NAG Library Function Document

nag_opt_conj_grad (e04dgc)

1 Purpose

nag_opt_conj_grad (e04dgc) minimizes an unconstrained nonlinear function of several variables using a pre-conditioned, limited memory quasi-Newton conjugate gradient method. The function is intended for use on large scale problems.

2 Specification

```
#include <nag.h>
#include <nage04.h>
void nag_opt_conj_grad (Integer n,
     void (*objfun)(Integer n, const double x[], double *objf, double g[],
          Nag_Comm *comm),
     double x[], double *objf, double g[], Nag_E04_Opt *options,
     Nag_Comm *comm, NagError *fail)
```

3 Description

nag_opt_conj_grad (e04dgc) uses a pre-conditioned conjugate gradient method and is based upon algorithm PLMA as described in Gill and Murray (1979) and Section 4.8.3 of Gill *et al.* (1981).

The algorithm proceeds as follows:

Let x_0 be a given starting point and let k denote the current iteration, starting with $k = 0$. The iteration requires g_k, the gradient vector evaluated at x_k, the kth estimate of the minimum. At each iteration a vector p_k (known as the direction of search) is computed and the new estimate x_{k+1} is given by $x_k + \alpha_k p_k$ where α_k (the step length) minimizes the function $F(x_k + \alpha_k p_k)$ with respect to the scalar α_k. At the start of each line search an initial approximation α_0 to the step α_k is taken as:

$$\alpha_0 = \min\{1, 2|F_k - F_{\mathrm{est}}|/g_k^{\mathrm{T}} g_k\}$$

where F_{est} is a user-supplied estimate of the function value at the solution. If F_{est} is not specified, the software always chooses the unit step length for α_0. Subsequent step length estimates are computed using cubic interpolation with safeguards.

A quasi-Newton method computes the search direction, p_k, by updating the inverse of the approximate Hessian (H_k) and computing

$$p_{k+1} = -H_{k+1} g_{k+1}. \tag{1}$$

The updating formula for the approximate inverse is given by

$$H_{k+1} = H_k - \frac{1}{y_k^{\mathrm{T}} s_k}\left(H_k y_k s_k^{\mathrm{T}} + s_k y_k^{\mathrm{T}} H_k\right) + \frac{1}{y_k^{\mathrm{T}} s_k}\left(1 + \frac{y_k^{\mathrm{T}} H_k y_k}{y_k^{\mathrm{T}} s_k}\right) s_k s_k^{\mathrm{T}} \tag{2}$$

where $y_k = g_{k-1} - g_k$ and $s_k = x_{k+1} - x_k = \alpha_k p_k$.

The method used by nag_opt_conj_grad (e04dgc) to obtain the search direction is based upon computing p_{k+1} as $-H_{k+1} g_{k+1}$ where H_{k+1} is a matrix obtained by updating the identity matrix with a limited number of quasi-Newton corrections. The storage of an n by n matrix is avoided by storing only the vectors that define the rank two corrections – hence the term limited-memory quasi-Newton method. The precise method depends upon the number of updating vectors stored. For example, the direction obtained with the 'one-step' limited memory update is given by (1) using (2) with H_k equal to the identity matrix, viz.

$$p_{k+1} = -g_{k+1} + \frac{1}{y_k^{\mathrm{T}} s_k}\left(s_k^{\mathrm{T}} g_{k+1} y_k + y_k^{\mathrm{T}} g_{k+1} s_k\right) - \frac{s_k^{\mathrm{T}} g_{k+1}}{y_k^{\mathrm{T}} s_k}\left(1 + \frac{y_k^{\mathrm{T}} y_k}{y_k^{\mathrm{T}} s_k}\right) s_k$$

nag_opt_conj_grad (e04dgc) uses a two-step method described in detail in Gill and Murray (1979) in which restarts and pre-conditioning are incorporated. Using a limited-memory quasi-Newton formula, such as the one above, guarantees p_{k+1} to be a descent direction if all the inner products $y_k^{\mathrm{T}} s_k$ are positive for all vectors y_k and s_k used in the updating formula.

The termination criteria of nag_opt_conj_grad (e04dgc) are as follows:

Let τ_F specify an argument that indicates the number of correct figures desired in F_k (τ_F is equivalent to **options.optim_tol** in the optional parameter list, see Section 11). If the following three conditions are satisfied:

(i) $F_{k-1} - F_k < \tau_F (1 + |F_k|)$

(ii) $\|x_{k-1} - x_k\| < \sqrt{\tau_F}(1 + \|x_k\|)$

(iii) $\|g_k\| \leq \tau_F^{1/3}(1 + |F_k|)$ or $\|g_k\| < \epsilon_A$, where ϵ_A is the absolute error associated with computing the objective function

then the algorithm is considered to have converged. For a full discussion on termination criteria see Chapter 8 of Gill *et al.* (1981).

4 References

Gill P E and Murray W (1979) Conjugate-gradient methods for large-scale nonlinear optimization *Technical Report SOL 79-15* Department of Operations Research, Stanford University

Gill P E, Murray W, Saunders M A and Wright M H (1983) Computing forward-difference intervals for numerical optimization *SIAM J. Sci. Statist. Comput.* **4** 310–321

Gill P E, Murray W and Wright M H (1981) *Practical Optimization* Academic Press

5 Arguments

1: **n** – Integer *Input*

On entry: the number n of variables.

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

2: **objfun** – function, supplied by the user *External Function*

objfun must calculate the objective function $F(x)$ and its gradient at a specified point x.

The specification of **objfun** is:

```
void objfun (Integer n, const double x[], double *objf, double g[],
     Nag_Comm *comm)
```

1: **n** – Integer *Input*

On entry: the number n of variables.

2: **x**[**n**] – const double *Input*

On entry: the point x at which the objective function is required.

3: **objf** – double * *Output*

On exit: the value of the objective function F at the current point x.

4: **g**[**n**] – double *Output*

On exit: **g**$[i-1]$ must contain the value of $\frac{\partial F}{\partial x_i}$ at the point x, for $i = 1, 2, \ldots, n$.

5: **comm** – Nag_Comm *

Pointer to structure of type Nag_Comm; the following members are relevant to **objfun**.

flag – Integer *Input/Output*

On entry: **comm**→**flag** is always non-negative.

On exit: if **objfun** resets **comm**→**flag** to some negative number then nag_opt_conj_grad (e04dgc) will terminate immediately with the error indicator NE_USER_STOP. If **fail** is supplied to nag_opt_conj_grad (e04dgc) **fail**.**errnum** will be set to your setting of **comm**→**flag**.

first – Nag_Boolean *Input*

On entry: will be set to Nag_TRUE on the first call to **objfun** and Nag_FALSE for all subsequent calls.

nf – Integer *Input*

On entry: the number of calculations of the objective function; this value will be equal to the number of calls made to **objfun** including the current one.

user – double *
iuser – Integer *
p – Pointer

The type Pointer will be `void *` with a C compiler that defines `void *` and `char *` otherwise. Before calling nag_opt_conj_grad (e04dgc) these pointers may be allocated memory and initialized with various quantities for use by **objfun** when called from nag_opt_conj_grad (e04dgc).

Note: **objfun** should be tested separately before being used in conjunction with nag_opt_conj_grad (e04dgc). The array **x** must **not** be changed by **objfun**.

3: **x**[**n**] – double *Input/Output*

On entry: x_0, an estimate of the solution point x^*.

On exit: the final estimate of the solution.

4: **objf** – double * *Output*

On exit: the value of the objective function $F(x)$ at the final iterate.

5: **g**[**n**] – double *Output*

On exit: the objective gradient at the final iterate.

6: **options** – Nag_E04_Opt * *Input/Output*

On entry/exit: a pointer to a structure of type Nag_E04_Opt whose members are optional parameters for nag_opt_conj_grad (e04dgc). These structure members offer the means of adjusting some of the argument values of the algorithm and on output will supply further details of the results. A description of the members of **options** is given below in Section 11.

If any of these optional parameters are required then the structure **options** should be declared and initialized by a call to nag_opt_init (e04xxc) and supplied as an argument to nag_opt_conj_grad (e04dgc). However, if the optional parameters are not required the NAG defined null pointer, `E04_DEFAULT`, can be used in the function call.

7: **comm** – Nag_Comm * *Input/Output*

Note: **comm** is a NAG defined type (see Section 2.3.1.1 in How to Use the NAG Library and its Documentation).

On entry/exit: structure containing pointers for communication with user-supplied functions; see the above description of **objfun** for details. If you do not need to make use of this communication feature the null pointer `NAGCOMM_NULL` may be used in the call to nag_opt_conj_grad (e04dgc); **comm** will then be declared internally for use in calls to user-supplied functions.

8: **fail** – NagError * *Input/Output*

The NAG error argument (see Section 2.7 in How to Use the NAG Library and its Documentation).

5.1 Description of Printed Output

Intermediate and final results are printed out by default. The level of printed output can be controlled with the structure member **options.print_level** (see Section 11.2). The default, **options.print_level** = Nag_Soln_Iter, provides the result of any derivative check, a single line of output at each iteration and the final result.

The derivative check performed by default will give the directional derivative, $g(x)^{\mathrm{T}}p$, of the objective gradient and its finite difference approximation, where p is a random vector of unit length. If the gradient is believed to be in error then nag_opt_conj_grad (e04dgc) will exit with **fail.code** = NE_DERIV_ERRORS.

The line of results printed at each iteration gives:

`Itn` the current iteration number k.

`Nfun` the cumulative number of calls to **objfun**. The evaluations needed for the estimation of the gradients by finite differences are not included in the total `Nfun`. The value of `Nfun` is a guide to the amount of work required for the linesearch. nag_opt_conj_grad (e04dgc) will perform at most 16 function evaluations per iteration.

`Objective` the current value of the objective function, $F(x_k)$.

`Norm g` the Euclidean norm of the gradient vector, $\|g(x_k)\|$.

`Norm x` the Euclidean norm of x_k.

`Norm (x(k-1)-x(k))`
the Euclidean norm of $x_{k-1} - x_k$.

`Step` the step α_k taken along the computed search direction p_k. On reasonably well-behaved problems, the unit step will be taken as the solution is approached.

The printout of the final result consists of:

`x` the final point, x^*.

`g` the final gradient vector, $g(x^*)$.

6 Error Indicators and Warnings

NE_ALLOC_FAIL

Dynamic memory allocation failed.

NE_BAD_PARAM

On entry, argument **options.print_level** had an illegal value.

On entry, argument **options.verify_grad** had an illegal value.

NE_DERIV_ERRORS

Large errors were found in the derivatives of the objective function.

This value of **fail** will occur if the verification process indicated that at least one gradient component had no correct figures. You should refer to the printed output to determine which elements are suspected to be in error.

As a first step, you should check that the code for the objective values is correct – for example, by computing the function at a point where the correct value is known. However, care should be taken that the chosen point fully tests the evaluation of the function. It is remarkable how often the values $x = 0$ or $x = 1$ are used to test function evaluation procedures, and how often the special properties of these numbers make the test meaningless.

Errors in programming the function may be quite subtle in that the function value is 'almost' correct. For example, the function may not be accurate to full precision because of the inaccurate calculation of a subsidiary quantity, or the limited accuracy of data upon which the function depends.

NE_GRAD_TOO_SMALL

The gradient at the starting point is too small, rerun the problem at a different starting point.

The value of $g(x_0)^{\mathrm{T}}g(x_0)$ is less than $\epsilon|F(x_o)|$, where ϵ is the ***machine precision***.

NE_INT_ARG_LT

On entry, **n** = ⟨*value*⟩.
Constraint: **n** ≥ 1.

NE_INVALID_INT_RANGE_1

Value ⟨*value*⟩ given to **options.max_iter** not valid. Correct range is **options.max_iter** ≥ 0.

NE_INVALID_REAL_RANGE_EF

Value ⟨*value*⟩ given to **options.f_prec** not valid. Correct range is $\epsilon \leq$ **options.f_prec** < 1.0.

Value ⟨*value*⟩ given to **options.optim_tol** not valid. Correct range is ⟨*value*⟩ $\leq$ **options.optim_tol** < 1.0.

NE_INVALID_REAL_RANGE_F

Value ⟨*value*⟩ given to **options.max_line_step** not valid. Correct range is **options.max_line_step** > 0.0.

NE_INVALID_REAL_RANGE_FF

Value ⟨*value*⟩ given to **options.linesearch_tol** not valid. Correct range is $0.0 \leq$ **options.linesearch_tol** < 1.0.

NE_NOT_APPEND_FILE

Cannot open file ⟨*string*⟩ for appending.

NE_NOT_CLOSE_FILE

Cannot close file ⟨*string*⟩.

NE_OPT_NOT_INIT

Options structure not initialized.

NE_USER_STOP

User requested termination, user flag value $= \langle value \rangle$.

This exit occurs if you set **comm→flag** to a negative value in **objfun**. If **fail** is supplied the value of **fail.errnum** will be the same as your setting of **comm→flag**.

NE_WRITE_ERROR

Error occurred when writing to file $\langle string \rangle$.

NW_NO_IMPROVEMENT

A sufficient decrease in the function value could not be attained during the final linesearch. Current point cannot be improved upon.

If **objfun** computes the function and gradients correctly, then this warning may occur because an overly stringent accuracy has been requested, i.e., **options.optim_tol** is too small or if the minimum lies close to a step length of zero. In this case you should apply the tests described in Section 3 to determine whether or not the final solution is acceptable. For a discussion of attainable accuracy see Gill *et al.* (1981).

If many iterations have occurred in which essentially no progress has been made or nag_opt_conj_grad (e04dgc) has failed to move from the initial point, then the function **objfun** may be incorrect. You should refer to the comments below under NE_DERIV_ERRORS and check the gradients using the **options.verify_grad** argument. Unfortunately, there may be small errors in the objective gradients that cannot be detected by the verification process. Finite difference approximations to first derivatives are catastrophically affected by even small inaccuracies.

NW_STEP_BOUND_TOO_SMALL

Computed upper-bound on step length was too small

The computed upper bound on the step length taken during the linesearch was too small. A rerun with an increased value of **options.max_line_step** (ρ say) may be successful unless $\rho \geq 10^{10}$ (the default value), in which case the current point cannot be improved upon.

NW_TOO_MANY_ITER

The maximum number of iterations, $\langle value \rangle$, have been performed.

If the algorithm appears to be making progress the value of **options.max_iter** value may be too small (see Section 11), you should increase its value and rerun nag_opt_conj_grad (e04dgc). If the algorithm seems to be 'bogged down', you should check for incorrect gradients or ill-conditioning as described below under NW_NO_IMPROVEMENT.

7 Accuracy

On successful exit the accuracy of the solution will be as defined by the optional parameter **options.optim_tol**.

8 Parallelism and Performance

nag_opt_conj_grad (e04dgc) is not threaded in any implementation.

9 Further Comments

9.1 Timing

Problems whose Hessian matrices at the solution contain sets of clustered eigenvalues are likely to be minimized in significantly fewer than n iterations. Problems without this property may require anything between n and $5n$ iterations, with approximately $2n$ iterations being a common figure for moderately difficult problems.

10 Example

This example minimizes the function

$$F = e^{x_1}\left(4{x_1}^2 + 2{x_2}^2 + 4x_1x_2 + 2x_2 + 1\right).$$

The data includes a set of user-defined column and row names, and data for the Hessian in a sparse storage format (see Section 10.2 for further details). The **options** structure is declared and initialized by nag_opt_init (e04xxc). Five option values are read from a data file by use of nag_opt_read (e04xyc).

10.1 Program Text

```
/* nag_opt_conj_grad (e04dgc) Example Program.
 *
 * NAGPRODCODE Version.
 *
 * Copyright 2016 Numerical Algorithms Group.
 *
 * Mark 26, 2016.
 *
 */

#include <nag.h>
#include <stdio.h>
#include <string.h>
#include <math.h>
#include <nag_stdlib.h>
#include <nage04.h>

#ifdef __cplusplus
extern "C"
{
#endif
  static void NAG_CALL objfun(Integer n, const double x[], double *objf,
                              double g[], Nag_Comm *comm);
#ifdef __cplusplus
}
#endif

int main(void)
{
  const char *optionsfile = "e04dgce.opt";
  static double ruser[1] = { -1.0 };
  Integer exit_status = 0;
  Nag_Boolean print;
  Integer n;
  Nag_E04_Opt options;
  double *g = 0, objf, *x = 0;
  Nag_Comm comm;
  NagError fail;

  INIT_FAIL(fail);

  printf("nag_opt_conj_grad (e04dgc) Example Program Results\n");

  /* For communication with user-supplied functions: */
  comm.user = ruser;

  fflush(stdout);
  /* Initialize options structure and read option values from file */
  print = Nag_TRUE;
  n = 2; /* Number of variables */
  if (n >= 1) {
    if (!(x = NAG_ALLOC(n, double)) || !(g = NAG_ALLOC(n, double)))
    {
      printf("Allocation failure\n");
      exit_status = -1;
      goto END;
    }
  }
  else {
    printf("Invalid n.\n");
    exit_status = 1;
    return exit_status;
  }
  /* nag_opt_init (e04xxc).
   * Initialization function for option setting
   */
  nag_opt_init(&options);
  /* nag_opt_read (e04xyc).
   * Read options from a text file
   */
  nag_opt_read("e04dgc", optionsfile, &options, print, "stdout", &fail);
  if (fail.code != NE_NOERROR) {
    printf("Error from nag_opt_read (e04xyc).\n%s\n", fail.message);
    exit_status = 1;
    goto END;
  }
  /* Set the initial estimate of the solution. */
  x[0] = -1.0;
  x[1] = 1.0;

  /* Solve the problem. */
  /* nag_opt_conj_grad (e04dgc), see above. */
  nag_opt_conj_grad(n, objfun, x, &objf, g, &options, &comm, &fail);
  if (fail.code != NE_NOERROR) {
    printf("Error from nag_opt_conj_grad (e04dgc).\n%s\n", fail.message);
    exit_status = 1;
    goto END;
  }

END:
  NAG_FREE(x);
  NAG_FREE(g);

  return exit_status;
}

static void NAG_CALL objfun(Integer n, const double x[], double *objf,
                            double g[], Nag_Comm *comm)
{
  /* Function to evaluate objective function and its 1st derivatives. */

  double ex1, x1, x2;

  if (comm->user[0] == -1.0) {
    printf("(User-supplied callback objfun, first invocation.)\n");
    fflush(stdout);
    comm->user[0] = 0.0;
  }

  ex1 = exp(x[0]);
  x1 = x[0];
  x2 = x[1];
  *objf = ex1 * (4 * x1 * x1 + 2 * x2 * x2 + 4 * x1 * x2 + 2 * x2 + 1);

  g[0] = 4 * ex1 * (2 * x1 + x2) + *objf;
  g[1] = 2 * ex1 * (2 * x2 + 2 * x1 + 1);
} /* objfun */
```

10.2 Program Data

```
nag_opt_conj_grad (e04dgc) Example Program Optional Parameters

Following options for e04dgc are read by e04xyc.

begin e04dgc

 print_level =       Nag_Soln  /* Print solution only */

 max_iter =                30  /* Set iteration limit */

 verify_grad =   Nag_CheckObj  /* Check objective gradient components */

 max_line_step =       1.0e+2  /* Maximum allowable step length */

 f_est = 1.0                   /* Estimate of optimal function value */

end
```

10.3 Program Results

```
nag_opt_conj_grad (e04dgc) Example Program Results

Optional parameter setting for e04dgc.
--------------------------------------

Option file: e04dgce.opt

print_level set to Nag_Soln
max_iter set to 30
verify_grad set to Nag_CheckObj
max_line_step set to 1.00e+02
f_est set to 1.00e+00

Parameters to e04dgc
--------------------

Number of variables..........   2

max_line_step..........  1.00e+02    machine precision.......  1.11e-16
optim_tol..............  3.26e-12    linesearch_tol..........  9.00e-01
f_est..................  1.00e+00    f_prec..................  4.37e-15
verify_grad.........  Nag_CheckObj    max_iter................       30
print_level.........      Nag_Soln    print_gcheck............      Nag_TRUE
outfile................    stdout
(User-supplied callback objfun, first invocation.)


Verification of the objective gradients.
----------------------------------------

All objective gradient elements have been set.

The objective gradient seems to be ok.

Directional derivative of the objective    -1.47151776e-01
Difference approximation                   -1.47151796e-01


Component-wise check:

   i     x[i]       dx[i]         g[i]       Difference approxn.   Itns.
   1  -1.00e+00   1.64e-07   3.67879441e-01   3.67879441e-01 OK     1
   2   1.00e+00   1.84e-07   7.35758882e-01   7.35758882e-01 OK     1

2 objective gradient elements out of the 2 assigned,
set in columns 1 through 2, seem to be ok.

The largest relative error was 1.02e-10 in element 1

Results from e04dgc:
-------------------

Final solution:

 Variable         x                g
    1         5.0000e-01       1.3247e-07
    2        -1.0000e+00       3.0215e-08

Final objective function value = 7.3217934e-16.

Exit after 9 iterations and 19 function evaluations.

Optimal solution found.
```

11 Optional Parameters

A number of optional input and output arguments to nag_opt_conj_grad (e04dgc) are available through the structure argument **options**, type Nag_E04_Opt. a argument may be selected by assigning an appropriate value to the relevant structure member; those arguments not selected will be assigned default values. If no use is to be made of any of the optional parameters you should use the NAG defined null pointer, `E04_DEFAULT`, in place of **options** when calling nag_opt_conj_grad (e04dgc); the default settings will then be used for all arguments.

Before assigning values to **options** directly the structure **must** be initialized by a call to the function nag_opt_init (e04xxc). Values may then be assigned to the structure members in the normal C manner.

Option settings may also be read from a text file using the function nag_opt_read (e04xyc) in which case initialization of the **options** structure will be performed automatically if not already done. Any subsequent direct assignment to the **options** structure must **not** be preceded by initialization.

If assignment of functions and memory to pointers in the **options** structure is required, then this must be done directly in the calling program, they cannot be assigned using nag_opt_read (e04xyc).

11.1 Optional Parameter Checklist and Default Values

For easy reference, the following list shows the members of **options** which are valid for nag_opt_conj_grad (e04dgc) together with their default values where relevant. The number ϵ is a generic notation for ***machine precision*** (see nag_machine_precision (X02AJC)).

`Boolean list`	Nag_TRUE
`Nag_PrintType print_level`	Nag_Soln_Iter
`char outfile[80]`	`stdout`
`void (*print_fun)()`	**NULL**
`Nag_GradChk verify_grad`	Nag_SimpleCheck
`Boolean print_gcheck`	Nag_TRUE
`Integer obj_check_start`	1
`Integer obj_check_stop`	**n**
`Integer max_iter`	$\max(50, 5\mathbf{n})$
`double f_prec`	$\epsilon^{0.9}$
`double optim_tol`	**options.f_prec**$^{0.8}$
`double linesearch_tol`	0.9
`double max_line_step`	10^{10}
`double f_est`	
`Integer iter`	
`Integer nf`	

11.2 Description of the Optional Parameters

list – Nag_Boolean Default = Nag_TRUE

On entry: if **options**.**list** = Nag_TRUE the argument settings in the call to nag_opt_conj_grad (e04dgc) will be printed.

print_level – Nag_PrintType Default = Nag_Soln_Iter

On entry: the level of results printout produced by nag_opt_conj_grad (e04dgc). The following values are available:

Nag_NoPrint	No output.
Nag_Soln	The final solution.
Nag_Iter	One line of output for each iteration.
Nag_Soln_Iter	The final solution and one line of output for each iteration.

Constraint: **options**.**print_level** = Nag_NoPrint, Nag_Soln, Nag_Iter or Nag_Soln_Iter.

outfile – const char[80] Default = `stdout`

On entry: the name of the file to which results should be printed. If **options**.**outfile**[0] = '\0' then the `stdout` stream is used.

print_fun – pointer to function Default = **NULL**

On entry: printing function defined by you; the prototype of **options**.**print_fun** is

```
    void (*print_fun)(const Nag_Search_State *st, Nag_Comm *comm);
```

See Section 11.3.1 below for further details.

verify_grad – Nag_GradChk Default = Nag_SimpleCheck

On entry: specifies the level of derivative checking to be performed by nag_opt_conj_grad (e04dgc) on the gradient elements defined in **objfun**.

options.**verify_grad** may have the following values:

Nag_NoCheck	No derivative check is performed.
Nag_SimpleCheck	Perform a simple check of the gradient.
Nag_CheckObj	Perform a component check of the gradient elements.

If **options**.**verify_grad** = Nag_SimpleCheck then a simple 'cheap' test is performed, which requires only one call to **objfun**. If **options**.**verify_grad** = Nag_CheckObj then a more reliable (but more expensive) test will be made on individual gradient components. This component check will be made in the range specified by **options**.**obj_check_start** and **options**.**obj_check_stop**, default values being 1 and **n** respectively. The procedure for the derivative check is based on finding an interval that produces an acceptable estimate of the second derivative, and then using that estimate to compute an interval that should produce a reasonable forward-difference approximation. The gradient element is then compared with the difference approximation. (The method of finite difference interval estimation is based on Gill *et al.* (1983)). The result of the test is printed out by nag_opt_conj_grad (e04dgc) if **options**.**print_gcheck** = Nag_TRUE.

Constraint: **options**.**verify_grad** = Nag_NoCheck, Nag_SimpleCheck or Nag_CheckObj.

print_gcheck – Nag_Boolean Default = Nag_TRUE

On entry: if Nag_TRUE the result of any derivative check (see **options**.**verify_grad**) will be printed.

obj_check_start – Integer Default $= 1$
obj_check_stop – Integer Default $= \mathbf{n}$

On entry: these options take effect only when **options.verify_grad** = Nag_CheckObj. They may be used to control the verification of gradient elements computed by the function **objfun**. For example, if the first 30 variables appear linearly in the objective, so that the corresponding gradient elements are constant, then it is reasonable for **options.obj_check_start** to be set to 31.

Constraint: $1 \leq$ **options.obj_check_start** $\leq$ **options.obj_check_stop** $\leq$ **n**.

max_iter – Integer Default $= \max(50, 5\mathbf{n})$

On entry: the limit on the number of iterations allowed before termination.

Constraint: **options.max_iter** ≥ 0.

f_prec – double Default $= \epsilon^{0.9}$

On entry: this argument defines ϵ_r, which is intended to be a measure of the accuracy with which the problem function F can be computed. The value of ϵ_r should reflect the relative precision of $1 + |F(x)|$; i.e., ϵ_r acts as a relative precision when $|F|$ is large, and as an absolute precision when $|F|$ is small. For example, if $F(x)$ is typically of order 1000 and the first six significant digits are known to be correct, an appropriate value for ϵ_r would be 1.0e$-$6. In contrast, if $F(x)$ is typically of order 10^{-4} and the first six significant digits are known to be correct, an appropriate value for ϵ_r would be 1.0e$-$10. The choice of ϵ_r can be quite complicated for badly scaled problems; see Chapter 8 of Gill *et al.* (1981), for a discussion of scaling techniques. The default value is appropriate for most simple functions that are computed with full accuracy. However when the accuracy of the computed function values is known to be significantly worse than full precision, the value of ϵ_r should be large enough so that nag_opt_conj_grad (e04dgc) will not attempt to distinguish between function values that differ by less than the error inherent in the calculation.

Constraint: $\epsilon \leq$ **options.f_prec** < 1.0.

optim_tol – double Default $=$ **options.f_prec**$^{0.8}$

On entry: specifies the accuracy to which you wish the final iterate to approximate a solution of the problem. Broadly speaking, **options.optim_tol** indicates the number of correct figures desired in the objective function at the solution. For example, if **options.optim_tol** is 10^{-6} and nag_opt_conj_grad (e04dgc) terminates successfully, the final value of F should have approximately six correct figures. nag_opt_conj_grad (e04dgc) will terminate successfully if the iterative sequence of x-values is judged to have converged and the final point satisfies the termination criteria (see Section 3, where τ_F represents **options.optim_tol**).

Constraint: **options.f_prec** $\leq$ **options.optim_tol** < 1.0.

linesearch_tol – double Default $= 0.9$

On entry: controls the accuracy with which the step α taken during each iteration approximates a minimum of the function along the search direction (the smaller the value of **options.linesearch_tol**, the more accurate the linesearch). The default value requests an inaccurate search, and is appropriate for most problems. A more accurate search may be appropriate when it is desirable to reduce the number of iterations – for example, if the objective function is cheap to evaluate.

Constraint: $0.0 \leq$ **options.linesearch_tol** < 1.0.

max_line_step – double Default $= 10^{10}$

On entry: defines the maximum allowable step length for the line search.

Constraint: **options.max_line_step** > 0.0.

f_est – double

On entry: specifies the user-supplied guess of the optimum objective function value. This value is used by nag_opt_conj_grad (e04dgc) to calculate an initial step length (see Section 3). If no value is supplied then an initial step length of 1.0 will be used but it should be noted that for badly scaled functions a unit step along the steepest descent direction will often compute the function at very large values of x.

iter – Integer

On exit: the number of iterations which have been performed in nag_opt_conj_grad (e04dgc).

nf – Integer

On exit: the number of times the objective function has been evaluated (i.e., number of calls of **objfun**). The total excludes the calls made to **objfun** for purposes of derivative checking.

11.3 Description of Printed Output

The level of printed output can be controlled with the structure members **options.list**, **options.print_gcheck** and **options.print_level** (see Section 11.2). If **options.list** = Nag_TRUE then the argument values to nag_opt_conj_grad (e04dgc) are listed, followed by the result of any derivative check if **options.print_gcheck** = Nag_TRUE. The printout of the optimization results is governed by the value of **options.print_level**. The default of **options.print_level** = Nag_Soln_Iter provides a single line of output at each iteration and the final result. This section describes all of the possible levels of results printout available from nag_opt_conj_grad (e04dgc).

If a simple derivative check, **options.verify_grad** = Nag_SimpleCheck, is requested then the directional derivative, $g(x)^{\mathrm{T}}p$, of the objective gradient and its finite difference approximation are printed out, where p is a random vector of unit length.

When a component derivative check, **options.verify_grad** = Nag_CheckObj, is requested then the following results are supplied for each component:

`x[i]` the element of x.

`dx[i]` the optimal finite difference interval.

`g[i]` the gradient element.

`Difference approxn.` the finite difference approximation.

`Itns` the number of trials performed to find a suitable difference interval.

The indicator, `OK` or `BAD?`, states whether the gradient element and finite difference approximation are in agreement.

If the gradient is believed to be in error nag_opt_conj_grad (e04dgc) will exit with **fail** set to NE_DERIV_ERRORS.

When **options.print_level** = Nag_Iter or Nag_Soln_Iter a single line of output is produced on completion of each iteration, this gives the following values:

`Itn` the current iteration number k.

`Nfun` the cumulative number of calls to **objfun**. The evaluations needed for the estimation of the gradients by finite differences are not included in the total `Nfun`. The value of `Nfun` is a guide to the amount of work required for the linesearch. nag_opt_conj_grad (e04dgc) will perform at most 16 function evaluations per iteration.

`Objective` the current value of the objective function, $F(x_k)$.

`Norm g` the Euclidean norm of the gradient vector, $\|g(x_k)\|$.

`Norm x` the Euclidean norm of x_k.

`Norm(x(k-1)-x(k))` the Euclidean norm of $x_{k-1} - x_k$.

`Step` the step α taken along the computed search direction p_k.

If **options.print_level** = Nag_Soln or Nag_Soln_Iter, the final result is printed out. This consists of:

x	the final point, x^*.
g	the final gradient vector, $g(x^*)$.

If **options.print_level** = Nag_NoPrint then printout will be suppressed; you can print the final solution when nag_opt_conj_grad (e04dgc) returns to the calling program.

11.3.1 Output of results via a user-defined printing function

You may also specify your own print function for output of the results of any gradient check, the optimization results at each iteration and the final solution. The user-defined print function should be assigned to the **options.print_fun** function pointer, which has prototype

```
void (*print_fun)(const Nag_Search_State *st, Nag_Comm *comm);
```

The rest of this section can be skipped if the default printing facilities provide the required functionality.

When a user-defined function is assigned to **options.print_fun** this will be called in preference to the internal print function of nag_opt_conj_grad (e04dgc). Calls to the user-defined function are again controlled by means of the **options.print_gcheck** and **options.print_level** members. Information is provided through **st** and **comm** the two structure arguments to **options.print_fun**.

If **comm→it_prt** = Nag_TRUE then the results from the last iteration of nag_opt_conj_grad (e04dgc) are in the following members of **st**:

n – Integer

The number of variables.

x – double *

Points to the **st→n** memory locations holding the current point x_k.

f – double

The value of the current objective function.

g – double *

Points to the **st→n** memory locations holding the first derivatives of F at the current point x_k.

step – double

The step α taken along the search direction p_k.

xk_norm – double

The Euclidean norm of $x_{k-1} - x_k$.

iter – Integer

The number of iterations performed by nag_opt_conj_grad (e04dgc).

nf – Integer

The cumulative number of calls made to **objfun**.

If **comm→g_prt** = Nag_TRUE then the following members are set:

n – Integer

The number of variables.

x – double *

Points to the **st→n** memory locations holding the initial point x_0.

g – double *

Points to the **st→n** memory locations holding the first derivatives of F at the initial point x_0.

Details of any derivative check performed by nag_opt_conj_grad (e04dgc) are held in the following substructure of **st**:

gprint – Nag_GPrintSt *

Which in turn contains two substructures **gprint→g_chk**, **gprint→f_sim** and a pointer to an array of substructures, $*$**gprint→f_comp**.

g_chk – Nag_Grad_Chk_St *

This substructure contains the members:

type – Nag_GradChk

The type of derivative check performed by nag_opt_conj_grad (e04dgc). This will be the same value as in **options.verify_grad**.

g_error – Integer

This member will be equal to one of the error codes NE_NOERROR or NE_DERIV_ERRORS according to whether the derivatives were found to be correct or not.

obj_start – Integer

Specifies the gradient element at which any component check started. This value will be equal to **options.obj_check_start**.

obj_stop – Integer

Specifies the gradient element at which any component check ended. This value will be equal to **options.obj_check_stop**.

f_sim – Nag_SimSt *

The result of a simple derivative check, **g_chk→type** $=$ Nag_SimpleCheck, will be held in this substructure which has members:

correct – Nag_Boolean

If Nag_TRUE then the objective gradient is consistent with the finite difference approximation according to a simple check.

dir_deriv – double *

The directional derivative $g(x)^T p$ where p is a random vector of unit length with elements of approximately equal magnitude.

fd_approx – double *

The finite difference approximation, $(F(x+hp)-F(x))/h$, to the directional derivative.

f_comp – Nag_CompSt *

The results of a component derivative check, **g_chk→type** $=$ Nag_CheckObj, will be held in the array of **st→n** substructures of type Nag_CompSt pointed to by **gprint→f_comp**. The procedure for the derivative check is based on finding an interval that produces an acceptable estimate of the second derivative, and then using that estimate to compute an interval that should produce a reasonable forward-difference approximation. The gradient element is then compared with the difference approximation. (The method of finite difference interval estimation is based on Gill *et al.* (1983)).

correct – Nag_Boolean

If Nag_TRUE then this objective gradient component is consistent with its finite difference approximation.

hopt – double *

The optimal finite difference interval. This is `dx[i]` in the NAG default printout.

gdiff – double *

The finite difference approximation for this gradient component.

iter – Integer

The number of trials performed to find a suitable difference interval.

comment – char

A character string which describes the possible nature of the reason for which an estimation of the finite difference interval failed to produce a satisfactory relative condition error of the second-order difference. Possible strings are: `"Constant?"`, `"Linear or odd?"`, `"Too nonlinear?"` and `"Small derivative?"`.

The relevant members of the structure **comm** are:

g_prt – Nag_Boolean

Will be Nag_TRUE only when the print function is called with the result of the derivative check of **objfun**.

it_prt – Nag_Boolean

Will be Nag_TRUE when the print function is called with the result of the current iteration.

sol_prt – Nag_Boolean

Will be Nag_TRUE when the print function is called with the final result.

user – double *
iuser – Integer *
p – Pointer

Pointers for communication of user information. If used they must be allocated memory either before entry to nag_opt_conj_grad (e04dgc) or during a call to **objfun** or **options.print_fun**. The type Pointer will be `void *` with a C compiler that defines `void *` and `char *` otherwise.