

## NAG Library Function Document

### nag\_zero\_sparse\_nonlin\_eqns\_easy (c05qsc)

#### 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

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

void nag_zero_sparse_nonlin_eqns_easy (
    void (*fcn)(Integer n, Integer lindf, 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:

$$f_i(x_1, x_2, \dots, x_n) = 0, \quad i = 1, 2, \dots, n.$$

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

Moré J J, Garbow B S and Hillstom K E (1980) User guide for MINPACK-1 *Technical Report ANL-80-74* Argonne National Laboratory

Powell M J D (1970) A hybrid method for nonlinear algebraic equations *Numerical Methods for Nonlinear Algebraic Equations* (ed P Rabinowitz) Gordon and Breach

Schubert L K (1970) Modification of a quasi-Newton method for nonlinear equations with a sparse 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:

```
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\_eqn\_s\_easy (c05qsc) you may allocate memory and initialize these pointers with various quantities for use by **fcn** when called from nag\_zero\_sparse\_nonlin\_eqn\_s\_easy (c05qsc) (see Section 2.3.1.1 in How to Use the NAG Library and its Documentation).

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  $f_i$ .
- 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 + *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 + *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 2.3.1.1 in How to Use the NAG Library and its Documentation).
- 12: **fail** – NagError \* *Input/Output*  
The NAG error argument (see Section 2.7 in How to Use the NAG Library and its Documentation).

## 6 Error Indicators and Warnings

### NE\_ALLOC\_FAIL

Dynamic memory allocation failed.

See Section 2.3.1.2 in How to Use the NAG Library and its Documentation for further information.

### NE\_BAD\_PARAM

On entry, argument  $\langle value \rangle$  had an illegal value.

### NE\_INT

On entry, **licomm** =  $\langle value \rangle$ .

Constraint: **licomm**  $\geq \langle value \rangle$ .

On entry, **lrcomm** =  $\langle value \rangle$ .

Constraint: **lrcomm**  $\geq \langle value \rangle$ .

On entry, **n** =  $\langle value \rangle$ .

Constraint: **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 2.7.6 in How to Use the NAG Library and its Documentation 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 `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  $\langle value \rangle$ .

### NE\_NO\_LICENCE

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

See Section 2.7.5 in How to Use the NAG Library and its Documentation for further information.

### NE\_REAL

On entry, **xtol** =  $\langle value \rangle$ .

Constraint: **xtol**  $\geq 0.0$ .

### NE\_TOO\_MANY\_FEVALS

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

### NE\_TOO\_SMALL

No further improvement in the solution is possible. **xtol** is too small: **xtol** =  $\langle value \rangle$ .

### NE\_USER\_STOP

**iflag** was set negative in **fcn**. **iflag** =  $\langle value \rangle$ .

## 7 Accuracy

If  $\hat{x}$  is the true solution, `nag_zero_sparse_nonlin_eqns_easy` (c05qsc) tries to ensure that

$$\|x - \hat{x}\|_2 \leq \mathbf{xtol} \times \|\hat{x}\|_2.$$

If this condition is satisfied with  $\mathbf{xtol} = 10^{-k}$ , 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  $\mathbf{xtol}$  is less than *machine precision* and the above test is satisfied with the *machine precision* in place of  $\mathbf{xtol}$ , 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  $\mathbf{xtol}$ .

## 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  $x_1, \dots, x_9$  which satisfy the tridiagonal equations:

$$\begin{aligned} (3 - 2x_1)x_1 - 2x_2 &= -1, \\ -x_{i-1} + (3 - 2x_i)x_i - 2x_{i+1} &= -1, \quad i = 2, 3, \dots, 8 \\ -x_8 + (3 - 2x_9)x_9 &= -1. \end{aligned}$$

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.
 *
 * NAGPRODCODE Version.
 *
 * Copyright 2016 Numerical Algorithms Group.
 *
 * Mark 26, 2016.
 */

#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("\nFinal 2-norm of the residuals = %12.4e\n", fnorm);
        printf("\nFinal 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%s\n",
              fail.message);
        if (fail.code == NE_TOO_MANY_FEVALS ||
            fail.code == NE_TOO_SMALL || fail.code == NE_NO_IMPROVEMENT) {
            printf("\nApproximate 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(icom);
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

---