NAG Toolbox

nag zeros poly real (c02ag)

1 Purpose

nag_zeros_poly_real (c02ag) finds all the roots of a real polynomial equation, using a variant of Laguerre's method.

2 Syntax

3 Description

nag zeros poly real (c02ag) attempts to find all the roots of the nth degree real polynomial equation

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

The roots are located using a modified form of Laguerre's method, originally proposed by Smith (1967).

The method of Laguerre (see Wilkinson (1965)) can be described by the iterative scheme

$$L(z_k) = z_{k+1} - z_k = \frac{-nP(z_k)}{P'(z_k) \pm \sqrt{H(z_k)}},$$

where
$$H(z_k) = (n-1) \left[(n-1)(P'(z_k))^2 - nP(z_k)P''(z_k) \right]$$
 and z_0 is specified.

The sign in the denominator is chosen so that the modulus of the Laguerre step at z_k , viz. $|L(z_k)|$, is as small as possible. The method can be shown to be cubically convergent for isolated roots (real or complex) and linearly convergent for multiple roots.

The function generates a sequence of iterates z_1, z_2, z_3, \ldots , such that $|P(z_{k+1})| < |P(z_k)|$ and ensures that $z_{k+1} + L(z_{k+1})$ 'roughly' lies inside a circular region of radius |F| about z_k known to contain a zero of P(z); that is, $|L(z_{k+1})| \le |F|$, where F denotes the Fejér bound (see Marden (1966)) at the point z_k . Following Smith (1967), F is taken to be $\min(B, 1.445nR)$, where B is an upper bound for the magnitude of the smallest zero given by

$$B = 1.0001 \times \min(\sqrt{n}L(z_k), |r_1|, |a_n/a_0|^{1/n}),$$

 r_1 is the zero X of smaller magnitude of the quadratic equation

$$\frac{P''(z_k)}{2n(n-1)}X^2 + \frac{P'(z_k)}{n}X + \frac{1}{2}P(z_k) = 0$$

and the Cauchy lower bound R for the smallest zero is computed (using Newton's Method) as the positive root of the polynomial equation

$$|a_0|z^n + |a_1|z^{n-1} + |a_2|z^{n-2} + \dots + |a_{n-1}|z - |a_n| = 0.$$

Starting from the origin, successive iterates are generated according to the rule $z_{k+1}=z_k+L(z_k)$, for $k=1,2,3,\ldots$, and $L(z_k)$ is 'adjusted' so that $|P(z_{k+1})|<|P(z_k)|$ and $|L(z_{k+1})|\leq |F|$. The iterative procedure terminates if $P(z_{k+1})$ is smaller in absolute value than the bound on the rounding error in $P(z_{k+1})$ and the current iterate $z_p=z_{k+1}$ is taken to be a zero of P(z) (as is its conjugate \bar{z}_p if z_p is complex). The deflated polynomial $\tilde{P}(z)=P(z)/(z-z_p)$ of degree n-1 if z_p is real $(\tilde{P}(z)=P(z)/((z-z_p)(z-\bar{z}_p)))$ of degree n-2 if z_p is complex) is then formed, and the above

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procedure is repeated on the deflated polynomial until n < 3, whereupon the remaining roots are obtained via the 'standard' closed formulae for a linear (n = 1) or quadratic (n = 2) equation.

Note that nag_zeros_quadratic_real (c02aj), nag_zeros_cubic_real (c02ak) and nag_zeros_quartic_real (c02al) can be used to obtain the roots of a quadratic, cubic (n = 3) and quartic (n = 4) polynomial, respectively.

4 References

Marden M (1966) Geometry of polynomials *Mathematical Surveys* 3 American Mathematical Society, Providence, RI

Smith B T (1967) ZERPOL: a zero finding algorithm for polynomials using Laguerre's method *Technical Report* Department of Computer Science, University of Toronto, Canada

Thompson K W (1991) Error analysis for polynomial solvers Fortran Journal (Volume 3) 3 10-13

Wilkinson J H (1965) The Algebraic Eigenvalue Problem Oxford University Press, Oxford

5 Parameters

5.1 Compulsory Input Parameters

1: $\mathbf{a}(\mathbf{n} + \mathbf{1}) - \text{REAL (KIND=nag wp)}$ array

if **a** is declared with bounds $(0:\mathbf{n})$, then $\mathbf{a}(i)$ must contain a_i (i.e., the coefficient of z^{n-i}), for $i=0,1,\ldots,n$.

Constraint: $\mathbf{a}(1) \neq 0.0$.

2: $\mathbf{n} - INTEGER$

n, the degree of the polynomial.

Constraint: $\mathbf{n} \geq 1$.

5.2 Optional Input Parameters

1: **scal** – LOGICAL

Suggested value: scal = true.

Default: true

Indicates whether or not the polynomial is to be scaled. See Section 9 for advice on when it may be preferable to set scal = false and for a description of the scaling strategy.

5.3 Output Parameters

1: $\mathbf{z}(\mathbf{2}, \mathbf{n}) - REAL (KIND=nag_wp) array$

The real and imaginary parts of the roots are stored in $\mathbf{z}(1,i)$ and $\mathbf{z}(2,i)$ respectively, for $i=1,2,\ldots,n$. Complex conjugate pairs of roots are stored in consecutive pairs of elements of \mathbf{z} ; that is, $\mathbf{z}(1,i+1)=\mathbf{z}(1,i)$ and $\mathbf{z}(2,i+1)=-\mathbf{z}(2,i)$.

2: **ifail** – INTEGER

ifail = 0 unless the function detects an error (see Section 5).

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6 Error Indicators and Warnings

Errors or warnings detected by the function:

ifail = 1

On entry,
$$\mathbf{a}(0) = 0.0$$
, or $\mathbf{n} < 1$.

$$ifail = 2$$

The iterative procedure has failed to converge. This error is very unlikely to occur. If it does, please contact NAG, as some basic assumption for the arithmetic has been violated. See also Section 9.

ifail = 3

Either overflow or underflow prevents the evaluation of P(z) near some of its zeros. This error is very unlikely to occur. If it does, please contact NAG. See also Section 9.

ifail
$$= -99$$

An unexpected error has been triggered by this routine. Please contact NAG.

ifail
$$= -399$$

Your licence key may have expired or may not have been installed correctly.

ifail
$$= -999$$

Dynamic memory allocation failed.

7 Accuracy

All roots are evaluated as accurately as possible, but because of the inherent nature of the problem complete accuracy cannot be guaranteed. See also Section 10.

8 Further Comments

If $\mathbf{scal} = true$, then a scaling factor for the coefficients is chosen as a power of the base b of the machine so that the largest coefficient in magnitude approaches $thresh = b^{e_{\max}-p}$. You should note that no scaling is performed if the largest coefficient in magnitude exceeds thresh, even if $\mathbf{scal} = true$. (b, e_{\max} and p are defined in Chapter X02.)

However, with **scal** = true, overflow may be encountered when the input coefficients $a_0, a_1, a_2, \ldots, a_n$ vary widely in magnitude, particularly on those machines for which $b^{(4p)}$ overflows. In such cases, **scal** should be set to false and the coefficients scaled so that the largest coefficient in magnitude does not exceed $b^{(e_{\max}-2p)}$.

Even so, the scaling strategy used by nag_zeros_poly_real (c02ag) is sometimes insufficient to avoid overflow and/or underflow conditions. In such cases, you are recommended to scale the independent variable (z) so that the disparity between the largest and smallest coefficient in magnitude is reduced. That is, use the function to locate the zeros of the polynomial dP(cz) for some suitable values of c and d. For example, if the original polynomial was $P(z) = 2^{-100} + 2^{100}z^{20}$, then choosing $c = 2^{-10}$ and $d = 2^{100}$, for instance, would yield the scaled polynomial $1 + z^{20}$, which is well-behaved relative to overflow and underflow and has zeros which are 2^{10} times those of P(z).

If the function fails with **ifail** = 2 or 3, then the real and imaginary parts of any roots obtained before the failure occurred are stored in \mathbf{z} in the reverse order in which they were found. Let n_R denote the number of roots found before the failure occurred. Then $\mathbf{z}(1,n)$ and $\mathbf{z}(2,n)$ contain the real and imaginary parts of the first root found, $\mathbf{z}(1,n-1)$ and $\mathbf{z}(2,n-1)$ contain the real and imaginary parts of the second root found, $\dots, \mathbf{z}(1,n-n_R+1)$ and $\mathbf{z}(2,n-n_R+1)$ contain the real and imaginary

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parts of the n_R th root found. After the failure has occurred, the remaining $2 \times (n - n_R)$ elements of \mathbf{z} contain a large negative number (equal to $-1/(x02\text{am}() \times \sqrt{2})$).

9 Example

For this function two examples are presented. There is a single example program for nag_zeros_poly_real (c02ag), with a main program and the code to solve the two example problems given in the functions EX1 and EX2.

Example 1 (EX1)

This example finds the roots of the fifth degree polynomial

$$z^5 + 2z^4 + 3z^3 + 4z^2 + 5z + 6 = 0$$
.

Example 2 (EX2)

This example solves the same problem as function EX1, but in addition attempts to estimate the accuracy of the computed roots using a perturbation analysis. Further details can be found in Thompson (1991).

9.1 Program Text

```
function c02ag_example
fprintf('c02ag example results\n\n');
a = [1;
                   3;
                          4;
                                  5;
                                       6];
n = nag_int(5);
ex1(n,a);
ex2(n,a);
function ex1(n,a)
  [z, ifail] = c02ag(a, n);
  disp('Computed roots of polynomial:');
  cz = z(1,:) + i*z(2,:);
  disp(cz');
function ex2(n,a)
  [z, ifail] = c02ag(a, n);
  % Estimate the accuracy of the computed roots using a perturbation analysis
  % Form the coefficients of the perturbed polynomial
  abar = a;
  epsbar = 3*x02aj;
  for j=1:2:n+1
    abar(j) = (1+epsbar)*abar(j);
  for j=2:2:n+1
    abar(j) = (1-epsbar)*abar(j);
  % Compute the roots of the perturbed polynomial
  [zbar, ifail] = c02ag(abar, nag_int(n));
  % Perform error analysis
  % Initialise markers to 0 (unmarked)
  m = zeros(n, 1);
  r = zeros(n, 1);
  rmax = x02a1;
  cz = z(1,:) + i*z(2,:);
```

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```
czbar = zbar(1,:) + i*zbar(2,:);
  for j=1:n
    deltai = rmax;
    r1 = abs(cz(j));
    % Loop over all perturbed roots (stored in zbar)
    for k=1:n
      % Compare the current unperturbed root to all unmarked perturbed roots.
      if m(k) == 0
        r2 = abs(czbar(k));
        deltac = abs(r1-r2);
        if deltac < deltai
          deltai = deltac;
          jmin = k;
        end
      end
    end
    % Mark the selected perturbed root
    m(jmin) = 1;
    % Compute the relative error
    if r1 \tilde{} = 0
     r3 = abs(czbar(jmin));
      di = min(r1,r3);
      r(j) = max(deltai/max(di,deltai/rmax),x02aj);
    end
  end
  fprintf('\nComputed Roots of Polynomial
                                            Error Estimate\n');
  fprintf('
                                          (machine dependent)\n');
  for j=1:n
    if^{-}(z(2,j)<0)
      fprintf('%9.4f - %7.4fi
                                         88.2e\n',z(1,j),-z(2,j),r(j));
      fprintf('%9.4f + %7.4fi
                                         88.2e\n',z(1,j),z(2,j),r(j));
    end
  end
9.2 Program Results
     c02ag example results
Computed roots of polynomial:
  -1.4918 + 0.0000i
  0.5517 - 1.2533i
  0.5517 + 1.2533i
  -0.8058 - 1.2229i
```

```
0.5517 + 1.2533i

-0.8058 - 1.2229i

-0.8058 + 1.2229i

Computed Roots of Polynomial Error Estimate

(machine dependent)

-1.4918 + 0.0000i 1.04e-15

0.5517 + 1.2533i 1.62e-16

0.5517 - 1.2533i 1.62e-16

-0.8058 + 1.2229i 1.52e-16

-0.8058 - 1.2229i 1.52e-16
```

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