1 Purpose

nag_zero_sparse_nonlin_eqns_easy (c05qsc) is an easy-to-use function that finds a solution of a sparse
system of nonlinear equations by a modification of the Powell hybrid method.

2 Specification

```c
#include <nag.h>
#include <nagc05.h>

void nag_zero_sparse_nonlin_eqns_easy (nag_zero_sparse_nonlin_eqns_easy_t fcn, Integer n, double x[], double fvec[],
                        const Integer indf[], const double x[], double fvec[], Nag_Comm *comm, Integer *iflag),
                        Integer n, double x[], double fvec[], double xtol, Nag_Boolean init,
                        double rcomm[], Integer lrcomm, Integer icomm[], Integer licomm,
                        Nag_Comm *comm, NagError *fail)
```

3 Description

The system of equations is defined as:

\[ f_i(x_1, x_2, \ldots, x_n) = 0, \quad i = 1, 2, \ldots, n. \]

nag_zero_sparse_nonlin_eqns_easy (c05qsc) is based on the MINPACK routine HYBRD1 (see Moré et
al. (1980)). It chooses the correction at each step as a convex combination of the Newton and scaled
gradient directions. The Jacobian is updated by the sparse rank-1 method of Schubert (see Schubert
(1970)). At the starting point, the sparsity pattern is determined and the Jacobian is approximated by
forward differences, but these are not used again until the rank-1 method fails to produce satisfactory
progress. Then, the sparsity structure is used to recompute an approximation to the Jacobian by forward
differences with the least number of function evaluations. The function you supply must be able to
compute only the requested subset of the function values. The sparse Jacobian linear system is solved at
each iteration with nag_superlu_lu_factorize (f11mec) computing the Newton step. For more details see
Powell (1970) and Broyden (1965).

4 References

Broyden C G (1965) A class of methods for solving nonlinear simultaneous equations Mathematics of
Computation 19(92) 577–593

74 Argonne National Laboratory

Nonlinear Algebraic Equations (ed P Rabinowitz) Gordon and Breach

Jacobian Mathematics of Computation 24(109) 27–30

5 Arguments

1:  **fcn** – function, supplied by the user

   *External Function*

   `fcn` must return the values of the functions \( f_i \) at a point \( x \).
The specification of `fcn` is:

```c
void fcn (Integer n, Integer lindf, const Integer indf[],
         const double x[], double fvec[], Nag_Comm *comm, Integer *iflag)
```

1: `n` – Integer  
   **Input**  
   *On entry:* `n`, the number of equations.

2: `lindf` – Integer  
   **Input**  
   *On entry:* `lindf` specifies the number of indices \(i\) for which values of \(f_i(x)\) must be computed.

3: `indf[lindf]` – const Integer  
   **Input**  
   *On entry:* `indf` specifies the indices \(i\) for which values of \(f_i(x)\) must be computed. The indices are specified in strictly ascending order.

4: `x[n]` – const double  
   **Input**  
   *On entry:* the components of the point \(x\) at which the functions must be evaluated. \(x[i-1]\) contains the coordinate \(x_i\).

5: `fvec[n]` – double  
   **Output**  
   *On exit:* `fvec[i-1]` must contain the function values \(f_i(x)\), for all indices \(i\) in `indf`.

6: `comm` – Nag_Comm *  
   Pointer to structure of type Nag_Comm; the following members are relevant to `fcn`.
   - `user` – double *  
   - `iuser` – Integer *  
   - `p` – Pointer
     The type Pointer will be `void *`. Before calling `nag_zero_sparse_nonlin_eqns_easy (c05qsc)` you may allocate memory and initialize these pointers with various quantities for use by `fcn` when called from `nag_zero_sparse_nonlin_eqns_easy (c05qsc)` (see Section 3.2.1.1 in the Essential Introduction).

7: `iflag` – Integer *  
   **Input/Output**  
   *On entry:* `iflag > 0`.  
   *On exit:* in general, `iflag` should not be reset by `fcn`. If, however, you wish to terminate execution (perhaps because some illegal point \(x\) has been reached), then `iflag` should be set to a negative integer.

---

2: `n` – Integer  
   **Input**  
   *On entry:* \(n\), the number of equations.  
   *Constraint:* \(n > 0\).

3: `x[n]` – double  
   **Input/Output**  
   *On entry:* an initial guess at the solution vector. \(x[i-1]\) must contain the coordinate \(x_i\).  
   *On exit:* the final estimate of the solution vector.
4: fvec[n] – double  
   Output
   On exit: the function values at the final point returned in x. fvec[i-1] contains the function values fj.

5: xtol – double  
   Input
   On entry: the accuracy in x to which the solution is required.
   Suggested value: \( \sqrt{\epsilon} \), where \( \epsilon \) is the machine precision returned by nag_machine_precision (X02AJC).
   Constraint: xtol \( \geq 0.0 \).

6: init – Nag_Boolean  
   Input
   On entry: init must be set to Nag_TRUE to indicate that this is the first time nag_zero_sparse_nonlin_eqns_easy (c05qsc) is called for this specific problem. nag_zero_sparse_nonlin_eqns_easy (c05qsc) then computes the dense Jacobian and detects and stores its sparsity pattern (in rcomm and icomm) before proceeding with the iterations. This is noticeably time consuming when n is large. If not enough storage has been provided for rcomm or icomm, nag_zero_sparse_nonlin_eqns_easy (c05qsc) will fail. On exit with fail.code = NE_NOERROR, NE_NO_IMPROVEMENT, NE_TOO_MANY_FEVALS or NE_TOO_SMALL, icomm[0] contains nnz, the number of nonzero entries found in the Jacobian. On subsequent calls, init can be set to Nag_FALSE if the problem has a Jacobian of the same sparsity pattern. In that case, the computation time required for the detection of the sparsity pattern will be smaller.

7: rcomm[lrcomm] – double  
   Communication Array
   rcomm MUST NOT be altered between successive calls to nag_zero_sparse_nonlin_eqns_easy (c05qsc).

8: lrcomm – Integer  
   Input
   On entry: the dimension of the array rcomm.
   Constraint: lrcomm \( \geq 12 + \text{nnz} \) where nnz is the number of nonzero entries in the Jacobian, as computed by nag_zero_sparse_nonlin_eqns_easy (c05qsc).

9: icomm[licomm] – Integer  
   Communication Array
   If fail.code = NE_NOERROR, NE_NO_IMPROVEMENT, NE_TOO_MANY_FEVALS or NE_TOO_SMALL on exit, icomm[0] contains nnz where nnz is the number of nonzero entries in the Jacobian.
   icomm MUST NOT be altered between successive calls to nag_zero_sparse_nonlin_eqns_easy (c05qsc).

10: licomm – Integer  
    Input
   On entry: the dimension of the array icomm.
   Constraint: licomm \( \geq 8 \times n + 19 + \text{nnz} \) where nnz is the number of nonzero entries in the Jacobian, as computed by nag_zero_sparse_nonlin_eqns_easy (c05qsc).

11: comm – Nag_Comm * 
   The NAG communication argument (see Section 3.2.1.1 in the Essential Introduction).

12: fail – NagError *  
    Input/Output
   The NAG error argument (see Section 3.6 in the Essential Introduction).
6 Error Indicators and Warnings

**NE_ALLOC_FAIL**
Dynamic memory allocation failed.
See Section 3.2.1.2 in the Essential Introduction for further information.

**NE_BAD_PARAM**
On entry, argument \(\text{value}\) had an illegal value.

**NE_INT**
On entry, \(\text{licomm} = \text{value}\).
Constraint: \(\text{licomm} \geq \text{value}\).
On entry, \(\text{lcomm} = \text{value}\).
Constraint: \(\text{lcomm} \geq \text{value}\).
On entry, \(\text{n} = \text{value}\).
Constraint: \(\text{n} > 0\).

**NE_INTERNAL_ERROR**
An internal error has occurred in this function. Check the function call and any array sizes. If the call is correct then please contact NAG for assistance.

An unexpected error has been triggered by this function. Please contact NAG.
See Section 3.6.6 in the Essential Introduction for further information.

**NE_NO_IMPROVEMENT**
The iteration is not making good progress. This failure exit may indicate that the system does not have a zero, or that the solution is very close to the origin (see Section 7). Otherwise, rerunning \text{nag_zero_sparse_nonlin_eqns_easy (c05qsc)} from a different starting point may avoid the region of difficulty. The condition number of the Jacobian is \(\text{value}\).

**NE_NO_LICENCE**
Your licence key may have expired or may not have been installed correctly.
See Section 3.6.5 in the Essential Introduction for further information.

**NE_REAL**
On entry, \(\text{xtol} = \text{value}\).
Constraint: \(\text{xtol} \geq 0.0\).

**NE_TOO_MANY_FEVALS**
There have been at least \(200 \times (\text{n} + 1)\) calls to \text{fcn}. Consider setting \text{init} = \text{Nag_FALSE} and restarting the calculation from the point held in \text{x}.

**NE_TOO_SMALL**
No further improvement in the solution is possible. \(\text{xtol}\) is too small: \(\text{xtol} = \text{value}\).

**NE_USER_STOP**
\(\text{iflag}\) was set negative in \text{fcn}. \(\text{iflag} = \text{value}\).
7 Accuracy

If \( \hat{x} \) is the true solution, nag_zero_sparse_nonlin_eqns_easy (c05qsc) tries to ensure that
\[
\|x - \hat{x}\|_2 \leq xtol \times \|\hat{x}\|_2.
\]
If this condition is satisfied with \( xtol = 10^{-k} \), then the larger components of \( x \) have \( k \) significant decimal digits. There is a danger that the smaller components of \( x \) may have large relative errors, but the fast rate of convergence of nag_zero_sparse_nonlin_eqns_easy (c05qsc) usually obviates this possibility.

If \( xtol \) is less than machine precision and the above test is satisfied with the machine precision in place of \( xtol \), then the function exits with fail code = NE_TOO_SMALL.

Note: this convergence test is based purely on relative error, and may not indicate convergence if the solution is very close to the origin.

The convergence test assumes that the functions are reasonably well behaved. If this condition is not satisfied, then nag_zero_sparse_nonlin_eqns_easy (c05qsc) may incorrectly indicate convergence. The validity of the answer can be checked, for example, by rerunning nag_zero_sparse_nonlin_eqns_easy (c05qsc) with a lower value for \( xtol \).

8 Parallelism and Performance

nag_zero_sparse_nonlin_eqns_easy (c05qsc) is threaded by NAG for parallel execution in multithreaded implementations of the NAG Library.

nag_zero_sparse_nonlin_eqns_easy (c05qsc) makes calls to BLAS and/or LAPACK routines, which may be threaded within the vendor library used by this implementation. Consult the documentation for the vendor library for further information.

Please consult the X06 Chapter Introduction for information on how to control and interrogate the OpenMP environment used within this function. Please also consult the Users’ Note for your implementation for any additional implementation-specific information.

9 Further Comments

Local workspace arrays of fixed lengths are allocated internally by nag_zero_sparse_nonlin_eqns_easy (c05qsc). The total size of these arrays amounts to \( 8 \times n + 2 \times q \) double elements and \( 10 \times n + 2 \times q + 5 \) integer elements where the integer \( q \) is bounded by \( 8 \times nnz \) and \( n^2 \) and depends on the sparsity pattern of the Jacobian.

The time required by nag_zero_sparse_nonlin_eqns_easy (c05qsc) to solve a given problem depends on \( n \), the behaviour of the functions, the accuracy requested and the starting point. The number of arithmetic operations executed by nag_zero_sparse_nonlin_eqns_easy (c05qsc) to process each evaluation of the functions depends on the number of nonzero entries in the Jacobian. The timing of nag_zero_sparse_nonlin_eqns_easy (c05qsc) is strongly influenced by the time spent evaluating the functions.

When init is Nag_TRUE, the dense Jacobian is first evaluated and that will take time proportional to \( n^2 \). Ideally the problem should be scaled so that, at the solution, the function values are of comparable magnitude.

10 Example

This example determines the values \( x_1, \ldots, x_9 \) which satisfy the tridiagonal equations:
\[
\begin{align*}
(3 - 2x_1)x_1 - 2x_2 &= -1, \\
-x_{i-1} + (3 - 2x_i)x_i - 2x_{i+1} &= -1, & i &= 2, 3, \ldots, 8 \\
-x_8 + (3 - 2x_9)x_9 &= -1.
\end{align*}
\]

It then perturbs the equations by a small amount and solves the new system.
10.1 Program Text

/* nag_zero_sparse_nonlin_eqns_easy (c05qsc) Example Program. */
/* Copyright 2014 Numerical Algorithms Group. */
/* Mark 23, 2011. */
*/
#include <nag.h>
#include <stdio.h>
#include <nag_stdlib.h>
#include <math.h>
#include <nagc05.h>
#include <nagx02.h>

static void NAG_CALL fcn(Integer n, Integer lindf, const Integer indf[],
const double x[], double fvec[], Nag_Comm *comm, Integer *iflag)
{
  double theta;
  Integer i, ind;

  *iflag = 0;
  theta = (double) (comm->iuser[0]) * pow(0.5, 7);
  for (ind = 0; ind < lindf; ind++) {
    i = indf[ind] - 1;
    fvec[i] = (3.0 - (2.0 + theta) * x[i]) * x[i] + 1.0;
    if (i > 0) fvec[i] = fvec[i] - x[i - 1];
    if (i < n-1) fvec[i] = fvec[i] - 2.0 * x[i + 1];
  }
}

int main(void)
{
  Integer exit_status = 0, n = 9, i, j, licomm, lrcomm;
  double fnorm, xtol;
  Nag_Boolean init;
  Nag_Comm comm;
  Integer iuser[1], *icomm = 0;
  double ruser[1], *rcomm = 0, *fvec = 0, *x = 0;
  NagError fail;

  printf("nag_zero_sparse_nonlin_eqns_easy (c05qsc) Example Program Results\n");
  lrcomm = 12 + 3 * n;
  licomm = 8 * n + 19 + 3 * n;
  if (! (fvec = NAG_ALLOC(n, double)) ||
      (x = NAG_ALLOC(n, double)) ||
      (rcomm = NAG_ALLOC(lrcomm, double)) ||
      (icomm = NAG_ALLOC(licomm, Integer)))
  {
    printf("Allocation failure\n");
    exit_status = -1;
    goto END;
  }
  comm.iuser = iuser;
  comm.user = ruser;
  xtol = sqrt(nag_machine_precision);
  /* The following starting values provide a rough solution. */
  for (j = 0; j < n; j++) x[j] = -1.0E0;
  for (i = 0; i <= 1; i++)
  {
    INIT_FAIL(fail);
    /* Perturb the system? */
    comm.iuser[0] = i;
    init = (i == 0 ? Nag_TRUE : Nag_FALSE);
    /* nag_zero_sparse_nonlin_eqns_easy (c05qsc). */
    /* Solution of a sparse system of nonlinear equations using function */
    /* values only (easy-to-use). */
    nag_zero_sparse_nonlin_eqns_easy(fcn, n, x, fvec, xtol, init, rcomm, lrcomm,
                                    icomm, licomm, &comm, &fail);

if (fail.code == NE_NOERROR) {
  /* Compute Euclidean norm. */
  fnorm = 0.0E0;
  for (j = 0; j < n; j++) fnorm = pow(fvec[j], 2);
  fnorm = sqrt(fnorm);
  printf("Final 2-norm of the residuals = %12.4e\n", fnorm);
  printf("Final approximate solution\n\n");
  for (j = 0; j < n; j++)
    printf("%12.4f%s", x[j], (j + 1) % 3 ? " " : "\n");
  printf("\n");
} else {
  printf("Error from nag_zero_sparse_nonlin_eqns_easy (c05qsc).\n", fail.message);
  if (fail.code == NE_TOO_MANY_FEVALS ||
      fail.code == NE_TOO_SMALL ||
      fail.code == NE_NO_IMPROVEMENT) {
    printf("Approximate solution\n");
    for (j = 0; j < n; j++)
      printf("%12.4f%s", x[j], (j + 1) % 3 ? " " : "\n");
    printf("\n");
  }
}
END:
NAG_FREE(fvec);
NAG_FREE(x);
NAG_FREE(rcomm);
NAG_FREE(icomm);
return exit_status;

10.2 Program Data

None.

10.3 Program Results

nag_zero_sparse_nonlin_eqns_easy (c05qsc) Example Program Results

Final 2-norm of the residuals = 1.7592e-09

Final approximate solution

-0.5707 -0.6816 -0.7017
-0.7042 -0.7014 -0.6919
-0.6658 -0.5960 -0.4164

Final 2-norm of the residuals = 2.6329e-13

Final approximate solution

-0.5697 -0.6804 -0.7004
-0.7029 -0.7000 -0.6906
-0.6646 -0.5951 -0.4159