{d}x$$

In Genstat, specify the function as an expression and its dummy arguments in a pointer, within the ARGS pointer

```
EXPRESSION fx; !e( Y =X*sin(30*X)/              \
                      SQRT(1-(X/(2*PI))**2))
POINTER pfx; !p( fx, Y, X)

NAG [NAME=D01AJF]  !p( pfx, A,B,EPSABS,EPSREL, \
           RESULT, ABSERR,W,LW,IW,LIW,IFAIL)
```

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D01BAF – Gaussian Quadrature

```
SCALAR N; VALUE = 8
SCALAR   A, B; VALUE = 0, 1

POINTER  ARGS; VALUES=   \
       !p('D01BAZ',0,1,8,    \
          !p(!e(Y=4/(1+X*X)),Y,X),  \
          IFAIL)

NAG      [NAME=D01BAF] ARGS; \
          RESULT=Integral
```

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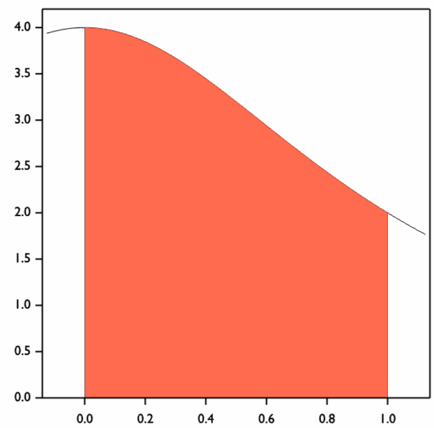
D01BAF – Gaussian Quadrature



$$\int_0^1 \frac{4}{1+x^2}\,\mathrm{d}x = \pi$$

8-point Gauss-Legendre gives the value 3.14159

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D02 – Systems of Diff. Equations

Lotka-Volterra Model: Predator - Prey

$$\frac{dx}{dt} = 2.0x - 0.01xy \qquad \frac{dy}{dt} = -0.8y + 0.0002xy$$

```
POINTER  [VALUES=X, XEND, N, Y, \
          !P(!E(F$[1]=2.0*Y$[1] - 0.01*Y$[1]*Y$[2]),\
             !E(F$[2]=-0.8*Y$[2] + \
                                  0.0002*Y$[1]*Y$[2]),\
             X,Y,F), J, \
           TOL, RELABS, O, 0, W, IW, IFAIL] ARGS

NAG      [NAME=D02EJF] ARGS
```

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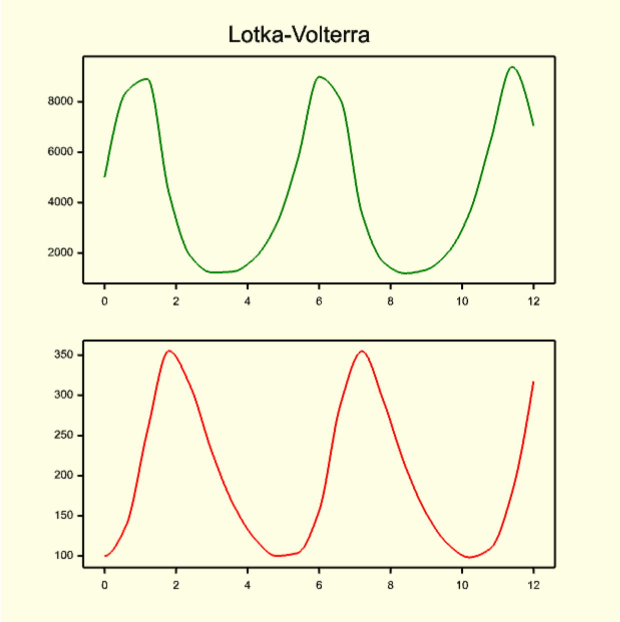
D02 – Systems of Diff. Equations



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GenStat 11th Edition

Our initial interest involves the following chapters of the NAG library:

C02 – Zeros of Polynomials
D01 – Quadrature
D02 – Ordinary Differential Equations
D04 – Numerical Differentiation
E02 – Curve and Surface Fitting
E04 – Minimizing or Maximizing a Function
G11 – Contingency Table Analysis
G12 – Survival Analysis
H02 – Operations Research
H03 – Operations Research

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As a start we have incorporated interfaces to 87 individual NAG algorithms:

C02AGF, D01AHF, D01AJF, D01AKF, D01ALF, D01AMF, D01ANF, D01APF, D01AQF, D01ARF, D01ASF, D01BAF, D01BBF, D01BCF, D01DAF, D01EAF, D01FBF, D01FCF, D01GAF, D01GBF, D01JAF, D01PAF, D02AGF, D02BGF, D02BHF, D02BJF, D02CJF, D02EJF, D02GAF, D02GBF, D02HAF, D02HBF, D02JAF, D02JBF, D02KAF, D02KDF, D02KEF, D02LAF, D02LXF, D02LYF, D02LZF, D02MVF, D02MZF, D02NBF, D02NCF, D02NDF, D02NGF, D02NHF, D02NJF, D02NMF, D02NNF, D02NRF, D02NSF, D02NTF, D02NUF, D02NVF, D02NWF, D02NXF, D02NYF, D02NZF, D02PCF, D02PDF, D02PVF, D02PWF, D02PXF, D02PYF, D02PZF, D02QFF, D02QGF, D02QWF, D02QXF, D02QYF, D02QZF, D02XJF, D02XKF, D04AAF, E02AHF, E02AKF, E04CCA, E04CCF, E04MFA, E04MFF, G11CAF, G12BAF, H02BBF, H02CBF, H03ADF

GenStat 12th Edition

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Proposed extensions to the NAG directive:

D03 – Partial Differential Equations
- e.g. Black-Scholes model

D05 – Integral Equations

D06 – Mesh Generation

E01 – Interpolation

E04 – Minimizing or Maximizing a Function
- additional methods

G13 - Multivariate Time Series (VARMA)

H02 – Operations Research
- transportation problem