

Conjugate Gradient Algorithms Closest to Self-Scaling Memoryless BFGS Method based on clustering the eigenvalues of the self-scaling memoryless BFGS iteration matrix or on minimizing the Byrd-Nocedal measure function with Different Wolfe Line Searches for Unconstrained Optimization

Neculai Andrei¹

Center for Advanced Modeling and optimization,
Academy of Romanian Scientists
E-mail: nandrei@ici.ro

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Abstract Three new procedures for computation the scaling parameter in the self-scaling memoryless Broyden-Fletcher-Goldfarb-Shanno search direction closest to the Perry and Shanno search direction are presented. The first two are based on clustering the eigenvalues of the self-scaling memoryless Broyden-Fletcher-Goldfarb-Shanno iteration matrix by using the determinant or the trace of this matrix. The third one is based on minimizing the measure function of Byrd and Nocedal (SIAM J Numer Anal 26:727-739, 1989). For all these three algorithms the sufficient descent condition is established. The stepsize is computed using three line search procedures based on: the standard Wolfe line search (SIAM Rev 11:226-235, 1969, SIAM Rev 13:185-188, 1971), the approximate Wolfe line search of Hager and Zhang (SIAM J Optim 16:170-192, 2005) or the improved Wolfe line search of Dai and Kou (SIAM J Optim 23:296-320, 2013). Under the improved Wolfe line search the global convergence of these algorithms is established. By using 80 unconstrained optimization test problems, with different structures and complexities, it is proved that the performances of the self-scaling memoryless algorithms with the approximate or the improved Wolfe line searches are better than the performances of the same algorithms with the standard Wolfe line search. For all procedures for the stepsize computation using the standard, the approximate, or the improved Wolfe line search, the performances of the self-scaling memoryless algorithms based on the determinant or on the trace of the iteration matrix are similar. Using the standard, the approximate or the improved Wolfe line search, the performances of the self-scaling memoryless algorithms based on the determinant or on the trace of the iteration matrix or on minimizing the measure function are better than those of CG-DESCENT with Wolfe or with the approximate Wolfe line search of Hager and Zhang (SIAM J Optim 16:170-192, 2005). For all three procedures for stepsize computation using the standard, the approximate or the improved Wolfe line search, the self-scaling memoryless algorithm based on minimizing the measure function of Byrd and Nocedal is top performer versus the same algorithms based

¹ Dr. Neculai Andrei is full member of Academy of Romanian Scientists.

The numerical results presented in this Technical Report are obtained with CG3x8.for package which is a modification of the CG-DESCENT (version 1.4) package implementing a conjugate gradient algorithm. CG3x8 implements three line searches: standard Wolfe, approximate Wolfe and improved Wolfe, with eight conjugate gradient methods: Hager and Zhang, Minim DETERMINANT (same as Dai and Kou), Minim TRACE, Minim measure function FI of Byrd and Nocedal, Hestenes and Stiefel, Dai and Yuan, Polak, Ribiere and Polyak, Combination trace & log(det).

on the determinant or on the trace of the iteration matrix.

Keywords Unconstrained optimization . Self-scaling . Quasi-Newton method . Standard Wolfe line search . Approximate Wolfe line search . Improved Wolfe line search

Mathematics Subject Classification (2000) 49M37. 90C30

1 Introduction

For solving large-scale unconstrained optimization problems the best very well known methods are the quasi-Newton Broyden-Fletcher-Goldfarb-Shanno (BFGS) [1-4] and the nonlinear conjugate gradient. The relationship between these two methods was given by Perry [5] and Shanno [6], who introduced the self-scaling memoryless BFGS method. For convex quadratic functions, if the line search is exact and if for the initial approximation to the Hessian matrix the identity matrix is used, then both the BFGS and the self-scaling memoryless BFGS will generate the same iterations as the conjugate gradient methods. For general nonlinear functions Shanno [6] proved that the conjugate gradient methods are precisely the BFGS quasi-Newton method, where the approximation to the inverse Hessian is restarted as the identity matrix at every step. Based on the self-scaling memoryless BFGS method by Perry and Shanno, Hager and Zhang [7, 8] and Dai and Kou [9] introduced two new conjugate gradient algorithms, called CG-DESCENT and CGOPT, respectively. Intensive numerical experiments proved that these two conjugate gradient methods are more efficient and more robust than the self-scaling memoryless BFGS method.

More exactly, if at every step the approximation to the inverse Hessian is restarted as a scaled identity matrix with a parameter, then the Perry-Shanno search direction is obtained which is dependent by the scaling parameter. Using an aggressive modification of the Perry-Shanno search direction by deleting its last term and selecting for the scaling parameter the value suggested by Oren and Spedicato [10], then the CG-DESCENT conjugate gradient is obtained. Some other conjugate gradient methods were suggested by considering other values for the scaling parameter, as those given by Oren [11], or Oren and Luenberger [12] or Al-Baali [13]. However, in this class of conjugate gradient algorithms, CG-DESCENT proved to be the best. Another approach, developed by Dai and Kou [9] was to seek the conjugate gradient direction that is closest to the Perry-Shanno search direction. Thus, Dai and Kou introduced a general family of conjugate gradient algorithms with a scaling parameter. If for this scaling parameter the value suggested by Oren and Luenberger is selected, then the CGOPT conjugate gradient algorithm is obtained. It is worth saying that the value of the scaling parameter suggested by Oren and Spedicato and used to get CG-DESCENT conjugate gradient algorithm is obtained by minimizing the condition number of $H_k^{-1}H_{k+1}$, where H_k is the approximation to the inverse Hessian. On the other hand, the value of the scaling parameter given by Oren and Luenberger and used to get CGOPT conjugate gradient algorithm is obtained by reducing the condition number of the matrix $H_k^{1/2}\nabla^2 f(x_k)H_k^{1/2}$. Observe that these values for the scaling parameters are obtained by using the singular values of the corresponding matrices.

In this paper we present another approach to determine the value of the scaling parameter in the search direction which is closest to the Perry and Shanno's. In this approach we suggest three procedures for computing the scaling parameter based on the clustering the spectrum of the iteration matrix corresponding to the search direction, or based on the measure function of Byrd and Nocedal [14]. In the first procedure, the value of the scaling parameter is determined by using the determinant of the self-scaling memoryless BFGS iteration matrix. The second one is based

on the trace of the same matrix. Finally, in the third procedure the value of the scaling parameter is obtained by minimizing the measure function of Byrd and Nocedal. It is proved that the first procedure based on the determinant of the iteration matrix leads to the CGOPT conjugate gradient of Dai and Kou. The others are new.

As it is known, in conjugate gradient algorithms the procedure for the stepsize computation is crucial. It is common to see that in conjugate gradient algorithms the search directions tend to be poorly scaled and as a consequence the line search procedure must perform more function and gradient evaluations in order to obtain a suitable stepsize. In other words, in conjugate gradient algorithm the stepsizes differ from 1 in a very unpredictable way [15]. They can be larger or smaller than 1 depending on how the problem is scaled. This is in very sharp contrast to the Newton or quasi-Newton methods, including the limited memory methods, which accept the unit stepsize most of the time along the iterations, and therefore usually they require only few function evaluations per search direction. Subject to the stepsize computation, in order to get more efficient and robust conjugate gradient algorithms two new procedures based on the Wolfe conditions have been developed. The first is the approximate Wolfe line search introduced by Hager and Zhang in CG-DESCENT [7, 8]. The second one is the improved Wolfe line search given by Dai and Kou in CGOPT [9].

The structure of the paper is as follows. For completeness, in Section 2 we present the Dai-Kou family of self-scaling memoryless BFGS quasi-Newton methods [9]. Both the CG-DESCENT and the CGOPT algorithms are particularized from the search direction closest to the Perry and Shanno self-scaling memoryless BFGS search direction. The main contribution of this paper is given in Section 3, where three new procedures for computing the scaling parameter in the search direction closest to the Perry and Shanno's are developed. The first two are based on clustering the eigenvalues of the self-scaling memoryless BFGS iteration matrix, and the third one is based on minimizing the measure function of Byrd and Nocedal. In Section 4 some comments on the approximate Wolfe line search and on the improved Wolfe line search are described. Both for strongly convex functions or for general nonlinear functions, the convergence of the self-scaling memoryless BFGS algorithms with the improved Wolfe line search is proved under the classical assumptions. Section 5 is devoted to present the numerical results with these algorithms on a set of 80 large-scale unconstrained optimization test functions, of different structures and complexities, under the standard Wolfe line search, the approximate Wolfe line search by Hager and Zhang [7] and the improved Wolfe line search by Dai and Kou [9], respectively. The numerical comparisons among these algorithms showed that for all procedures for stepsize computation, the performances of the suggested algorithms based on clustering the eigenvalues of the self-scaling memoryless BFGS iteration matrix H_{k+1} using the determinant or the trace of H_{k+1} are similar. For the standard, the approximate or the improved Wolfe line searches, the self-scaling memoryless BFGS algorithms based on minimizing the measure function of Byrd and Nocedal is more efficient and more robust versus the algorithms based on the determinant or on the trace of H_{k+1} . Under the standard, the approximate or the improved Wolfe line search, the performances of the suggested algorithms based on the determinant or on the trace of the iteration matrix H_{k+1} , or based on minimizing the measure function defined by Byrd and Nocedal, are substantially better than those of CG-DESCENT with Wolfe or with the approximate Wolfe line search.

2 The Dai-Kou Family of Self-Scaling Memoryless Broyden-Fletcher-Goldfarb-Shanno Quasi-Newton Methods

Let us consider the unconstrained optimization problem

$$\min_{x \in \mathbb{R}^n} f(x), \quad (1)$$

where $f : \mathbb{R}^n \rightarrow \mathbb{R}$ is a real valued, twice differentiable function f of n variables with known gradient $g(x) = \nabla f(x)$. Suppose that f satisfies the following assumption.

Assumption 2.1: f is bounded below and its gradient g is Lipschitz continuous, namely there exists a constant $L > 0$ such that $\|g(x) - g(y)\| \leq L\|x - y\|$, for any $x, y \in \mathbb{R}^n$, where $\|\cdot\|$ stands for the Euclidian norm.

As we know, given the initial point x_0 , the iterations of the quasi-Newton methods are generated in the following form

$$x_{k+1} = x_k + \alpha_k d_k, \quad k = 0, 1, \dots, \quad (2)$$

where $d_k \in \mathbb{R}^n$ is the search direction along which the values of function f are reduced, and $\alpha_k \in \mathbb{R}$ is the stepsize determined by a line search procedure. Often, for determination of the stepsize, the standard Wolfe line search conditions [16, 17] are used:

$$f(x_k + \alpha_k d_k) \leq f(x_k) + \rho \alpha_k g_k^T d_k, \quad (3)$$

$$g(x_k + \alpha_k d_k)^T d_k \geq \sigma g_k^T d_k, \quad (4)$$

where $0 < \rho < \sigma < 1$. The search directions in the quasi-Newton methods are computed as

$$d_k = -\bar{H}_k g_k, \quad (5)$$

where $\bar{H}_k \in \mathbb{R}^{n \times n}$ is an approximation to the inverse Hessian of the minimizing function. At the iteration k , the approximation \bar{H}_k to the inverse Hessian is updated to achieve \bar{H}_{k+1} as a new approximation to the inverse Hessian in such a way that \bar{H}_{k+1} satisfies a particular equation, namely the secant equation, which includes the second order information. The most used equation is the standard secant equation

$$\bar{H}_{k+1} y_k = s_k, \quad (6)$$

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

Given the initial approximation \bar{H}_0 to the inverse Hessian, as an arbitrary symmetric and positive definite matrix, the most known quasi-Newton updating formula is the BFGS update

$$\bar{H}_{k+1} = \bar{H}_k - \frac{s_k y_k^T \bar{H}_k + \bar{H}_k y_k s_k^T}{y_k^T s_k} + \left(1 + \frac{y_k^T \bar{H}_k y_k}{y_k^T s_k} \right) \frac{s_k s_k^T}{y_k^T s_k}. \quad (7)$$

The self-scaling memoryless BFGS method of Perry [5] and Shanno [6] is obtained by updating the scaled identity matrix $(1/\tau_k)I$ by the BFGS updating formula (7), i.e. by considering in (7) $\bar{H}_k = (1/\tau_k)I$, where I is the $n \times n$ identity matrix and τ_k is a scaling parameter. Therefore, the search direction in the self-scaling memoryless BFGS method is computed as

$$d_{k+1} = -H_{k+1}g_{k+1}, \quad (8)$$

where

$$H_{k+1} = \frac{1}{\tau_k} \left(I - \frac{s_k y_k^T + y_k s_k^T}{y_k^T s_k} \right) + \left(1 + \frac{1}{\tau_k} \frac{\|y_k\|^2}{y_k^T s_k} \right) \frac{s_k s_k^T}{y_k^T s_k}, \quad (9)$$

and τ_k is the scaling parameter. Now, substituting (9) in (8), the self-scaling memoryless BFGS search direction of Perry and Shanno (with a multiplier difference) is obtained as

$$d_{k+1}^{PS} = -g_{k+1} + \left[\frac{g_{k+1}^T y_k}{y_k^T s_k} - \left(\tau_k + \frac{\|y_k\|^2}{y_k^T s_k} \right) \frac{g_{k+1}^T s_k}{y_k^T s_k} \right] s_k + \frac{g_{k+1}^T s_k}{y_k^T s_k} y_k. \quad (10)$$

Thus, subject to the parameter τ_k , a family of the Perry-Shanno self-scaling memoryless BFGS quasi-Newton methods is obtained. To this end the following particularizations of the search direction d_{k+1}^{PS} may be considered.

1) Having in view that $s_k = \alpha_k d_k$, the deletion of the last term in (10) gives the following search direction

$$d_{k+1} = -g_{k+1} + \left[\frac{g_{k+1}^T y_k}{y_k^T d_k} - \left(\tau_k + \frac{\|y_k\|^2}{y_k^T s_k} \right) \frac{g_{k+1}^T s_k}{y_k^T d_k} \right] d_k. \quad (11)$$

Now, if τ_k is selected as the value given by Oren and Spedicato [10]

$$\tau_k^{OS} = \frac{\|y_k\|^2}{y_k^T s_k}, \quad (12)$$

then (11) reduces to the very well known conjugate gradient algorithm CG-DESCENT proposed by Hager and Zhang [7]:

$$d_{k+1} = -g_{k+1} + \beta_k^{CG-DESCENT} d_k, \quad (13)$$

where

$$\beta_k^{CG-DESCENT} = \frac{g_{k+1}^T y_k}{y_k^T d_k} - 2 \frac{\|y_k\|^2}{y_k^T s_k} \frac{g_{k+1}^T s_k}{y_k^T d_k}. \quad (14)$$

To establish the global convergence, for general nonlinear functions, the conjugate gradient parameter (14) is truncated as

$$\beta_k^{CG-DESCENT+} = \max \left\{ \frac{g_{k+1}^T y_k}{y_k^T d_k} - 2 \frac{\|y_k\|^2}{y_k^T s_k} \frac{g_{k+1}^T s_k}{y_k^T d_k}, \frac{-1}{\|d_k\| \min\{\eta, \|g_k\|\}} \right\}, \quad (15)$$

where $\eta > 0$ is a constant ($\eta = 0.0001$) (see [7]).

The numerical experiments showed that CG-DESCENT is more efficient and more robust than the self-scaling memoryless BFGS method given by (10) [9].

Some other proposals for the parameter τ_k in (11) were given by Oren and Luenberger [12] as

$$\tau_k^{OL} = \frac{y_k^T s_k}{\|s_k\|^2} \quad (16)$$

and by Al-Baali [13]

$$\tau_k^{B1} = \min \left\{ 1, \frac{\|y_k\|^2}{y_k^T s_k} \right\} \quad \text{and} \quad \tau_k^{B2} = \min \left\{ 1, \frac{y_k^T s_k}{\|s_k\|^2} \right\}. \quad (17)$$

For a general nonlinear convex objective function, Nocedal and Yuan [18] proved the global convergence of the self-scaling BFGS method with τ_k given by (16) and with Wolfe line search. They also presented results indicating that the unscaled BFGS method in general is superior to the self-scaling BFGS with τ_k given by (16). Also, the proposals (17) for τ_k , analyzed by Al-Baali, ensure global convergence of the self-scaling BFGS method which is competitive with the unscaled BFGS method.

2) Observe that (10) is a three-term conjugate gradient algorithm. A more reasonable way to deal with the last term in (10) was suggested by Dai and Kou [9] who proposed to seek the search direction as a vector on the manifold $S_{k+1} = \{-g_{k+1} + \beta d_k : \beta \in \mathbb{R}\}$ that is closest to d_{k+1}^{PS} . The search direction in S_{k+1} closest to d_{k+1}^{PS} is obtained as solution of the following minimization problem

$$d_{k+1} = \arg \min \left\{ \|d - d_{k+1}^{PS}\|_2 : d \in S_{k+1} \right\}; \quad (18)$$

which is

$$d_{k+1} = -g_{k+1} + \beta_k(\tau_k) d_k, \quad (19)$$

where

$$\beta_k(\tau_k) = \frac{g_{k+1}^T y_k}{y_k^T d_k} - \left(\tau_k + \frac{\|y_k\|^2}{y_k^T s_k} - \frac{s_k^T y_k}{\|s_k\|^2} \right) \frac{g_{k+1}^T s_k}{y_k^T d_k}. \quad (20)$$

In order to avoid the non-convergence of the algorithm, similarly to Gilbert and Nocedal [19], who proved the global convergence of the PRP methods for general nonlinear functions by restricting $\beta_k \geq 0$, (20) is truncated, being replaced by

$$\beta_k^+(\tau_k) = \max \left\{ \beta_k(\tau_k), \eta \frac{g_{k+1}^T d_k}{\|d_k\|^2} \right\}, \quad (21)$$

where $\eta \in [0,1)$ is a parameter. ($\eta = 0.5$) Thus, the family of Dai-Kou self-scaling memoryless BFGS quasi-Newton methods is obtained. The following result shows that the search direction given by (19) and (20) satisfies the Dai and Liao conjugacy condition [20].

Proposition 2.1 *The search direction (19), where the parameter $\beta_k(\tau_k)$ is determined by (20) satisfies the Dai and Liao conjugacy condition $d_{k+1}^T y_k = -t_k (g_{k+1}^T s_k)$, where*

$$t_k = \tau_k + \frac{\|y_k\|^2}{y_k^T s_k} - \frac{s_k^T y_k}{\|s_k\|^2}$$

for any $k \geq 0$.

Proof From (19) and (20) by direct computation we get

$$d_{k+1}^T y_k = - \left(\tau_k + \frac{\|y_k\|^2}{y_k^T s_k} - \frac{s_k^T y_k}{\|s_k\|^2} \right) (g_{k+1}^T s_k) \equiv -t_k (g_{k+1}^T s_k). \quad \blacksquare$$

Proposition 2.1 is a generalization of the result of Shanno [6] who proved that the conjugate gradient methods are precisely the BFGS quasi-Newton method, where the approximation to the inverse Hessian is restarted as the identity matrix at every step. In our case, at every step the approximation to the inverse Hessian is restarted as a scaled identity matrix. Therefore, (2), (19) and (20) is a conjugate gradient algorithm.

It is worth mentioning that if τ_k in (20) is selected as τ_k^{OL} , then the CGOPT conjugate gradient algorithm of Dai and Kou [9] is obtained, where in this case the search direction is computed as

$$d_{k+1} = -g_{k+1} + \beta_k^{CGOPT} d_k, \quad (22)$$

where

$$\beta_k^{CGOPT} = \frac{g_{k+1}^T y_k}{y_k^T d_k} - \frac{\|y_k\|^2}{y_k^T s_k} \frac{g_{k+1}^T s_k}{y_k^T d_k}. \quad (23)$$

Observe that the difference between the conjugate gradient parameters of CG-DESCENT given by (14) and of the CGOPT given by (23) is the absence of the constant factor 2 in the second term of the parameter from (23). Again, the numerical experiments showed that CGOPT performs more efficiently than the self-scaling memoryless BFGS method given by (10) [9]. Observe that if the line search is exact, i.e. $g_{k+1}^T s_k = 0$, then the second term in (20), (or in (14), or (23)) is missing and the search direction reduces to that of Hestenes and Stiefel [21].

Dai and Kou [9, Lemma 2.1] proved that if $y_k^T d_k > 0$, then the search direction given by (19) and (20) satisfies

$$g_{k+1}^T d_{k+1} \leq -\min \left\{ \tau_k \frac{\|s_k\|^2}{y_k^T s_k}, \frac{3}{4} \right\} \|g_{k+1}\|^2. \quad (24)$$

More general, if function f is continuously differentiable and bounded below, and its gradient g is Lipschitz continuous, then Dai and Kou [9, Lemma 2.2] proved that the search direction (19) where τ_k in (20) is chosen to be any of τ_k^{OS} , τ_k^{OL} , τ_k^{B1} or τ_k^{B2} and $y_k^T s_k > 0$, then $g_{k+1}^T d_{k+1} \leq -c \|g_{k+1}\|^2$, for some positive constant $c > 0$.

Dai and Kou [9] implemented the algorithm (2), (19) and (20) endowed with two ingredients which improve its performances. The first ingredient is an improved Wolfe line search, which avoid the numerical drawback of the first Wolfe line search condition and guarantee the global convergence of the algorithm. The second one is an adaptive restart of the algorithm along the negative gradient based on how the minimizing function is close to some quadratic function. The numerical experiments with this family of self-scaling memoryless BFGS methods, given by Dai and Kou [9], where the parameter τ_k in (20) is chosen as τ_k^{OS} , τ_k^{OL} , τ_k^{B1} or τ_k^{B2} , proved that the selection τ_k^{OL} of τ_k is the most efficient one. With this selection of the parameter τ_k Dai and Kou [9] showed that the algorithm (2), (19) and (20) with improved Wolfe line search is more efficient and more robust than CG-DESCENT.

3 New Conjugate Gradient Algorithms based on Self-Scaling Memoryless Broyden-Fletcher-Goldfarb-Shanno Quasi-Newton Algorithms

The Dai-Kou family of the self-scaling memoryless BFGS quasi-Newton methods, given by (2) and (19) with (20), depends by the scaling parameter τ_k . In this section we present three different ways to choose the scaling parameter τ_k . For the very beginning observe that H_{k+1} given by (9) is symmetric and positive definite. Therefore it has n positive eigenvalues. If $y_k^T s_k > 0$, which always is satisfied when the setsize is determined by the Wolfe line search, then there exists a set of mutually orthogonal unit vectors $\{u_k^i\}_{i=1}^{n-2}$ such that

$$s_k^T u_k^i = y_k^T u_k^i = 0, \quad i = 1, \dots, n-2,$$

which leads to

$$H_{k+1} u_k^i = \frac{1}{\tau_k} u_k^i, \quad i = 1, \dots, n-2.$$

Thus, the vectors u_k^i , $i = 1, \dots, n-2$, are the eigenvectors of H_{k+1} correspondent to the eigenvalues $1/\tau_k$. Therefore, H_{k+1} given by (9) has $n-2$ eigenvalues all equal to $1/\tau_k$. Let λ_k^{n-1} and λ_k^n be the two remaining eigenvalues of H_{k+1} .

As we know, in a small neighborhood of the current point, the nonlinear objective function f in the unconstrained optimization problem (1) behaves like a quadratic one for which the results from the linear conjugate gradient can be applied. For faster convergence of linear conjugate gradient algorithms some approaches can be considered as follows: the presence of isolated smallest and/or largest eigenvalues of the matrix H_{k+1} as well as gaps inside the eigenvalues

spectrum [22], clustering of the eigenvalues about one point [23] or about several points [24], or preconditioning [25]. If the matrix has a number of certain distinct eigenvalues contained in m disjoint intervals of very small length, then the linear conjugate gradient method will produce a very small residual after m iterations [26]. This is an important property of linear conjugate gradient method and we try to use it in nonlinear case. Therefore, we consider the extension of the method of clustering the eigenvalues of the matrix defining the search direction from linear conjugate gradient algorithm to nonlinear case. For this we need to compute the determinant and the trace of the self-scaling memoryless BFGS matrix H_{k+1} . After some simple algebraic manipulation from (9) we get

$$\det(H_{k+1}) = \frac{1}{\tau_k^{n-1}} \frac{\|s_k\|^2}{y_k^T s_k} \quad (25)$$

and

$$\text{tr}(H_{k+1}) = \frac{n-2}{\tau_k} + \left(1 + \frac{1}{\tau_k} \frac{\|y_k\|^2}{y_k^T s_k}\right) \frac{\|s_k\|^2}{y_k^T s_k}. \quad (26)$$

The extension of the clustering the eigenvalues from the linear case to the nonlinear one can be achieved in the following two ways.

1) The first extension of the clustering the eigenvalues from the linear case to the nonlinear one is based on the determinant of the self-scaling memoryless BFGS matrix H_{k+1} given by (9). The idea of this variant of the self-scaling memoryless BFGS algorithm is to determine τ_k by clustering the eigenvalues of H_{k+1} in a point. Since H_{k+1} has $n-2$ eigenvalues all equal to $1/\tau_k$, then imposing that the remaining eigenvalues to have the same value, i.e. $\lambda_k^{n-1} = \lambda_k^n = 1/\tau_k$, from the equality

$$\det(H_{k+1}) = \frac{1}{\tau_k^n},$$

where $\det(H_{k+1})$ is given by (25), we get

$$\tau_k = \frac{y_k^T s_k}{\|s_k\|^2}. \quad (27)$$

From (23) we see that this choice of τ_k , based on determinant, is exactly the choice proposed by

Dai and Kou in their CGOPT algorithm [9], using the Oren and Luenberger choice [12]: $\frac{y_k^T s_k}{s_k^T B_k s_k}$,

with $B_k = H_k^{-1}$ for the BFGS method, where H_k is the identity matrix. Substituting (27) into (20) leads to the conjugate gradient parameter

$$\beta_k^{DE} = \frac{g_{k+1}^T y_k}{y_k^T d_k} - \frac{\|y_k\|^2}{y_k^T s_k} \frac{g_{k+1}^T s_k}{y_k^T d_k} \quad (28)$$

and from (21) the truncated form is obtained as

$$\beta_k^{DE+} = \max \left\{ \frac{g_{k+1}^T y_k}{y_k^T d_k} - \frac{\|y_k\|^2}{y_k^T s_k} \frac{g_{k+1}^T s_k}{y_k^T d_k}, \eta \frac{g_{k+1}^T d_k}{\|d_k\|^2} \right\}, \quad (29)$$

based on determinant. Observe that $\beta_k^{DE} = \beta_k^{CGOPT}$, i.e. the algorithm obtained by clustering the eigenvalues of the iteration matrix H_{k+1} is exactly the CGOPT algorithm of Dai and Kou. The formula (28) differs from (14) only with a constant coefficient in the second term of the Hager and Zhang method.

In the following we show that for strongly (uniformly) convex functions f the search directions (8) and (9), where τ_k is computed as in (27), satisfy the sufficient descent condition $g_k^T d_k \leq -c \|g_k\|^2$ for any $k \geq 0$, where c is a positive constant. Recall that a differential function f is said to be strongly convex on a nonempty open convex set S if there exists a positive constant μ such that

$$(g(x) - g(y))^T (x - y) \geq \mu \|x - y\|^2, \text{ for any } x, y \in S,$$

where $g(x) = \nabla f(x)$.

Theorem 3.1 *Suppose that the Assumption 2.1 holds. For the method (2), (8) and (9), if f is a strongly convex function on the level set $S = \{x \in \mathbb{R}^n : f(x) \leq f(x_0)\}$, and the stepsize α_k is determined by the Wolfe line search (3) and (4), then the search directions (8) and (9), where the parameter τ_k is computed as in (27), satisfy the sufficient descent condition $g_k^T d_k \leq -c \|g_k\|^2$ for any $k \geq 0$, where c is a positive constant.*

Proof As we know H_{k+1} given by (9) has $n-2$ eigenvalues all equal to $1/\tau_k$, as well as λ_k^{n-1} and λ_k^n . Since $\text{tr}(H_{k+1})$ is equal to the summation of the eigenvalues of H_{k+1} and $\det(H_{k+1})$ is equal to the product of them, from (26) and (25) it is easy to see that

$$\lambda_k^{n-1} + \lambda_k^n = \left(1 + \frac{1}{\tau_k} \frac{\|y_k\|^2}{y_k^T s_k} \right) \frac{\|s_k\|^2}{y_k^T s_k} \quad (30)$$

and

$$\lambda_k^{n-1} \lambda_k^n = \frac{1}{\tau_k} \frac{\|s_k\|^2}{y_k^T s_k}. \quad (31)$$

Now, from the Assumption 2.1 we have $\|y_k\| \leq L \|s_k\|$. On the other hand, from the strong convexity of function f on S we have $y_k^T s_k \geq \mu \|s_k\|^2$. Assume that $\lambda_k^n \leq \lambda_k^{n-1}$. With these, from (31) and (30) we get

$$\lambda_k^n = \frac{1}{\tau_k} \frac{\|s_k\|^2}{y_k^T s_k} \frac{1}{\lambda_k^{n-1}} \geq \frac{1}{\tau_k} \frac{\|s_k\|^2}{y_k^T s_k} \frac{1}{(\lambda_k^{n-1} + \lambda_k^n)} = \frac{y_k^T s_k}{\tau_k (y_k^T s_k) + \|y_k\|^2}. \quad (32)$$

But, from (27)

$$\tau_k (y_k^T s_k) = \frac{(y_k^T s_k)^2}{\|s_k\|^2} \leq L^2 \|s_k\|^2.$$

Therefore,

$$\lambda_k^n \geq \frac{\mu \|s_k\|^2}{L^2 \|s_k\|^2 + L^2 \|s_k\|^2} = \frac{\mu}{2L^2}. \quad (33)$$

Now, from (8) and (33), for all $k \geq 0$, we have

$$d_{k+1}^T g_{k+1} = -g_{k+1}^T H_{k+1} g_{k+1} \leq -\lambda_k^n \|g_{k+1}\|^2 \leq -\frac{\mu}{2L^2} \|g_{k+1}\|^2,$$

i.e. the search direction (8), where τ_k is determined as in (27) satisfy the sufficient descent condition $g_k^T d_k \leq -c \|g_k\|^2$ with $c = \mu / (2L^2)$. \blacksquare

2) The second extension of the clustering the eigenvalues from the linear case to nonlinear one is based on the trace of the self-scaling memoryless BFGS matrix H_{k+1} . Again, the idea of this variant of the self-scaling memoryless BFGS algorithm is to determine τ_k by clustering the eigenvalues of H_{k+1} in a point, but this time using trace of H_{k+1} . Since H_{k+1} has $n-2$ eigenvalues, all equal to $1/\tau_k$, then imposing that the remaining eigenvalues to have the same value, i.e. $\lambda_k^{n-1} = \lambda_k^n = 1/\tau_k$, from the equality

$$\text{tr}(H_{k+1}) = \frac{n}{\tau_k}$$

where $\text{tr}(H_{k+1})$ is given by (26) we get

$$\tau_k = \left(2 - \frac{\|y_k\|^2 \|s_k\|^2}{(y_k^T s_k)^2} \right) \frac{y_k^T s_k}{\|s_k\|^2}. \quad (34)$$

Now, substituting (34) into (20) leads to the conjugate gradient parameter

$$\beta_k^{TR} = \frac{g_{k+1}^T y_k}{y_k^T d_k} - \frac{y_k^T s_k}{\|s_k\|^2} \frac{g_{k+1}^T s_k}{y_k^T d_k}, \quad (35)$$

and from (21) the truncated form is obtained as

$$\beta_k^{TR+} = \max \left\{ \frac{g_{k+1}^T y_k}{y_k^T d_k} - \frac{y_k^T s_k}{\|s_k\|^2} \frac{g_{k+1}^T s_k}{y_k^T d_k}, \eta \frac{g_{k+1}^T d_k}{\|d_k\|^2} \right\}, \quad (36)$$

based on trace of H_{k+1} .

Theorem 3.2 Suppose that the Assumption 2.1 holds. For the method (2), (8) and (9), if f is a strongly convex function on the level set $S = \{x \in \mathbb{R}^n : f(x) \leq f(x_0)\}$, and the stepsize α_k is determined by the Wolfe line search (3) and (4), then the search directions (8) and (9), where the parameter τ_k is computed as in (34), satisfy the sufficient descent condition $g_k^T d_k \leq -c \|g_k\|^2$ for any $k \geq 0$, where c is a positive constant.

Proof The scaling parameter τ_k from (34) can be written as

$$\tau_k = 2 \frac{y_k^T s_k}{\|s_k\|^2} - \frac{\|y_k\|^2}{y_k^T s_k}.$$

From (32) it is easy to see that

$$\lambda_k^n \geq \frac{\mu \|s_k\|^2}{3L^2 \|s_k\|^2 + L^2 \|s_k\|^2} = \frac{\mu}{4L^2}. \quad (37)$$

Now, from (8) and (37), for all $k \geq 0$, we have

$$d_{k+1}^T g_{k+1} = -g_{k+1}^T H_{k+1} g_{k+1} \leq -\lambda_k^n \|g_{k+1}\|^2 \leq -\frac{\mu}{4L^2} \|g_{k+1}\|^2,$$

i.e. the search directions (8), where τ_k is determined as in (34) satisfy the sufficient descent condition $g_k^T d_k \leq -c \|g_k\|^2$ with $c = \mu / (4L^2)$. ■

3) Another possibility to determine a value for the scaling parameter τ_k in the self-scaling memoryless BFGS method, we consider in this paper, is to minimize a combination of the determinant and the trace of the iteration matrix H_{k+1} given by (9). Byrd and Nocedal [14] introduced such a combination of $\det(H_{k+1})$ and $tr(H_{k+1})$ as the function:

$$\varphi(H_{k+1}) = tr(H_{k+1}) - \ln(\det(H_{k+1})), \quad (38)$$

where $\ln(\cdot)$ denotes the natural logarithm, known as the measure function. Since H_{k+1} is positive definite, it follows that $\varphi(H_{k+1})$ is well defined. Fletcher [27] observed that the BFGS formula can be derived by a variational argument using function φ . This is an elegant and efficient tool for analyzing the global behavior of quasi-Newton methods and now we intend to use it to generate new and efficient algorithms for unconstrained optimization. Observe that function φ works simultaneously with trace and determinant, thus simplifying the analysis of the quasi-Newton methods. In fact, this function is a measure of matrices involving all the eigenvalues of the iteration matrix, not only the smallest and the largest as it is traditionally used in the analysis

of the quasi-Newton methods based on the condition number of matrices (see [28–32]). Observe that this function is strictly convex on the set of symmetric and positive definite matrices and it is minimized by $H_{k+1} = I$. Besides, it becomes unbounded as H_{k+1} becomes singular or infinite and therefore it works as a barrier function that keeps H_{k+1} positive definite.

Therefore, the idea of this variant of the self-scaling memoryless BFGS algorithm is to determine τ_k by minimizing the measure function $\varphi(H_{k+1})$ of Byrd and Nocedal, defined in (38). From (25) and (26) we have

$$\varphi(H_{k+1}) = \frac{n-2}{\tau_k} + \frac{\|s_k\|^2}{y_k^T s_k} + \frac{1}{\tau_k} \frac{\|y_k\|^2 \|s_k\|^2}{(y_k^T s_k)^2} + (n-1) \ln(\tau_k) - \ln \left(\frac{\|s_k\|^2}{y_k^T s_k} \right). \quad (39)$$

It is easy to see that the solution of the problem $\min \varphi(H_{k+1})$, where $\varphi(H_{k+1})$ is given by (39), is the solution of the equation

$$\frac{\partial \varphi(H_{k+1})}{\partial \tau_k} = -\frac{n-2}{\tau_k^2} - \frac{1}{\tau_k^2} \frac{\|y_k\|^2 \|s_k\|^2}{(y_k^T s_k)^2} + (n-1) \frac{1}{\tau_k} = 0,$$

which is

$$\tau_k = \frac{n-2}{n-1} + \frac{1}{n-1} \frac{\|y_k\|^2 \|s_k\|^2}{(y_k^T s_k)^2} > 0. \quad (40)$$

The measure function $\varphi(H_{k+1})$ of Byrd and Nocedal is a special combination of the determinant and of the trace of the iteration matrix H_{k+1} . Observe that the determinant in $\varphi(H_{k+1})$ is under the natural logarithm. Since H_{k+1} is positive definite, it follows that $\text{tr}(H_{k+1}) > 0$. It is quite possible that along the iterations $\ln(\det(H_{k+1})) < 0$, this being more harmful for minimization of $\varphi(H_{k+1})$. Therefore a variant of the algorithm based on minimizing the measure function $\varphi(H_{k+1})$ is to update the value of the parameter τ_k using (40) only when $\det(H_{k+1}) > 1$, otherwise τ_k remains to be updated by (34).

Hence, to minimize the measure function $\varphi(H_{k+1})$ we consider the following procedure. From (25) compute $\det(H_{k+1})$ with τ_k given by (34). With this value of $\det(H_{k+1})$ compute:

$$\bar{\tau}_k = \begin{cases} \left(2 - \frac{\|y_k\|^2 \|s_k\|^2}{(y_k^T s_k)^2} \right) \frac{y_k^T s_k}{\|s_k\|^2}, & \text{if } \det(H_{k+1}) \leq 1, \\ \frac{n-2}{n-1} + \frac{1}{n-1} \frac{\|y_k\|^2 \|s_k\|^2}{(y_k^T s_k)^2} & \text{if } \det(H_{k+1}) > 1. \end{cases} \quad (41)$$

Now, considering $\tau_k = \bar{\tau}_k$ into (20) we get

$$\beta_k^{FI} = \frac{g_{k+1}^T y_k}{y_k^T d_k} - \left(\bar{\tau}_k + \frac{\|y_k\|^2}{y_k^T s_k} - \frac{s_k^T y_k}{\|s_k\|^2} \right) \frac{g_{k+1}^T s_k}{y_k^T d_k} \quad (42)$$

and its truncated value

$$\beta_k^{FI+} = \max \left\{ \frac{g_{k+1}^T y_k}{y_k^T d_k} - \left(\bar{\tau}_k + \frac{\|y_k\|^2}{y_k^T s_k} - \frac{s_k^T y_k}{\|s_k\|^2} \right) \frac{g_{k+1}^T s_k}{y_k^T d_k}, \eta \frac{g_{k+1}^T d_k}{\|d_k\|^2} \right\}, \quad (43)$$

based on minimizing the measure function of Byrd and Nocedal. Besides, based on the insights gained from the example given by Powell [33], we constrain β_k^{FI+} parameter to be positive, i.e.

$$\beta_k^{FI+} = \max\{\beta_k^{FI+}, 0\}. \quad (44)$$

Theorem 3.3 Suppose that the Assumption 2.1 holds. For the method (2), (8) and (9), if f is a strongly convex function on the level set $S = \{x \in \mathbb{R}^n : f(x) \leq f(x_0)\}$, and the stepsize α_k is determined by the Wolfe line search (3) and (4), then the search directions (8) and (9), where the parameter τ_k is computed as in (40), satisfy the sufficient descent condition $g_k^T d_k \leq -c\|g_k\|^2$ for any $k \geq 0$, where c is a positive constant.

Proof Having in view that $\|y_k\| \leq L\|s_k\|$ and $y_k^T s_k \geq \mu\|s_k\|^2$, following the same procedure as in previous theorems, from (40) the quantity $\tau_k(y_k^T s_k)$ in (32) can be estimated as

$$\begin{aligned} \tau_k(y_k^T s_k) &= \frac{n-2}{n-1}(y_k^T s_k) + \frac{1}{n-1} \frac{\|y_k\|^2 \|s_k\|^2}{y_k^T s_k} \leq y_k^T s_k + \frac{\|y_k\|^2 \|s_k\|^2}{y_k^T s_k} \\ &\leq \|y_k\| \|s_k\| + \frac{\|y_k\|^2 \|s_k\|^2}{\mu \|s_k\|^2} \leq \left(L + \frac{L^2}{\mu} \right) \|s_k\|^2. \end{aligned} \quad (45)$$

Therefore, from (32), using (45) we get

$$\lambda_k^n \geq \frac{y_k^T s_k}{\tau_k(y_k^T s_k) + \|y_k\|^2} \geq \frac{\mu^2}{L^2 + \mu(L + L^2)}. \quad (46)$$

Now, from (8) and (46), for all $k \geq 0$, we have

$$d_{k+1}^T g_{k+1} = -g_{k+1}^T H_{k+1} g_{k+1} \leq -\lambda_k^n \|g_{k+1}\|^2 \leq -\frac{\mu^2}{L^2 + \mu(L + L^2)} \|g_{k+1}\|^2,$$

i.e. the search directions (8), where τ_k is determined as in (40) satisfy the sufficient descent condition $g_k^T d_k \leq -c\|g_k\|^2$ with $c = \mu^2 / [L^2 + \mu(L + L^2)]$. \blacksquare

With these developments the following general self-scaling memoryless BFGS quasi-Newton algorithm may be presented.

Algorithm CGSSML (Conjugate Gradient Self-Scaling MemoryLess BFGS algorithm)

1. Initialization. Choose an initial point $x_0 \in \mathbb{R}^n$. Choose the constants σ, ρ with $0 < \rho < \sigma < 1$ and $\varepsilon > 0$ sufficiently small. Compute $g_0 = \nabla f(x_0)$. Set $d_0 = -g_0$ and $k = 0$
 2. Test a criterion for stopping the iterations. For example, if $\|g_k\|_\infty < \varepsilon$, then stop the iterations
 3. Compute the stepsize $\alpha_k > 0$ using the Wolfe line search conditions, or some modifications of them
 4. Update the variables $x_{k+1} = x_k + \alpha_k d_k$ and compute f_{k+1} and g_{k+1}
 5. Compute the scaling parameter τ_k using clustering the eigenvalues of the iteration matrix, or by minimizing the measure function of Byrd and Nocedal
 6. Compute the parameter β_k according the values of parameter τ_k
 7. Update the search direction $d_{k+1} = -g_{k+1} + \beta_k d_k$
 8. Restart criterion. If $|g_{k+1}^T g_k| > 0.2 \|g_{k+1}\|^2$ then set $d_{k+1} = -g_{k+1}$
 9. Set $k = k + 1$ and go to step 2
-

For computing the stepsize α_k in step 3 of the algorithm, the Wolfe line search (3) and (4) or the approximate Wolfe line search of Hager and Zhang [7, 8], or the improved Wolfe line search of Dai and Kou [9] may be implemented, as it is described in the next section. Observe that in step 5 the parameter τ_k may be computed using the clustering the eigenvalues of H_{k+1} by the determinant of H_{k+1} (27), or by the trace of H_{k+1} (34), or by minimizing the measure function of Byrd and Nocedal (41). In our algorithm, when the Powell restart condition is satisfied (step 8), then we restart the algorithm with the negative gradient $-g_{k+1}$. Some other restarting procedures may be implemented in CGSSML, like $d_{k+1}^T g_{k+1} \geq 10^{-3} \|d_{k+1}\| \|g_{k+1}\|$ of Birgin and Martínez [34], or the adaptive restarting strategy of Dai and Kou [9], but we are interesting to see the performances of CGSSML implementing the Powell restarting technique.

4 Line Search in CGSSML and Convergence Analysis

As it is known the stepsize is crucial in the efficiency of any line search algorithm like CGSSML. Usually, the Wolfe line search (3) and (4) are implemented in line search algorithms. However, in order to improve the performances of the line search algorithms the approximate Wolfe and the improved Wolfe line searches were introduced.

Hager and Zhang [7, 8] introduced the *approximate Wolfe line search*:

$$\sigma d_k^T g_k \leq d_k^T g_{k+1} \leq (2\rho - 1) d_k^T g_k, \quad (47)$$

where $0 < \rho < 1/2$ and $\rho < \sigma < 1$. This approximate line search is implemented in the CG-DESCENT algorithm. The first inequality in (47) is the same as (4). When f is quadratic, the second inequality in (47) is equivalent to (3). As shown by Hager and Zhang [7], the first Wolfe condition (3) limits the accuracy of a conjugate gradient method to the order of the square root of the machine precision, while with the approximate Wolfe line search we can achieve accuracy to the order of the machine precision. In practical computations, the first Wolfe condition (3) may never be satisfied because of the numerical errors, even for tinny values for ρ . In order to avoid

the numerical drawback of the Wolfe line search, Hager and Zhang [7] introduced a combination of the original Wolfe conditions and the approximate Wolfe conditions (47). Their line search is working very well in numerical computations, but cannot guarantee the global convergence of the algorithm in theory. Details on the global convergence of the CG-DESCENT algorithm with the approximate Wolfe line search are given by Hager and Zhang [7, 8].

In order to overcome the deficiencies of the approximate Wolfe line search, Dai and Kou [9] introduced the so called *improved Wolfe line search*: given a constant parameter $\varepsilon > 0$, a positive sequence $\{\eta_k\}$ satisfying $\sum_{k \geq 1} \eta_k < \infty$ as well as the parameters ρ and σ satisfying $0 < \rho < \sigma < 1$, Dai and Kou proposed the following modified Wolfe condition

$$f(x_k + \alpha d_k) \leq f(x_k) + \min\left\{\varepsilon |g_k^T d_k|, \rho \alpha g_k^T d_k + \eta_k\right\}. \quad (48)$$

The line search satisfying (48) and (4) is called the improved Wolfe line search. If f is continuously differentiable and bounded below, the gradient g is Lipschitz continuous and d_k is a descent direction (i.e. $g_k^T d_k < 0$), then there must exist a suitable stepsize satisfying (4) and (48), since they are weaker than the standard Wolfe conditions.

Under the improved Wolfe line search the search direction satisfies the Zoutendijk condition [35]. This condition has a crucial role in proving the convergence of the CGSSML algorithm with improved Wolfe line search.

Proposition 4.1 *Suppose that the Assumption 2.1 holds. Consider the method (2) where the search direction d_k satisfies the descent condition $g_k^T d_k < 0$ and the stepsize α_k satisfies the improved Wolfe line search conditions (4) and (48). Then*

$$\sum_{k \geq 1} \frac{(g_k^T d_k)^2}{\|d_k\|^2} < \infty. \quad (49)$$

Proof Like in [9] from the Lipschitz continuity and (4) we can write

$$L \alpha_k \|d_k\|^2 \geq (g_{k+1} - g_k)^T d_k \geq (\sigma - 1) g_k^T d_k.$$

Therefore

$$\alpha_k \geq \frac{\sigma - 1}{L} \frac{g_k^T d_k}{\|d_k\|^2}. \quad (50)$$

From (48) we have

$$f_{k+1} \leq f_k + \min\left\{\varepsilon |g_k^T d_k|, \rho \alpha g_k^T d_k + \eta_k\right\} \leq f_k + \rho \alpha g_k^T d_k + \eta_k.$$

Now, from (50) we get

$$f_k - f_{k+1} + \eta_k \geq c \frac{(g_k^T d_k)^2}{\|d_k\|^2}, \quad (51)$$

where $c = \rho(1 - \sigma) / L$. Since f is bounded below, summing (51) over k and having in view that the sequence $\{\eta_k\}$ satisfies $\sum_{k \geq 1} \eta_k < \infty$ it follows that (49) holds. \blacksquare

For strongly convex functions, the following theorem prove the global convergence of the algorithm (2), (19) and (20), where the scaling parameter τ_k is chosen as in (27), (34) or (40), under the improved Wolfe line search.

Theorem 4.1 *Suppose that the Assumption 2.1 holds. Consider the algorithm (2) in which the search direction is defined by (19) and (20), where τ_k is chosen to be as in (27), (34) or (40) and the stepsize α_k is determined by the improved Wolfe line search (4) and (48). If the function f is strongly convex, then the algorithm CGSSML is global convergent, i.e. $\lim_{k \rightarrow \infty} \|g_k\| = 0$.*

Proof From the Assumption 2.1 and the strong convexity of function f it follows that $\|y_k\| \leq L\|s_k\|$ and $y_k^T s_k \geq \mu\|s_k\|^2$. Therefore, for any τ_k given by (27), (34) and (40), there exists a positive constant c_τ such that $|\tau_k| \leq c_\tau$. From (19) and (20) we have

$$\begin{aligned} \|d_{k+1}\| &\leq \|g_{k+1}\| + \left| \frac{g_{k+1}^T y_k}{y_k^T d_k} \right| \|d_k\| + \left| \tau_k + \frac{\|y_k\|^2}{y_k^T s_k} + \frac{s_k^T y_k}{\|s_k\|^2} \right| \left| \frac{g_{k+1}^T s_k}{y_k^T d_k} \right| \|d_k\| \\ &\leq \|g_{k+1}\| + \frac{\|g_{k+1}\| L \|s_k\|}{\mu \|s_k\|^2} \|s_k\| + \left(c_\tau + \frac{L^2 \|s_k\|^2}{\mu \|s_k\|^2} + \frac{L \|s_k\|^2}{\|s_k\|^2} \right) \frac{\|g_{k+1}\| \|s_k\|}{\mu \|s_k\|^2} \|s_k\| \\ &\leq \left(1 + \frac{L^2 + 2\mu L + \mu c_\tau}{\mu^2} \right) \|g_{k+1}\|. \end{aligned} \quad (52)$$

On the other hand, since from the Theorems 3.1-3.3 for any τ_k given by (27), (34) or (40) the search direction (19) and (20) satisfies the sufficient descent condition, it follows that

$$\sum_{k \geq 1} \frac{\|g_k\|^4}{\|d_k\|^2} < \infty. \quad (53)$$

By (52) and (53) we get

$$\sum_{k \geq 1} \|g_k\|^2 < \infty,$$

which implies that $\lim_{k \rightarrow \infty} \|g_k\| = 0$. \blacksquare

For general nonlinear functions, the global convergence of the algorithm (2) with (19) and (20), where the scaling parameter τ_k is chosen as in (27), (34) or (40) under the improved Wolfe line search follows the methodology given by Gilbert and Nocedal [19]. Dai and Kou [9] proved that if function f satisfies the Assumption 2.1 and there exists $\gamma > 0$ such that $\|g_k\| \geq \gamma$ for any $k \geq 1$, then for the family of conjugate gradient algorithms given by (2), in which the search

direction d_{k+1} is computed as in (19) and (20), and the stepsize α_k is determined by the improved Wolfe line search (4) and (48), then $d_k \neq 0$ and

$$\sum_{k \geq 2} \|u_k - u_{k-1}\|^2 < \infty, \quad (54)$$

where $u_k = d_k / \|d_k\|$.

This result, similar to Lemma 4.1 in [19], is used for proving the global convergence of the CGSSML algorithm with improved Wolfe line search. For this in the following proposition we prove that $\beta_k(\tau_k)$ in (20) has Property (*) defined in [19] (see also [36]).

Proposition 4.2 *Suppose that the Assumption 2.1 holds. Consider the family of conjugate gradient algorithms given by (2) in which the search direction d_{k+1} is computed as in (19) and (20) and the stepsize α_k is determined by the improved Wolfe line search (4) and (48). If the sequence $\{x_k\}$ generated by the algorithm CGSSML is bounded and if τ_k is chosen as in (27), (34) or (40), then $\beta_k(\tau_k)$ in (20) has Property (*).*

Proof The proof follows by contradiction, like in [9]. Suppose that $\|g_k\| \geq \gamma$ for any $k \geq 1$. From continuity of the gradient and the boundedness of $\{x_k\}$ it follows that there exists a positive constant $\bar{\gamma}$ such that

$$\|x_k\| \leq \bar{\gamma}, \quad \|g_k\| \leq \bar{\gamma}, \quad \text{for any } k \geq 1. \quad (55)$$

From (4) it follows that

$$g_{k+1}^T d_k \geq \sigma g_k^T d_k. \quad (56)$$

From Theorems 3.1 – 3.3 it follows that for any values of τ_k given by (27), or (34), or (40) we have $g_k^T d_k \leq -c \|g_k\|^2$, where c is a constant. Therefore, from (56) we get

$$d_k^T y_k = d_k^T g_{k+1} - d_k^T g_k \geq -(1-\sigma) d_k^T g_k \geq c(1-\sigma) \gamma^2. \quad (57)$$

Now, from (56) and since $g_k^T d_k < 0$, it follows that

$$\frac{\sigma}{\sigma-1} \leq \frac{g_{k+1}^T d_k}{d_k^T y_k} \leq 1. \quad (58)$$

As it was proved in Theorems 3.1 – 3.3, it is easy to see that for any values of τ_k given by (27), or (34), or (40) there exists a positive constant c_τ such that

$$|\tau_k(y_k^T s_k)| \leq c_\tau \|s_k\|^2, \quad \text{for any } k \geq 1. \quad (59)$$

It is easy to see that $\beta_k(\tau_k)$ from (20) can be written as

$$\beta_k(\tau_k) = \frac{g_{k+1}^T y_k}{d_k^T y_k} - \left(1 - \frac{(d_k^T y_k)^2}{\|d_k\|^2 \|y_k\|^2} \right) \frac{\|y_k\|^2}{d_k^T y_k} \frac{g_{k+1}^T d_k}{d_k^T y_k} - \frac{\tau_k (y_k^T s_k)}{d_k^T y_k} \frac{g_{k+1}^T d_k}{d_k^T y_k}. \quad (60)$$

Observe that $\|y_k\| \leq L\|s_k\|$ and $0 \leq (d_k^T y_k)^2 \leq \|d_k\|^2 \|y_k\|^2$, for any $k \geq 1$. Since by (55), $\|s_k\| = \|x_{k+1} - x_k\| \leq \|x_{k+1}\| + \|x_k\| \leq 2\bar{\gamma}$, using (57), (59) and (60) we get that there exists a constant $c_\beta > 0$ such that for any $k \geq 1$,

$$|\beta_k(\tau_k)| \leq c_\beta \|s_k\|. \quad (61)$$

Now, like in [19] define $b = 2c_\beta \bar{\gamma}$ and $\lambda = 1/(2c_\beta^2 \bar{\gamma})$. From (61) and (55) it follows that for all $k \geq 1$ we have that

$$|\beta_k(\tau_k)| \leq b, \quad (62)$$

and

$$\|s_k\| \leq \lambda \Rightarrow |\beta_k(\tau_k)| \leq \frac{1}{b}. \quad (63)$$

Therefore, (62) and (63) show that $\beta_k(\tau_k)$ defined by (20) has Property (*) (see [19]) ■

Theorem 4.2 *Suppose that the Assumption 2.1 holds. Consider the algorithm (2) in which the search direction is defined by (19) and (20), where τ_k is chosen to be as in (27), (34) or (40) and the stepsize α_k is determined by the improved Wolfe line search (4) and (48). If the sequence $\{x_k\}$ generated by the algorithm CGSSML is bounded, then the algorithm is global convergent, i.e. $\liminf_{k \rightarrow \infty} \|g_k\| = 0$.*

Proof By contradiction suppose that $\|g_k\| \geq \gamma$ for any $k \geq 1$. Since $-g_k^T d_k \geq c\|g_k\|^2$ for some positive constant $c > 0$ and for any $k \geq 1$, from Zoutendijk condition (49) it follows that

$$\|d_k\| \rightarrow +\infty. \quad (64)$$

From the continuity of the gradient, it follows that there exists a positive constant $\bar{\gamma}$ such that

$$\|g_k\| \leq \bar{\gamma}, \text{ for any } k \geq 1. \text{ By (21), (64) means that } \beta_k(\tau_k) \text{ can only be less than } \eta \frac{g_{k+1}^T d_k}{\|d_k\|^2} \text{ for}$$

finite times, since otherwise, we have that

$$\|d_{k+1}\| = \left\| -g_{k+1} + \eta \frac{g_{k+1}^T d_k}{\|d_k\|^2} d_k \right\| \leq (1 + \eta) \|g_{k+1}\| \leq (1 + \eta) \bar{\gamma}$$

for infinite k 's and therefore we get a contradiction with (64). Hence, we can suppose that along the iterations $\beta_k^+(\tau_k) = \beta_k(\tau_k)$ for sufficiently large k . With this, from (54) and Lemma 4.2 in [19] and the boundedness of the sequence $\{x_k\}$, we get a contradiction similarly to the proof of Theorem 4.3 in [19]. This contradiction shows that $\liminf_{k \rightarrow \infty} \|g_k\| = 0$. ■

5 Numerical Results and Comparisons

In this section we report some numerical results of the CGSSML algorithm for solving large-scale unconstrained optimization problems. Algorithm CGSSML was implemented by modifying the CG-DESCENT code (Fortran version 1.4) of Hager and Zhang [8] in order to incorporate the self-scaling memoryless BFGS algorithms in which the conjugate gradient parameter β_k in the search direction is computed by clustering the eigenvalues of the iteration matrix H_{k+1} or by minimizing the measure function of Byrd and Nocedal, presented in Section 3, and respectively with the standard Wolfe or with the approximate Wolfe or with the improved Wolfe line searches, discussed in Section 4.

Remark: Notice that, the algorithm CGSSML can be implemented by modifying the most recent C version 6.8 of CG-DESCENT code of Hager and Zhang [37], i.e. the preconditioned CG-DESCENT, where a limited memory conjugate gradient algorithm is used: L-CG-DESCENT. However, in this paper we do not implement CGSSML into the frame of L-CG-DESCENT because our interest here is to see the performances of β_k^{DE+} , β_k^{TR+} and β_k^{FI+} subject to different line search conditions, for solving large-scale unconstrained optimization problems, without any ingredients like: preconditioning, limited memory or adaptive restart of the algorithm. ■

The algorithms compared in this section are as follows: DESW, DEAW and DEIW, i.e. CGSSML algorithm with β_k^{DE+} given by (29) and with the standard Wolfe line search (3) and (4), with the approximate Wolfe line search of Hager and Zhang given by (47), with the improved Wolfe line search of Dai and Kou (48) and (4), respectively. TRSW, TRAW and TRIW, i.e. CGSSML algorithm with β_k^{TR+} given by (36) and with the standard Wolfe line search (3) and (4), with the approximate Wolfe line search of Hager and Zhang given by (47), with the improved Wolfe line search of Dai and Kou (48) and (4), respectively. FISW, FIAW and FIW, i.e. CGSSML algorithm with β_k^{FI+} given by (44) and with the standard Wolfe line search (3) and (4), with the approximate Wolfe line search of Hager and Zhang given by (47), with the improved Wolfe line search of Dai and Kou (48) and (4), respectively. The code is compiled with f77 (default compiler settings) on a Workstation Intel Pentium 4 with 1.8 GHz. We selected a number of 80 large-scale unconstrained optimization test functions in generalized or extended form [38]. In this collection, some problems are quadratic and some of them are highly nonlinear. The problems are presented in extended (separable) or generalized (chained) form. The Hessian for the problems in extended form has a block-diagonal structure. On the other hand, the Hessian for the problems in generalized form has a banded structure with small bandwidth, often being tri- or penta-diagonal. For some other optimization problems from this set, the corresponding Hessian has a sparse structure or it is a dense (full) matrix. The vast majority of the optimization problems included in our collection described in [38] is taken from CUTER collection [39]. For each test function, we have taken 10 numerical experiments with the number of variables $n = 1000, 2000, \dots, 10,000$.

The parameters in the standard Wolfe line searches are $\rho = 0.0001$ and $\sigma = 0.8$. All the algorithms use the same stopping criterion $\|g_k\|_\infty \leq 10^{-6}$, where $\|\cdot\|_\infty$ is the maximum absolute component of a vector, or when the number of iterations exceeds 2000 iterations. The rest of parameters are the same defined in CG-DESCENT by Hager and Zhang [8] and Algorithm 4.1 of Dai and Kou [9]. In all algorithms, we considered in our numerical experiments, the Powell restart criterion, described in step 8 of the CGSSML algorithm, is used.

The algorithms which we compare in these numerical experiments find local solutions. Therefore, the comparisons of the algorithms are given in the following context. Let f_i^{ALG1} and f_i^{ALG2} be the optimal value found by ALG1 and ALG2 for problem $i = 1, \dots, 80$, respectively. We say that, in the particular problem i , the performance of ALG1 was better than the performance of ALG2 if:

$$|f_i^{ALG1} - f_i^{ALG2}| < 10^{-3} \quad (65)$$

and if the number of iterations (#iter), or the number of function-gradient evaluations (#fg), or the CPU time of ALG1 was less than the number of iterations, or the number of function-gradient evaluations, or the CPU time corresponding to ALG2, respectively. The performances of the algorithms are displayed by the Dolan and Moré performance profiles [40].

It is worth emphasizing that in our numerical experiments we compare algorithms included in CGSSML versus CG-DESCENT version 1.4. The idea was to see the performances of the algorithms using β_k^{DE+} given by (29), β_k^{TR+} given by (36), β_k^{FI+} given by (44) and $\beta_k^{CG-DESCENT+}$ given by (15) without any other ingredients included in the limited memory conjugate gradient algorithm proposed by Hager and Zhang [37], or in the CGOPT by Dai and Kou [9]. Our interests were to see the power the conjugate gradient parameters β_k^{DE+} , β_k^{TR+} , β_k^{FI+} , and $\beta_k^{CG-DESCENT+}$ with different line searches for solving large-scale unconstrained optimization problems.

In the first set of numerical experiments we compare the performance of CGSSML algorithms with standard Wolfe line search, namely DESW versus TRSW, DESW versus FISW and TRSW versus FISW for solving the set of problems considered in this numerical study. Figure 1 shows the Dolan and Moré CPU performance profiles of these algorithms. When comparing DESW versus TRSW subject to the CPU time metric we see that DESW is top performer. Comparing DESW versus TRSW (see Fig. 1), subject to the number of iterations, we see that DESW was better in 250 problems (i.e. it achieved the minimum number of iterations in 250 problems). TRSW was better in 143 problems and they achieved the same number of iterations in 370 problems, etc. Out of 800 problems, only for 763 problems does the criterion (65) holds. Observe that DESW and TRSW have similar performances, DESW being slightly more efficient and more robust. It seems that from the viewpoint of clustering of the eigenvalues of H_{k+1} using the determinant or the trace of the iteration matrix leads to algorithms with similar performances. From Figure 1 we see that FISW is top performer versus DESW and versus TRSW. This is because the FISW algorithm is based on an *ad hoc* procedure for minimizing a special combination of the determinant and of the trace of the iteration matrix H_{k+1} .

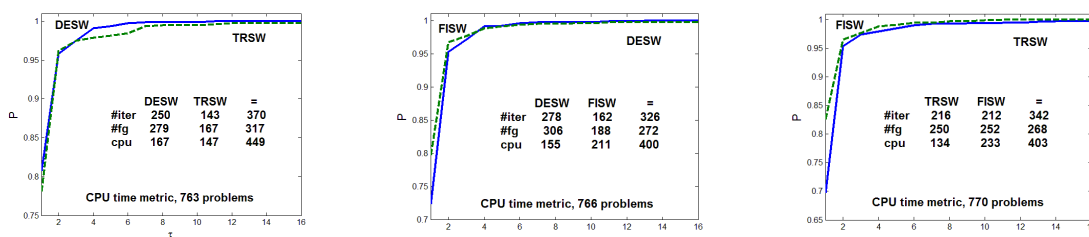


Fig. 1 Performance profiles of DESW versus TRSW, of DESW versus FISW and of TRSW versus FISW

In the second set of numerical experiments we compare DESW, TRSW and FISW versus CG-DESCENT (version 1.4) with truncated conjugate gradient parameter (15) and with standard Wolfe line search (3) and (4). CG-DESCENT was devised in order to ensure sufficient descent,

independent of the accuracy of the line search. In CG-DESCENT the search direction (13), where the conjugate gradient parameter is computed as in (14), satisfies the sufficient descent condition $g_k^T d_k \leq -(7/8)\|g_k\|^2$, provided that $y_k^T d_k \neq 0$. The search directions in CG-DESCENT do not satisfy the conjugacy condition. When iterates jam the expression $\|y_k\|^2 (g_{k+1}^T s_k) / (y_k^T s_k)^2$ in (14) becomes negligible. If the minimizing function f is quadratic and the line search is exact, then CG-DESCENT reduces to the Hestenes and Stiefel algorithm [21]. Figure 2 presents the Dolan and Moré performance profiles of these algorithms. From Figure 2 we see that DESW, TRSW and FISW are top performers versus CG-DESCENT and the differences are significant. Since all these algorithms use the same line search based on Wolfe conditions (3) and (4), it follows that DESW, TRSW and FISW generates a better search direction. Notice that the difference between DESW and CG-DESCENT is only in a constant coefficient of the second term of the Hager and Zhang method. Besides, the truncation mechanisms in these algorithms are different and this explains the differences between these algorithms.

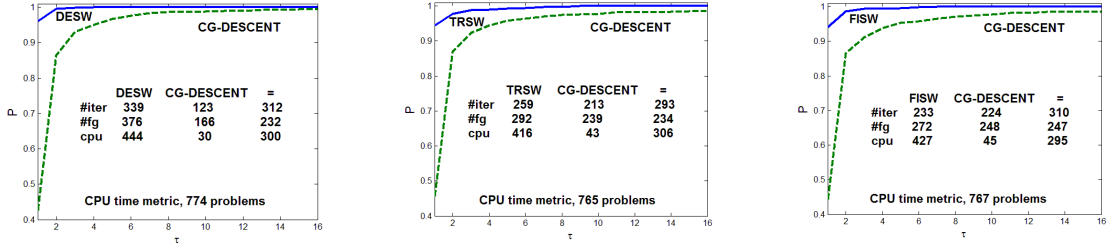


Fig. 2 Performance profiles of DESW, TRSW and FISW versus CG-DESCENT

In the third set of numerical experiments we compare the performance of CGSSML algorithms with approximate Wolfe line search, namely DEAW versus TRAW, DEAW versus FIAW and TRAW versus FIAW for solving the set of problems we considered in this numerical study. Figure 3 presents the Dolan and Moré performance profiles of these algorithms. From Figure 3 we see that both DEAW and TRAW have similar performances. However, FIAW is top performer versus both DEAW and TRAW.

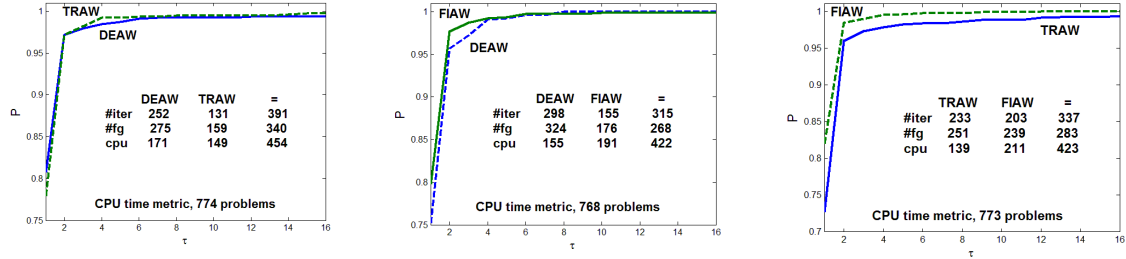


Fig. 3 Performance profiles of DEAW versus TRAW, of DEAW versus FIAW and of TRAW versus FIAW

In the fourth set of numerical experiment we compare DEAW, TRAW and FIAW versus CG-DESCENT with truncated conjugate gradient parameter (15) and with approximate Wolfe line search (47) (CG-DESCENTa). The CG-DESCENTa algorithm of Hager and Zhang [7, 8] implements advanced features of line search including: an approximation to the Wolfe line search

condition that can be evaluated with a greater accuracy, a special secant procedure that leads to a rapid and accurate reduction in the width of the interval bracketing the stepsize, and a quadratic step that retains the n -step quadratic convergence property of the algorithm [41]. Figure 4 shows the performances of these algorithms. Observe that all DEAW, TRAW and FIAW are top performers versus CG-DESCENTa. The greatest difference is between FIAW and CG-DESCENTa.

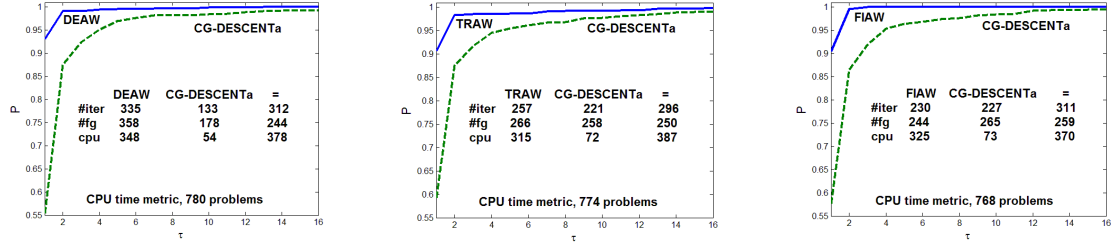


Fig. 4 Performance profiles of DEAW, TRAW and FIAW versus CG-DESCENTa

In the fifth set of numerical experiments we compare the performance of CGSSML algorithms with improved Wolfe line search, namely DEIW versus TRIW, DEIW versus FIIW and TRIW versus FIIW for solving the set of problems considered in this numerical study. Figure 5 presents the performances of these algorithms. Both DEIW and TRIW have similar performances. Observe that FIIW is slightly top performer versus DEIW and TRIW. However, they have similar performances, at least for this set of unconstrained optimization problems considered in this paper.

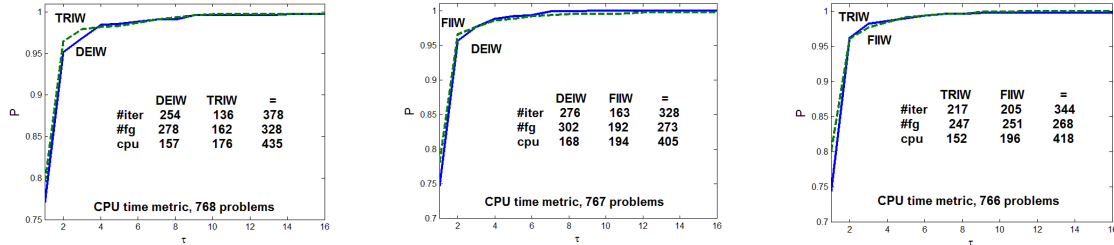


Fig. 5 Performance profiles of DEIW versus TRIW, of DEIW versus FIIW and of TRIW versus FIIW

In the sixth set of numerical experiments we compare DEIW, TRIW and FIIW versus CG-DESCENT with truncated conjugate gradient parameter (15) and with Wolfe line search (3) and (4). Figure 6 shows the performances of these algorithms. We see that DEIW, TRIW and FIIW are more efficient and more robust than CG-DESCENT with Wolfe line search. We see that using the determinant, the trace or the measure function of Byrd and Nocedal, we get conjugate gradient algorithms more efficient and more robust. All these methods are based on clustering the eigenvalues of the iteration matrix H_{k+1} given by (9) with corresponding values for τ_k .

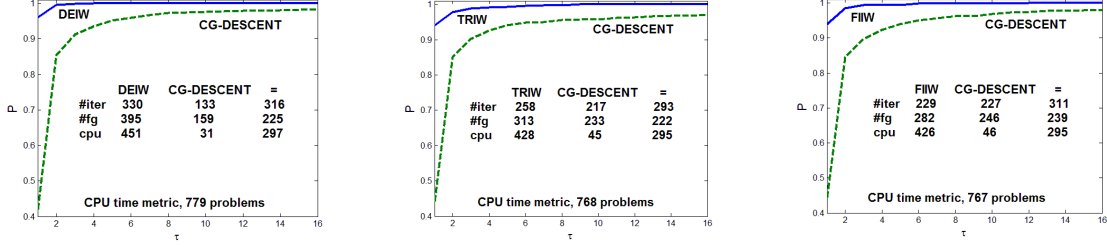


Fig. 6 Performance profiles of DEIW, TRIW and FIW versus CG-DESCENT

In the next set of numerical experiments we compare the performance of the CGSSML algorithms based on determinant or on trace or on minimizing the measure function of Byrd and Nocedal with different line searches. Figure 7 presents the performances of DESW versus DEAW, of DESW versus DEIW and of DEAW versus DEIW. We see that both the CGSSML algorithms based on determinant with the approximate Wolfe and with the improved Wolfe line search are more robust than the algorithm with standard Wolfe line search. The CGSSML algorithms based on determinant with approximate Wolfe and with the improved Wolfe line searches have similar performances, subject to the CPU time metric.

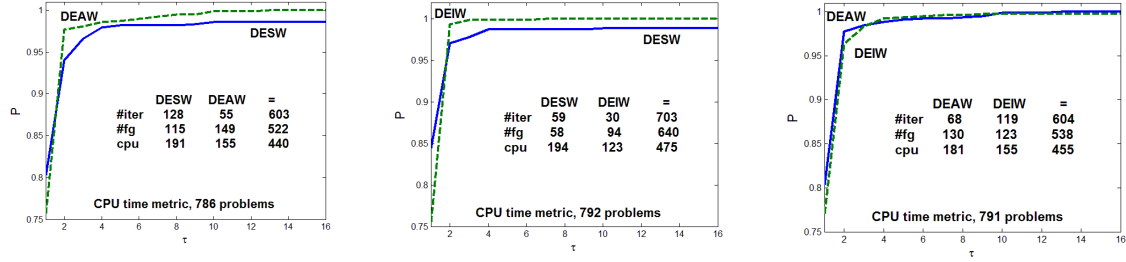


Fig. 7 Performance profiles of DESW versus DEAW, of DESW versus DEIW and of DEAW versus DEIW

Figure 8 shows the performances of TRSW versus TRAW, of TRSW versus TRIW and of TRAW versus TRIW. We see that both the CGSSML algorithms based on trace with the approximate Wolfe and with the improved Wolfe line search are more robust than the algorithm with standard Wolfe line search. Again the CGSSML algorithms based on trace with the approximate Wolfe and with the improved Wolfe line searches have similar performances, TRIW being slightly more efficient. In other words, the improved Wolfe line search is more efficient versus the approximate Wolfe line search, at least for this set of optimization problems.

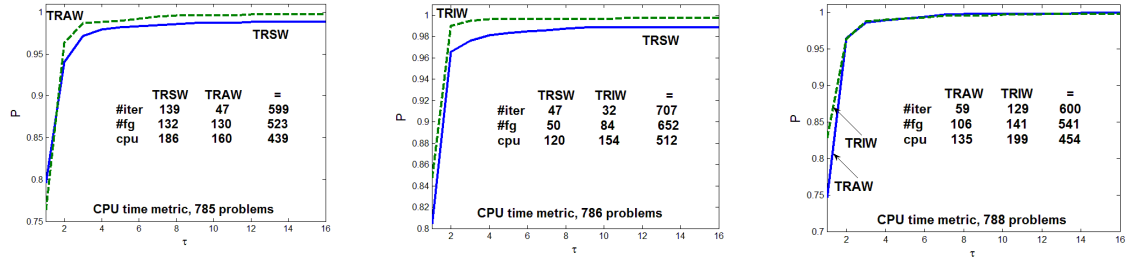


Fig. 8 Performance profiles of TRSW versus TRAW, of TRSW versus TRIW and of TRAW versus TRIW

Figure 9 shows the performances of FISW versus FIAW, of FISW versus FIIW and of FIAW versus FIIW. We see that the CGSSML algorithms based on minimizing the measure function of Byrd and Nocedal endowed with approximate Wolfe line search or with improved Wolfe line search are more robust than the algorithms with standard Wolfe line search. Besides, we have computational evidence that the algorithms minimizing the measure function with approximate Wolfe line search and with improved Wolfe line search have similar performances, FIAW being slightly more efficient.

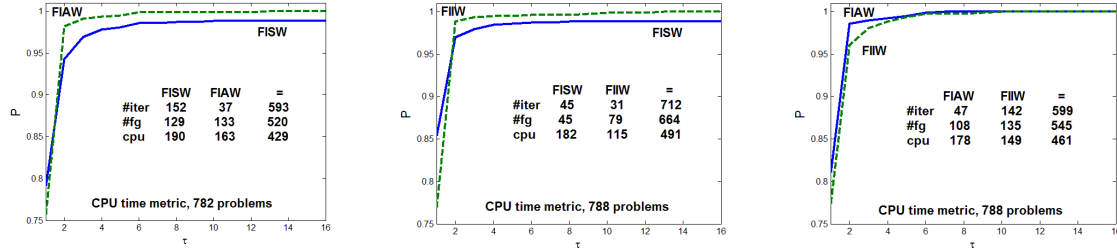


Fig. 9 Performance profiles of FISW versus FIAW, of FISW versus FIIW and of FIAW versus FIIW

Some remarks are in order.

- 1) Both the approximate Wolfe line search and the improved Wolfe line search are important ingredients for the efficiency and robustness of the self-scaling memoryless BFGS algorithms with clustering the eigenvalues. The performances of the CGSSML algorithms with approximate or improved line searches are better than the performances of the same algorithms with the standard Wolfe line search.
- 2) No matter how the stepsize is computed, using the standard, the approximate or the improved Wolfe line search, the performances of the CGSSML algorithms based on the determinant or on the trace of the iteration matrix H_{k+1} , or based on minimizing the measure function $\varphi(H_{k+1})$ defined by Byrd and Nocedal, are better than those of CG-DESCENT with Wolfe or with the approximate Wolfe line search.
- 3) For all procedures for stepsize computation using the standard, the approximate, or the improved Wolfe line search, the performances of the CGSSML algorithms based on the determinant or on the trace of the iteration matrix H_{k+1} are similar.
- 4) For the standard, the approximate or the improved Wolfe line searches, the self-scaling memoryless BFGS algorithms based on minimizing the measure function of Byrd and Nocedal is more efficient and more robust versus the algorithms based on the determinant or on the trace of H_{k+1} .

Both the CG-DESCENT and CGOPT are self-scaling memoryless BFGS algorithms obtained by using the singular values of some associated matrices. In our approach we followed the idea to cluster the eigenvalues of the iteration matrix, based on the determinant or on the trace of this matrix, or to minimize the measure function associated to all the eigenvalues of the iteration matrix. We conclude that the self-scaling memoryless BFGS algorithms based on minimizing the measure function of Byrd and Nocedal, which is a combination of the determinant and of the trace of the iteration matrix, are top performers versus the same algorithms based on the determinant or on the trace of the iteration matrix.

6 Conclusions

In this paper we have presented new procedures for selecting the parameter in the family of conjugate gradient algorithms of Dai and Kou [9], in which the search direction is closest to the Perry and Shanno self-scaling memoryless BFGS search direction. Three procedures have been developed. Two of them are based on clustering the eigenvalues of the self-scaling memoryless BFGS matrix H_{k+1} using the determinant or using the trace of H_{k+1} . The third one is based on minimizing the measure function of Byrd and Nocedal. The algorithm based on clustering the eigenvalues of H_{k+1} using the determinant is the same as CGOPT established by Dai and Kou [9]. The sufficient descent condition was established for all three members of the family. For stepsize computation, all these algorithms are endowed with the standard, the approximate and the improved Wolfe line search. In our numerical experiment we implemented the Powell restarting criterion. Our intensive numerical experiments showed that the algorithms using the clustering the eigenvalues of H_{k+1} based on determinant or on the trace of this matrix have similar performances. All the self-scaling memoryless BFGS algorithms endowed with the standard, or the approximate, or the improved Wolfe line search, are top performers versus the CG-DESCENT algorithm of Hager and Zhang. Besides, the self-scaling memoryless BFGS algorithm based on minimizing the measure function of Byrd and Nocedal is superior to the self-scaling memoryless BFGS algorithms based on the determinant or on the trace of the iteration matrix H_{k+1} , including here the CGOPT algorithm by Dai and Kou.

As an extension of the ideas presented in this paper, instead of minimizing the measure function $\varphi(H_{k+1})$ of Byrd and Nocedal, to determine a value for the parameter τ_k in (20) we may consider minimizing another measures function given by Dennis and Wolkowicz [42]

$$\omega(H_{k+1}) = \frac{\text{tr}(H_{k+1})}{n(\det(H_{k+1}))^{1/n}}. \quad (66)$$

Another possibility is to consider the self-scaling memoryless Broyden family of methods which include two parameters. We mention the possibility to implement in step 8 of CGSSML the adaptive restart criterion of Dai and Kou [9]. Finally, another extension is to implement CGSSML by modifying the most recent C version 6.8 of CG-DESCENT code of Hager and Zhang [37]

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April 18, 2019

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APPENDIX (Fortran program CG3x8.FOR)

```
c-----
c
c                               January 17, 2019
c
c                               Main program.
c
c                               All subroutines are included.
c
c The program is a modification of the CG-DESCENT of Hager and Zhang (2005)
c to include different formulae for parameter beta computation under the
c three line search conditions: standard Wolfe, Approximate Wolfe and
c Improved Wolfe.
c
c-----
c The program is that of Hager and Zhang (CG-DESCENT), where
c the formula for beta computation is modified as:
c
c  ibeta      Algorithm
c  -----
c    1      Hager and Zhang (2005)
c    2      Minim DETERMINANT (Andrei, Thechnical Report No.2/2019)
c    3      Minim TRACE (Andrei, Thechnical Report No.2/2019)
c    4      Minim Fi - measure function of Byrd and Nocedal
c           (Andrei, Thechnical Report No.2/2019)
c    5      Hestenes - Stiefel
c    6      Dai - Yuan
c    7      Polak-Ribiere-Polyak
c    8      Minim of combination of DETERMINANT and TRACE (Andrei, Thechnical
c           Report No.2/2019)
c
c
c The algorithms are described in:
c
c   N. Andrei, A Conjugate Gradient Algorithms Closest to Self-Scaling
c   Memoryless BFGS Method based on minimizing the Byrd-Nocedal measure
c   function with Different Wolfe Line Searches for Unconstrained Optimization.
c   Technical Report No.2/2019,
c   April 18, 2019.
c   28 pages.
c
c The program implements optimization of 80 unconstrained optimization test
c problems
c described in:
c
c   N. Andrei, UOP - A collection of 80 unconstrained optimization test
c   problems.
c   Technical Report No. 7/2018, November 17,
c   Research Institute for Informatics, Bucharest, Romania. (2018)
c
c The functions are implemented in Fortran.
c The subroutine CG_VALUE contains the Fortran expressions of the minimizing
c functions.
c The subroutine CG_GRAD contains the Fortran expressions of the gradient of
c the minimizing functions.
c
c The subroutine INIPOINT contains the initial point for starting the
c optimization.
c
c The parameters are defined in the subroutine CG_DESCENT. (See subroutine
c CG_INIT.)
c
c
c
```

```

c Dr. Neculai Andrei
c Center for Advanced Modeling and optimization,
c Academy of Romanian Scientists
c E-mail: nandrei@ici.ro

c-----
      parameter (maxsize = 100000)

      real*8 x (maxsize), d (maxsize), g (maxsize),
&          xtemp (maxsize), gtemp (maxsize), gnorm, f, timp

      real*8 tol

      logical AWolfe,IWolfe,SWolfe

      integer n, status, iter, nfunc, ngrad,ibeta
      integer*4 gh,gm,gs,gc, ght,gmt,gst,gct, timpexp
      integer*2 iyear, imonth, iday
      character*70 numef, fnumef(200)

      external cg_value, cg_grad

c Input file

      open(unit=7,file='fun80.txt',status='old')

c Output files

      open(unit=8,file='fisw.out',status='unknown')
      open(unit=9,file='fisw.rez',status='unknown')

c-----Select the line search procedure

      SWolfe = .true.
      AWolfe = .false.
      IWolfe = .false.

*-----
c
c----- Select beta parameter

c ibeta = 1: Hager and Zhang
c ibeta = 2: Minim DETERMINANT (same as Dai and Kou)
c ibeta = 3: Minim TRACE
c ibeta = 4: Minim measure function FI (Byrd-Nocedal)
c ibeta = 5: Hestenes and Stiefel
c ibeta = 6: Dai and Yuan
c ibeta = 7: Polak, Ribiere and Polyak
c ibeta = 8: Combination trace & log(det)

      ibeta = 8

c----- Range of numerical experiments

      nexpini = 1
      nexptot = 80

c----- Stop rule

c          StopRule = F: |g|_infty <= tol
      tol = 0.000001d0

c-----

```

```

    write(8,90)
90    format(1x,52('*'))
    write(8,91)
91    format(1x,'* FCG - Fast Conjugate Gradient Project      *')
    write(8,92)
92    format(1x,'*                                           *')
    call getdat(iyear, imonth, iday)
    write(8,1) imonth, iday, iyear
1    format(1x,'* Date: Month:',i2,' Day:',i2,' Year: ',i4,15x,'*')

c-----
-
    if(SWolfe) write(8,111)
111    format(1x,'* Standard Wolfe line search              *')
    if(IWolfe) write(8,112)
112    format(1x,'* Improved Wolfe line search              *')
    if(AWolfe) write(8,113)
113    format(1x,'* Approximate Wolfe line search           *')
c-----
--

    if(ibeta .eq. 1) write(8,211)
211    format(1x,'* Hager - Zhang conjugate gradient algorithm *')
    if(ibeta .eq. 2) write(8,212)
212    format(1x,'* MINIM DETERMINANT conjugate gradient algorithm *')
    if(ibeta .eq. 3) write(8,213)
213    format(1x,'* MINIM TRACE conjugate gradient algorithm *')
    if(ibeta .eq. 4) write(8,214)
214    format(1x,'* MINIM FI conjugate gradient algorithm *')
    if(ibeta .eq. 5) write(8,215)
215    format(1x,'* Hestenes-Stiefel conjugate gradient algorithm *')
    if(ibeta .eq. 6) write(8,216)
216    format(1x,'* Dai-Yuan conjugate gradient algorithm *')
    if(ibeta .eq. 7) write(8,217)
217    format(1x,'* Polak-Ribiere-Polyak conjugate gradient algorithm*')
    if(ibeta .eq. 8) write(8,218)
218    format(1x,'* Min TRACE & DET conjugate gradient algorithm *')

    write(8,90)

    do i=1,80
        read(7,21) numef
        fnumef(i)=numef
21    format(a70)
    end do

*----- Start experiments

    do nexp = nexpini, nexptot

        itert = 0
        nfunct= 0
        ngradt= 0
        timp = 0

        numef = fnumef(nexp)

        call printbeta(ibeta, SWolfe,AWolfe,IWolfe, numef,nexp)

    write(8,19)
19    format(9x,'n',5x,'iter',4x,'nfunc',4x,'ngrad',2x,'time(c) ',
*        15x,'f',18x,'gnorm',9x,'s')
    write(8,20)

```

```

20    format(1x,94('-'))

        do  n = 1000, 10000, 1000

c Call INIPOINT    (initial guess)

        call inipoint (n,x, nexp)

c Call CG_DESCENT for optimization

        call gettim(gh,gm,gs,gc)

        call cg_descent (tol, x, n, cg_value, cg_grad,
&                        status, gnorm,
&                        f,iter, nfunc, ngrad, d, g, xtemp, gtemp,
&                        SWolfe,IWolfe,AWolfe,ibeta,nexp)

        call gettim(ght,gmt,gst,gct)
        call exetim(gh,gm,gs,gc, ght,gmt,gst,gct)
*
        timpexp = ght*360000 + gmt*6000 + gst*100 + gct

        itert = itert + iter
        nfunc = nfunc + nfunc
        ngradt = ngradt + ngrad
        timp = timp + float(timpexp)

*----- *.out

        write(8,51) n, iter, nfunc, ngrad, timpexp, f, gnorm,status
51    format(3x,i7,3x,i6,3x,i6,3x,i6,3x,i6,5x,e20.13,2x,e20.13,1x,i1)

        write(*,851) n, iter, nfunc, ngrad, timpexp, f, gnorm
851  format(1x,i6,2x,i4,2x,i5,2x,i5,2x,i5,2x,e20.13,2x,e20.13)

*----- *.rez

        if(n .eq. 1000) then
            write(9,611)nexp, n,iter, nfunc, timpexp,f,gnorm
611    format(i2,i6,2x,i6,2x,i6,2x,i6,2x,e20.13,2x,e20.13)
        else
            write(9,61)      n,iter, nfunc, timpexp,f,gnorm
61    format(2x,i6,2x,i6,2x,i6,2x,i6,2x,e20.13,2x,e20.13)
        end if
*-----

        end do

c----- End do n

        write(8,20)
        write(8,71) itert, nfunc, ngradt, timp/100.d0
        write(*,71) itert, nfunc, ngradt, timp/100.d0
71    format(6x,'TOTAL',2x,i6,3x,i6,3x,i6,2x,f7.2,' (seconds) ')

        end do

c-----End do nexp

        write(9,1)imonth, iday, iyear

        stop
        end

c

```


c ----- Last line Main program

```

*-----
*   Date created       : May 30, 1995
*   Date last modified : May 30, 1995
*
*   Subroutine for execution time computation.
*
*-----
*
*       subroutine exetim(tih,tim,tis,tic,tfh,tfm,tfs,tfc)
*
*           integer*4 tih,tim,tis,tic
*           integer*4 tfh,tfm,tfs,tfc
*
*           integer*4 ti,tf
*           integer*4 ch,cm,cs
*           data ch,cm,cs/360000,6000,100/
*
*           ti=tih*ch+tim*cm+tis*cs+tic
*           tf=tfh*ch+tfm*cm+tfs*cs+tfc
*           tf=tf-ti
*           tfh=tf/ch
*           tf=tf-tfh*ch
*           tfm=tf/cm
*           tf=tf-tfm*cm
*           tfs=tf/cs
*           tfc=tf-tfs*cs
*
*       return
*       end
*----- Last line exetim

```

```

subroutine printbeta(ibeta, SWolfe,AWolfe,IWolfe,numef,nexp)
integer ibeta,nexp
character*70 numef
logical SWolfe, AWolfe, IWolfe

c-----ibeta=1
        if(ibeta .eq. 1) then
            if(SWolfe) then
                write(8,11) nexp, numef
                write(*,11) nexp, numef
11         format(/,2x,i3,2x,'Hager-Zhang. Standard WLS. Function:',a40,/)
            end if
            if(IWolfe) then
                write(8,12) nexp, numef
                write(*,12) nexp, numef
12         format(/,2x,i3,2x,'Hager-Zhang. Improved WLS. Function:',a40,/)
            end if
            if(AWolfe) then
                write(8,13) nexp, numef
                write(*,13) nexp, numef
13         format(/,2x,i3,2x,'Hager-Zhang. Approximate WLS. Function:',a40,/)
            end if
        end if

```

```

c-----ibeta=2
      if(ibeta .eq. 2) then
        if(SWolfe) then
          write(8,21) nexp, numef
          write(*,21) nexp, numef
21      format(/,2x,i3,2x,'min DET. Standard WLS. Function:',a40,/)
        end if
        if(IWolfe) then
          write(8,22) nexp, numef
          write(*,22) nexp, numef
22      format(/,2x,i3,2x,'min DET. Improved WLS. Function:',a40,/)
        end if
        if(AWolfe) then
          write(8,23) nexp, numef
          write(*,23) nexp, numef
23      format(/,2x,i3,2x,'min DET. Approximate WLS. Function:',a40,/)
        end if
      end if

c-----ibeta=3
      if(ibeta .eq. 3) then
        if(SWolfe) then
          write(8,31) nexp, numef
          write(*,31) nexp, numef
31      format(/,2x,i3,2x,'min TRACE. Standard WLS.',
*          ' Function:',a40,/)
        end if
        if(IWolfe) then
          write(8,32) nexp, numef
          write(*,32) nexp, numef
32      format(/,2x,i3,2x,'min TRACE. Improved WLS.',
*          ' Function:',a40,/)
        end if
        if(AWolfe) then
          write(8,33) nexp, numef
          write(*,33) nexp, numef
33      format(/,2x,i3,2x,'min TRACE. Approximate WLS.',
*          ' Function:',a40,/)
        end if
      end if

c-----ibeta=4
      if(ibeta .eq. 4) then
        if(SWolfe) then
          write(8,41) nexp, numef
          write(*,41) nexp, numef
41      format(/,2x,i3,2x,'Min FI (Byrd-Nocedal). Standard WLS.',
*          ' Function:',a40,/)
        end if
        if(IWolfe) then
          write(8,42) nexp, numef
          write(*,42) nexp, numef
42      format(/,2x,i3,2x,'Min FI (Byrd-Nocedal). Improved WLS.',
*          ' Function:',a40,/)
        end if
        if(AWolfe) then
          write(8,43) nexp, numef
          write(*,43) nexp, numef
43      format(/,2x,i3,2x,'Min FI (Byrd-Nocedal). Approximate WLS.',

```

```

*           ' Function:',a40,/)
end if
end if

c-----ibeta=5
if(ibeta .eq. 5) then
if(SWolfe) then
write(8,51) nexp, numef
write(*,51) nexp, numef
51 format(/,2x,i3,2x,'Hestenes-Stiefel. Standard WLS.',
*           ' Function:',a40,/)
end if
if(IWolfe) then
write(8,52) nexp, numef
write(*,52) nexp, numef
52 format(/,2x,i3,2x,'Hestenes-Stiefel. Improved WLS.',
*           ' Function:',a40,/)
end if
if(AWolfe) then
write(8,53) nexp, numef
write(*,53) nexp, numef
53 format(/,2x,i3,2x,'Hestenes-Stiefel. Approximate WLS.',
*           ' Function:',a40,/)
end if
end if

c-----ibeta=6
if(ibeta .eq. 6) then
if(SWolfe) then
write(8,61) nexp, numef
write(*,61) nexp, numef
61 format(/,2x,i3,2x,'Dai-Yuan. Standard WLS.',
*           ' Function:',a40,/)
end if
if(IWolfe) then
write(8,62) nexp, numef
write(*,62) nexp, numef
62 format(/,2x,i3,2x,'Dai-Yuan. Improved WLS.',
*           ' Function:',a40,/)
end if
if(AWolfe) then
write(8,63) nexp, numef
write(*,63) nexp, numef
63 format(/,2x,i3,2x,'Dai-Yuan. Approximate WLS.',
*           ' Function:',a40,/)
end if
end if

c-----ibeta=7
if(ibeta .eq. 7) then
if(SWolfe) then
write(8,71) nexp, numef
write(*,71) nexp, numef
71 format(/,2x,i3,2x,'Polak-Ribiere-Polyak. Standard WLS.',
*           ' Function:',a40,/)
end if
if(IWolfe) then
write(8,72) nexp, numef
write(*,72) nexp, numef
72 format(/,2x,i3,2x,'Polak-Ribiere-Polyak. Improved WLS.',
*           ' Function:',a40,/)

```

```

        end if
        if(AWolfe) then
            write(8,73) nexp, numef
            write(*,73) nexp, numef
73    format(/,2x,i3,2x,'Polak-Ribiere-Polyak. Approximate WLS.',
*        ' Function:',a40,/)
        end if
        end if

c-----ibeta=8
        if(ibeta .eq. 8) then
            if(SWolfe) then
                write(8,81) nexp, numef
                write(*,81) nexp, numef
81    format(/,2x,i3,2x,'TRACE & DETERMINANT (det<1). Standard WLS.',
*        ' Function:',a40,/)
            end if
            if(IWolfe) then
                write(8,82) nexp, numef
                write(*,82) nexp, numef
82    format(/,2x,i3,2x,'TRACE & DETERMINANT (det<1). Improved WLS.',
*        ' Function:',a40,/)
            end if
            if(AWolfe) then
                write(8,83) nexp, numef
                write(*,83) nexp, numef
83    format(/,2x,i3,2x,'TRACE & DETERMINANT (det<1). Approximate WLS.',
*        ' Function:',a40,/)
            end if
            end if

        return
        end

c ----- Last line Printbeta

```

```

c | -----
c | A conjugate gradient method with guaranteed descent
c | January 15, 2004
c | William W. Hager and Hongchao Zhang
c | hager@math.ufl.edu hzhang@math.ufl.edu
c | Department of Mathematics
c | University of Florida
c | Gainesville, Florida 32611 USA
c | 352-392-0281 x 244
c |
c | copyright by William W. Hager
c |
c | http://www.math.ufl.edu/~hager/papers/cg_descent.ps
c | http://www.math.ufl.edu/~hager/papers/cg_compare.ps
c | http://www.math.ufl.edu/~hager/papers/cg_manual.ps
c |
c | INPUT:
c |
c | (double) grad_tol-- StopRule = F: |g|_infty <= grad_tol[default]
c | StopRule = T: |g|_infty <= grad_tol(1+|f|)
c |
c | (double) x --starting guess (length n)
c |

```

```
(int)      dim          --problem dimension (also denoted n)

cg_value--name of cost evaluation subroutine
           (external in main program, cg_value(f, x, n)
           puts value of cost function at x in f
           f is double precision scalar and x is
           double precision array of length n)

cg_grad   --name gradient evaluation subroutine
           (external in main program, cg_grad (g, x, n)
           puts gradient at x in g, g and x are
           double precision arrays of length n)

(double) gnorm    --if the parameter Step in cg.parm is .true.,
                   then gnorm contains the initial step used at
                   iteration 0 in the line search

(double) d        --direction (work array, length n)

(double) g        --gradient (work array, length n)

(double) xtemp    --work array (work array, length n)

(double) gtemp    --work array (work array, length n)

OUTPUT:

(int) status     -- 0 (convergence tolerance satisfied)
                  1 (change in func <= feeps*|f|)
                  2 (total iterations exceeded maxit)
                  3 (slope always negative in line search)
                  4 (number secant iterations exceed nsecant)
                  5 (search direction not a descent direction)
                  6 (line search fails in initial interval)
                  7 (line search fails during bisection)
                  8 (line search fails during interval update)

(double) gnorm    --max abs component of gradient

(double) f        --function value at solution

(double) x        --solution (length n)

(int) iter       --number of iterations

(int) nfunc      --number of function evaluations

(int) ngrad      --number of gradient evaluations

Note: The file cg.parm must be placed in the directory where
the code is run
-----

subroutine cg_descent (grad_tol, x, dim, cg_value, cg_grad,
& status, gnorm, f, iter, nfunc, ngrad,
& d, g, xtemp, gtemp, SWolfe,IWolfe,AWolfe,ibeta,nexp)

double precision x (1), d (1), g (1), xtemp (1), gtemp (1),
& delta, sigma, epsilon, theta, gamma, rho, tol,
& eta, fpert, f0, wolfe_hi, wolfe_lo,
& awolfe hi, QuadCutOff, zero, feeps,
```

```

      subroutine cg_descent (grad_tol, x, dim, cg_value, cg_grad,
&      status, gnorm, f, iter, nfunc, ngrad,
&      d, g, xtemp, gtemp, SWolfe,IWolfe,AWolfe,ibeta,nexp)

      double precision x (1), d (1), g (1), xtemp (1), gtemp (1),
&      delta, sigma, epsilon, theta, gamma, rho, tol,
&      eta, fpert, f0, wolfe_hi, wolfe_lo,
&      awolfe hi, QuadCutOff, zero, feps,

```

```

&          psi0, psi1, psi2,
&          grad_tol, delta2, eta_sq,   gtgprev,z1,z2,
&          f, ftemp, gnorm, xnorm, gnorm2, dnorm2, denom,
&          t, t1, t2, t3, t4, dphi, dphi0, alpha, talpha,
&          yk, yk2, ykgk, dkyk, beta,dkdk,etta, gkgk,tauu,
&          a8, y(100000),trh,deth,bn

      integer      nrestart, nexpand, nsecant, maxit,
&                n, n5, n6, nf, ng, info,
&                iter, status, nfunc, ngrad,ibeta,
&                i, j, i1, i2, i3, i4, dim

      logical QuadOK, QuadStep, PrintLevel, PrintFinal,
&            StopRule, ERule, AWolfe, Step, cg_tol,IWolfe,SWolfe

      external      cg_value, cg_grad

      common /cgparms/delta, sigma, epsilon, theta, gamma, rho, tol,
&            eta, fpert, f0, wolfe_hi, wolfe_lo,
&            awolfe_hi, QuadCutOff, zero, feps,
&            psi0, psi1, psi2,
&            n, n5, n6, nf, ng, info,
&            nrestart, nexpand, nsecant, maxit,
&            QuadStep, PrintLevel, PrintFinal, StopRule,
&            ERule, Step, QuadOK

c initialize the parameters

      call cg_init (grad_tol, dim)

      delta2 = 2*delta - 1
      eta_sq = eta*eta
      iter = 0

      z1 = 1.d0/(float(n)-1.d0)           ! For FI only
      z2 = (float(n)-2.d0)/(float(n)-1.d0) !

c initial function and gradient evaluations, initial direction

      call cg_value (f, x, n, nexp)
      nf = nf + 1
      call cg_grad (g, x, n, nexp)         !g = gradient(x0)  d(0)=-g(0)
      ng = ng + 1
      f0 = f + f
      gnorm = zero
      xnorm = zero
      gnorm2 = zero
      do i = 1, n5
         xnorm = dmax1 (xnorm, dabs (x (i)))
         t = g (i)
         d (i) = -t
         gnorm = dmax1 (gnorm, dabs(t))
         gnorm2 = gnorm2 + t*t
      enddo
      do i = n6, n, 5
         xnorm = dmax1 (xnorm, dabs (x (i)))
         t = g (i)
         gnorm = dmax1 (gnorm, dabs (t))
         d (i) = -t
         j = i + 1
         t1 = g (j)

```

```

        d (j) = -t1
        gnorm = dmax1 (gnorm, dabs (t1))
        xnorm = dmax1 (xnorm, dabs (x (j)))
        j = i + 2
        t2 = g (j)
        d (j) = -t2
        gnorm = dmax1 (gnorm, dabs (t2))
        xnorm = dmax1 (xnorm, dabs (x (j)))
        j = i + 3
        t3 = g (j)
        d (j) = -t3
        gnorm = dmax1 (gnorm, dabs (t3))
        xnorm = dmax1 (xnorm, dabs (x (j)))
        j = i + 4
        t4 = g (j)
        d (j) = -t4
        gnorm = dmax1 (gnorm, dabs (t4))
        xnorm = dmax1 (xnorm, dabs (x (j)))
        gnorm2 = gnorm2 + t*t + t1*t1 + t2*t2 + t3*t3 + t4*t4
    enddo

c   gnorm2 = g(k)T*g(k) (=gtg)

    if ( PrintLevel ) then
        write (*, 10) iter, f, gnorm
10      format ('iter: ', i5, ' f= ', e14.6, ' gnorm= ', e14.6)
    endif

    if ( cg_tol (f, gnorm) ) goto 100

    dphi0 = -gnorm2          ! dphi0 = d(0)T*g(0) = g(0)T*g(0)
    if ( Step ) then
        alpha = gnorm
    else
        alpha = psi0*xnorm/gnorm
        if ( xnorm .eq. zero ) then
            if ( f .ne. zero ) then
                alpha = psi0*dabs (f)/gnorm2
            else
                alpha = 1.d0
            endif
        endif
    endif
endif

c start the conjugate gradient iteration

c
c   alpha starts as old step, ends as initial step for next iteration
c   f is function value for alpha = 0
c   QuadOK = .true. means that a quadratic step was taken
c
c=====
c
    do iter = 1, maxit

        etta = 1.d0/float(iter)/float(iter)
c       etta is used in improved Wolfe I

        QuadOK = .false.
        alpha = psi2*alpha

        if ( QuadStep ) then
            if ( f .ne. zero ) then

```

```

        t = dabs ((f-f0)/f)
    else
        t = 1.d0
    endif
    if ( t .gt. QuadCutoff ) then
        talpha = psil*alpha
        call cg_step (xtemp, x, d, talpha)
        call cg_value (ftemp, xtemp, n, nexp)
        nf = nf + 1
        if ( ftemp .lt. f ) then
            denom = 2.0d0*(((ftemp-f)/talpha)-dphi0)
            if ( denom .gt. zero ) then
                QuadOK = .true.
                alpha = -dphi0*talpha/denom
            endif
        endif
    endif
    endif
    f0 = f

    if ( PrintLevel ) then
        write (*, 20) QuadOK, alpha, f0, dphi0
        format ('QuadOK:', l2, ' initial a:',
20      &      e14.6, ' f0:', e14.6, ' dphi', e14.6)
    endif

c Parameters in Wolfe and approximate Wolfe conditions, and in update

    if ( ERule ) then
        fpert = f + epsilon
    else
        fpert = f + epsilon*dabs (f)
    endif

    wolfe_hi = delta*dphi0
    wolfe_lo = sigma*dphi0
    awolfe_hi = delta2*dphi0

    call cg_line (alpha, f, dphi, dphi0, x, xtemp, d, gtemp,
&      cg_value, cg_grad, SWolfe, IWolfe, AWolfe, etta, nexp)

    do i=1,n
        y(i) = gtemp(i) - g(i)
    end do

    gnorm8 = cg_dot(g,g)

c
c -----

        if ( info .gt. 0 ) goto 100

c
c Test for convergence to within machine epsilon
c (set feps to zero to remove this test)
c
        if ( -alpha*dphi0 .le. feps*dabs (f) ) then
            info = 1
            goto 100
        endif

c compute beta, yk2, gnorm, gnorm2, dnorm2, update x and g,

```



```
gtgprev = cg_dot(g,g)      ! For PR only
```

```
c-----
      if ( mod (iter, nrestart) .ne. 0 ) then      ! Powell restart test

        gnorm = zero
        dnorm2 = zero
        yk2 = zero
        ykgk = zero
        do i = 1, n5
          x (i) = xtemp (i)
          t = gtemp (i)
          yk = t - g (i)
          yk2 = yk2 + yk**2
          ykgk = ykgk + yk*t
          g (i) = t
          gnorm = dmax1 (gnorm, dabs (t))
          dnorm2 = dnorm2 + d (i)**2
        enddo
        do i = n6, n, 5
          x (i) = xtemp (i)
          t = gtemp (i)
          yk = t - g (i)
          yk2 = yk2 + yk**2
          ykgk = ykgk + yk*t
          i1 = i + 1
          x (i1) = xtemp (i1)
          t1 = gtemp (i1)
          i2 = i + 2
          x (i2) = xtemp (i2)
          t2 = gtemp (i2)
          i3 = i + 3
          x (i3) = xtemp (i3)
          t3 = gtemp (i3)
          i4 = i + 4
          x (i4) = xtemp (i4)
          t4 = gtemp (i4)
          yk2 = yk2 + (t1-g (i1))**2 + (t2-g (i2))**2
          &          + (t3-g (i3))**2 + (t4-g (i4))**2
          ykgk = ykgk + (t1-g (i1))*t1 + (t2-g (i2))*t2
          &          + (t3-g (i3))*t3 + (t4-g (i4))*t4
          g (i) = t
          gnorm = dmax1 (gnorm, dabs (t))
          g (i1) = t1
          gnorm = dmax1 (gnorm, dabs (t1))
          g (i2) = t2
          gnorm = dmax1 (gnorm, dabs (t2))
          g (i3) = t3
          gnorm = dmax1 (gnorm, dabs (t3))
          g (i4) = t4
          gnorm = dmax1 (gnorm, dabs (t4))
          dnorm2 = dnorm2 + d (i)**2 + d (i1)**2 + d (i2)**2
          &          + d (i3)**2 + d (i4)**2
        enddo

        if ( cg_tol (f, gnorm) ) goto 100
        dkyk = dphi - dphi0
```

```
*
*                                     *
*                                     ***
*                                     *****
*                                     ***
*                                     *
*
C                                     BETA computation:
C                                     =====
C
C HAGER - ZHANG
      if (ibeta .eq. 1) then
        beta = (ykgk - 2.d0*dphi*yk2/dkyk)/dkyk
        beta = dmax1(beta,
          &           -1.d0/dsqrt(dmin1(eta_sq, gnorm2)*dnorm2))
      end if
C-----

c Minim DETERMINANT (same as CGOPT by Dai and Kou)
      if (ibeta .eq. 2) then
        dkdk = cg_dot(d,d)
        tauu = dkyk/dkdk
        beta = ykgk/dkyk - (tauu+yk2/dkyk-dkyk/dkdk)*dphi/dkyk
        beta = dmax1(beta , 0.5d0*dphi/dkdk)
      end if
C-----

c Minim TRACE
      if (ibeta .eq. 3) then
        dkdk = cg_dot(d,d)
        a8 = (yk2*dkdk)/(dkyk*dkyk)
        tauu = (2.d0 - a8)*dkyk/dkdk                                ! minTR
        beta = ykgk/dkyk - tauu*dphi/dkyk -
          &       yk2*dphi/(dkyk*dkyk) + dphi/dkdk
        beta = dmax1(beta , 0.5d0*dphi/dkdk )
      end if
C-----

c Minim measure function FI (Byrd-Nocedal)
      if (ibeta .eq. 4) then
        dkdk = cg_dot(d,d)
        a8 = (yk2*dkdk)/(dkyk*dkyk)
        tauu = z2 + z1*a8
        beta = ykgk/dkyk - tauu*dphi/dkyk -
          &       yk2*dphi/(dkyk*dkyk) + dphi/dkdk
        beta = dmax1(beta , 0.5d0*dphi/dkdk )
      end if
C-----

c HESTENES-STIEFEL
      if (ibeta .eq. 5) then
        beta = ykgk/dkyk
        beta = dmax1(0.d0 , beta)
      end if
```

```

c-----
c  DAI-YUAN
      if(ibeta .eq. 6) then
            gkgk = cg_dot(g,g)
            beta = gkgk/dkyk
            beta = dmax1(beta , 0.d0)
      end if
c-----

c  POLAK-RIBIERE-POLYAK
      if(ibeta .eq. 7) then
            beta = ykgk/gtgprev
            beta = dmax1(beta , 0.d0)
      end if
c-----

c  Minim TRACE & LOG(DET)
      if (ibeta .eq. 8) then
            dkdk = cg_dot(d,d)
            a8 = (yk2*dkdk)/(dkyk*dkyk)
            tauu = z2 + z1*a8

c  Compute log(Det)

            deth = dkdk/( dkyk*(tauu**(n-1)) )
            if(deth .le. 1.d0) then
                  tauu = dkyk/dkdk                                ! min DET
c                  tauu = (2.d0 - a8)*dkyk/dkdk                    ! min TRACE

            beta = ykgk/dkyk - tauu*dphi/dkyk -
&              yk2*dphi/(dkyk*dkyk) + dphi/dkdk
            beta = dmax1( beta , 0.5d0*dphi/dkdk )
            else
                  tauu = z2 + z1*a8                                ! min fi (Byrd-Nocedal)
&              beta = ykgk/dkyk - tauu*dphi/dkyk -
                  yk2*dphi/(dkyk*dkyk) + dphi/dkdk
            beta = dmax1( beta , 0.5d0*dphi/dkdk )
            end if

            if(beta .lt. 0.d0) then
                  beta = 0.d0
            end if

      end if
c-----
c                  End BETA computation
c                  =====

c  update search direction: (Normal direction)

      gnorm2 = zero

      do i = 1, n5
            t = g (i)
            d (i) = -t + beta*d (i)
            gnorm2 = gnorm2 + t*t
      enddo

```

```

do i = n6, n, 5
  d (i) = -g (i) + beta*d (i)
  i1 = i + 1
  d (i1) = -g (i1) + beta*d (i1)
  i2 = i + 2
  d (i2) = -g (i2) + beta*d (i2)
  i3 = i + 3
  d (i3) = -g (i3) + beta*d (i3)
  i4 = i + 4
  d (i4) = -g (i4) + beta*d (i4)

  gnorm2 = gnorm2 + g (i)**2 + g (i1)**2 + g (i2)**2
&      + g (i3)**2 + g (i4)**2
enddo

dphi0 = -gnorm2 + beta*dphi

else

c   search direction d = -g (Restart)

  if ( PrintLevel ) then
    write (*, *) "RESTART CG"
  endif
  gnorm = zero
  gnorm2 = zero
  do i = 1, n5
    x (i) = xtemp (i)
    t = gtemp (i)
    g (i) = t
    d (i) = -t
    gnorm = dmax1 (gnorm, dabs(t))
    gnorm2 = gnorm2 + t*t
  enddo
  do i = n6, n, 5
    x (i) = xtemp (i)
    t = gtemp (i)
    g (i) = t
    d (i) = -t
    gnorm = dmax1 (gnorm, dabs(t))
    j = i + 1
    x (j) = xtemp (j)
    t1 = gtemp (j)
    g (j) = t1
    d (j) = -t1
    gnorm = dmax1 (gnorm, dabs(t1))
    j = i + 2
    x (j) = xtemp (j)
    t2 = gtemp (j)
    g (j) = t2
    d (j) = -t2
    gnorm = dmax1 (gnorm, dabs(t2))
    j = i + 3
    x (j) = xtemp (j)
    t3 = gtemp (j)
    g (j) = t3
    d (j) = -t3
    gnorm = dmax1 (gnorm, dabs(t3))
    j = i + 4
    x (j) = xtemp (j)
    t4 = gtemp (j)
    g (j) = t4
    d (j) = -t4

```

```

        gnorm = dmax1 (gnorm, dabs(t4))
        gnorm2 = gnorm2 + t*t + t1*t1 + t2*t2 + t3*t3 + t4*t4
    enddo
    if ( cg_tol (f, gnorm) ) goto 100
    dphi0 = -gnorm2
endif
if ( PrintLevel ) then
    write (*, 10) iter, f, gnorm
endif
if ( dphi0 .gt. zero ) then
    info = 5
    goto 100
endif
enddo
c***

100    info = 2
    nfunc = nf
    ngrad = ng
    status = info
    if ( info .gt. 2 ) then
        gnorm = zero
        do i = 1, n
            x (i) = xtemp (i)
            g (i) = gtemp (i)
            gnorm = dmax1 (gnorm, dabs(g (i)))
        enddo
    endif
    if ( PrintFinal ) then
        write (6, *)
        &    'nexp=', nexp, ' n=', n, ' Termination status:', status
        if ( status .eq. 0 ) then
            write (6, 200)
        else if ( status .eq. 1 ) then
            write (6, 210)
        else if ( status .eq. 2 ) then
            write (6, 220) maxit
            write (6, 300)
            write (6, 400) grad_tol
        else if ( status .eq. 3 ) then
            write (6, 230)
            write (6, 300)
            write (6, 430)
            write (6, 410)
        else if ( status .eq. 4 ) then
            write (6, 240)
            write (6, 400) grad_tol
        else if ( status .eq. 5 ) then
            write (6, 250)
        else if ( status .eq. 6 ) then
            write (6, 260)
            write (6, 300)
            write (6, 400) grad_tol
            write (6, 410)
            write (6, 420)
        else if ( status .eq. 7 ) then
            write (6, 260)
            write (6, 400) grad_tol
        else if ( status .eq. 8 ) then
            write (6, 260)
            write (6, 300)
            write (6, 400) grad_tol
            write (6, 410)

```

```

        write (6, 420)
    endif
    write (6, 500) gnorm
    write (6, *) 'function value:', f
    write (6, *) 'cg iterations:', iter
    write (6, *) 'function evaluations:', nfunc
    write (6, *) 'gradient evaluations:', ngrad
    endif
    return
200 format (' Convergence tolerance for gradient satisfied')
210 format (' Terminating since change in function value <= feps*|f|')
220 format (' Total number of iterations exceed max allow:', i10)
230 format (' Slope always negative in line search')
240 format (' Line search fails, too many secant steps')
250 format (' Search direction not a descent direction')
260 format (' Line search fails')
300 format (' Possible causes of this error message:')
400 format (' - your tolerance (grad_tol = ', d10.4,
&      ' ) is too strict')
410 format (' - your gradient routine has an error')
420 format (' - the parameter epsilon in cg.parm is too small')
430 format (' - your cost function has an error')
500 format (' absolute largest component of gradient: ', d10.4)
    end

c    PARAMETERS:
c
c    delta - range (0, .5), used in the Wolfe conditions
c    sigma - range [delta, 1), used in the Wolfe conditions
c    epsilon- range [0, infy), determines when to test approximate Wolfe
c    theta - range (0,1), used in interval update rules
c    gamma - range (0,1), determines when to perform bisection step
c    rho - range (1, infy), growth factor when finding initial interval
c    eta - range (0, infy), used in lower bound for beta
c    psi0 - range (0, 1), factor used in very initial starting guess
c    psi1 - range (0, 1), factor previous step multiplied by in QuadStep
c    psi2 - range (1, infy), factor previous step is multiplied by for
startup
c    QuadCutOff - lower bound on rel change in f before QuadStep
c    restart_fac - range (0, infy) restart cg when iter = n*restart
c    maxit_fac - range (0, infy) terminate in maxit = maxit_fac*n iterations
c    feps - stop when -alpha*dphi0 (est. change in value) <= feps*|f|
c            (feps = 0 removes this test, example: feps = eps*1.e-5
c            where eps is machine epsilon)
c    tol - range (0, infy), convergence tolerance
c    nexpand - range [0, infy), number of grow/shrink allowed in bracket
c    nsecant - range [0, infy), maximum number of secant steps
c    QuadStep- .true. (use quadratic step) .false. (no quadratic step)
c    PrintLevel- .false. (no printout) .true. (print intermediate results)
c    PrintFinal- .false. (no printout) .true. (print messages, final error)
c    StopRule - .false. (max abs grad <= tol) .true. (... <= tol*(1+|f|))
c    ERule - .false. (eps_k = epsilon|f|) .true. (eps_k = epsilon)
c    AWolfe - .false. (use standard Wolfe only)
c            - .true. (use approximate + standard Wolfe)
c    Step - .false. (program computing starting step at iteration 0)
c            - .true. (user provides starting step in gnorm argument of
cg_descent
c    info - same as status
c
c    DEFAULT PARAMETER VALUES:
c
c    delta : 0.1
c    sigma : 0.9

```

```

c      epsilon: 1.e-6
c      theta : 0.5
c      gamma : 0.66
c      rho   : 5.0
c      restart: 1.0
c      eta   : 0.01
c      psi0  : 0.01
c      psi1  : 0.1
c      psi2  : 2.0
c      QuadCutoff: 1.d-12
c      tol   : grad_tol
c      maxit : 500*n
c      nrestart: n
c      nexpand: 50
c      nsecant: 50
c      QuadStep: .true.
c      PrintLevel: .false.
c      PrintFinal: .true.
c      StopRule: .false.
c      Step: .false.
c      info  : 0
c      feps  : 0.0
c
c
c      CG_INIT
c-----
c
c      subroutine cg_init (grad_tol, dim)
c
c      double precision delta, sigma, epsilon, theta, gamma, rho, tol,
c      &          eta, fpert, f0, wolfe_hi, wolfe_lo,
c      &          awolfe_hi, QuadCutoff, zero, feps,
c      &          psi0, psi1, psi2,
c      &          grad_tol, restart_fac, maxit_fac
c
c      integer      nrestart, nexpand, nsecant, maxit,
c      &          n, n5, n6, nf, ng, info,
c      &          dim
c
c      logical      QuadOK, QuadStep, PrintLevel, PrintFinal,
c      &          StopRule, ERule, AWolfe, IWolfe, SWolfe, Step
c
c      common /cgparms/delta, sigma, epsilon, theta, gamma, rho, tol,
c      &          eta, fpert, f0, wolfe_hi, wolfe_lo,
c      &          awolfe_hi, QuadCutoff, zero, feps,
c      &          psi0, psi1, psi2,
c      &          n, n5, n6, nf, ng, info,
c      &          nrestart, nexpand, nsecant, maxit,
c      &          QuadStep, PrintLevel, PrintFinal, StopRule,
c      &          ERule, Step, QuadOK
c
c      n = dim
c      tol = grad_tol
c
c      delta = 0.1
c      sigma = 0.9
c      epsilon= 1.e-6
c      theta = 0.5
c      gamma = 0.66
c      rho   = 5.0
c      restart= 1.0
c      restart_fac=1.d0
c      eta   = 0.01

```

```

        psi0 = 0.01
        psi1 = 0.1
        psi2 = 2.0
        QuadCutOff= 1.d-12
        tol = grad_tol
c      maxit = 500*n
        maxit = 2000
        maxit_fac = 15
        nexpanse= 50
        nsecant= 50
        QuadStep= .true.
        PrintLevel= .false.
        PrintFinal= .false.
        StopRule= .false.
        ERule= .false.
        Step= .false.
        feps = 0.0

c
c-----
c
        nrestart = n*restart_fac
c      maxit = n*maxit_fac
        maxit=2000
        zero = 0.d0
        info = 0
        n5 = mod (n, 5)
        n6 = n5 + 1
        nf = 0
        ng = 0
        return
        end

c
c-----
c
c      CG_WOLFE
c-----

c check whether the Wolfe or the approximate Wolfe conditions
c are satisfied

        logical function cg_Wolfe(alpha,f,dphi,SWolfe,IWolfe,AWolfe,etta)

                double precision delta, sigma, epsilon, theta, gamma, rho, tol,
&                eta, fpert, f0, wolfe_hi, wolfe_lo,
&                awolfe_hi, QuadCutOff, zero, feps,
&                psi0, psi1, psi2,
&                alpha, f, dphi, etta

                integer      nrestart, nexpanse, nsecant, maxit,
&                n, n5, n6, nf, ng, info

                logical      QuadOK, QuadStep, PrintLevel, PrintFinal,
&                StopRule, ERule, Step, SWolfe, IWolfe, AWolfe

        common /cgparms/ delta, sigma, epsilon, theta, gamma, rho, tol,
&                eta, fpert, f0, wolfe_hi, wolfe_lo,
&                awolfe_hi, QuadCutOff, zero, feps,
&                psi0, psi1, psi2,
&                n, n5, n6, nf, ng, info,
&                nrestart, nexpanse, nsecant, maxit,
&                QuadStep, PrintLevel, PrintFinal, StopRule,
&                ERule, Step, QuadOK

```



```

        if ( dphi .ge. wolfe_lo ) then

c test original Wolfe conditions

        if(SWolfe) then
            if ( f-f0 .le. alpha*wolfe_hi ) then      ! Wolfe line search
                cg_Wolfe = .true.
                return
            end if
        end if

c test improved Wolfe

        if(IWolfe) then
            if(f-f0 .le. dmin1(epsilon*dabs(wolfe_hi/delta),
&      0.0001d0*alpha*wolfe_hi/delta+etta)) then    ! Improved Wolfe
                cg_Wolfe = .true.
                return
            end if
        end if

c test approximate Wolfe conditions

        if ( AWolfe ) then    ! Approximate Wolfe line search

            if ( (f .le. fpert) .and. (dphi .le. awolfe_hi) ) then
                cg_Wolfe = .true.
                return
            endif
        endif

        cg_Wolfe = .false.

        return
    end

c                                     CG_TOL
c-----

c check for convergence of the cg iterations

    logical function cg_tol (f, gnorm)

    double precision delta, sigma, epsilon, theta, gamma, rho, tol,
&      eta, fpert, f0, wolfe_hi, wolfe_lo,
&      awolfe_hi, QuadCutOff, zero, feps,
&      psi0, psi1, psi2,
&      f, gnorm

    integer          nrestart, nexpand, nsecant, maxit,
&      n, n5, n6, nf, ng, info

    logical          QuadOK, QuadStep, PrintLevel, PrintFinal,
&      StopRule, ERule, AWolfe, Step

    common /cgparms/delta, sigma, epsilon, theta, gamma, rho, tol,
&      eta, fpert, f0, wolfe_hi, wolfe_lo,
&      awolfe_hi, QuadCutOff, zero, feps,
&      psi0, psi1, psi2,

```

```

&          n, n5, n6, nf, ng, info,
&          nrestart, nexpand, nsecant, maxit,
&          QuadStep, PrintLevel, PrintFinal, StopRule,
&          ERule, Step, QuadOK

      if ( StopRule ) then
        if ( gnorm .le. tol*(1.0 + dabs (f)) ) then
          cg_tol = .true.
          return
        endif
      else
        if ( gnorm .le. tol ) then
          cg_tol = .true.
          return
        endif
      endif

      cg_tol = .false.

      return
    end

c ----- CG_DOT -----
c
c compute dot product of x and y

      double precision function cg_dot (x, y)

      double precision delta, sigma, epsilon, theta, gamma, rho, tol,
&          eta, fpert, f0, wolfe_hi, wolfe_lo,
&          awolfe_hi, QuadCutOff, zero, feps,
&          psi0, psil, psi2,
&          x (1), y(1), t

      integer          nrestart, nexpand, nsecant, maxit,
&          n, n5, n6, nf, ng, info, i

      logical          QuadOK, QuadStep, PrintLevel, PrintFinal,
&          StopRule, ERule, AWolfe, Step

      common /cgparms/delta, sigma, epsilon, theta, gamma, rho, tol,
&          eta, fpert, f0, wolfe_hi, wolfe_lo,
&          awolfe_hi, QuadCutOff, zero, feps,
&          psi0, psil, psi2,
&          n, n5, n6, nf, ng, info,
&          nrestart, nexpand, nsecant, maxit,
&          QuadStep, PrintLevel, PrintFinal, StopRule,
&          ERule, Step, QuadOK

      t = zero
      do i = 1, n5
        t = t + x (i)*y (i)
      enddo
      do i = n6, n, 5
        t = t + x (i)*y(i) + x (i+1)*y (i+1) + x (i+2)*y (i+2)
&          + x (i+3)*y (i+3) + x (i+4)*y (i+4)
      enddo
      cg_dot = t
      return
    end

```

```

c                                     CG_STEP
c-----

c
c compute xtemp = x + alpha d
c
      subroutine cg_step (xtemp, x, d, alpha)

      double precision delta, sigma, epsilon, theta, gamma, rho, tol,
&          eta, fpert, f0, wolfe_hi, wolfe_lo,
&          awolfe_hi, QuadCutOff, zero, feps,
&          psi0, psil, psi2,
&          xtemp (1), x (1), d (1), alpha

      integer          nrestart, nexpand, nsecant, maxit,
&          n, n5, n6, nf, ng, info, i, j

      logical          QuadOK, QuadStep, PrintLevel, PrintFinal,
&          StopRule, ERule, AWolfe, Step

      common /cgparms/delta, sigma, epsilon, theta, gamma, rho, tol,
&          eta, fpert, f0, wolfe_hi, wolfe_lo,
&          awolfe_hi, QuadCutOff, zero, feps,
&          psi0, psil, psi2,
&          n, n5, n6, nf, ng, info,
&          nrestart, nexpand, nsecant, maxit,
&          QuadStep, PrintLevel, PrintFinal, StopRule,
&          ERule, Step, QuadOK

      do i = 1, n5
        xtemp (i) = x(i) + alpha*d(i)
      enddo
      do i = n6, n, 5
        xtemp (i) = x (i) + alpha*d (i)
        j = i + 1
        xtemp (j) = x (j) + alpha*d (j)
        j = i + 2
        xtemp (j) = x (j) + alpha*d (j)
        j = i + 3
        xtemp (j) = x (j) + alpha*d (j)
        j = i + 4
        xtemp (j) = x (j) + alpha*d (j)
      enddo

      return
      end

c                                     CG_LINE
c-----

      subroutine cg_line (alpha, phi, dphi, dphi0, x, xtemp, d, gtemp,
&          cg_value, cg_grad, SWolfe, IWolfe, AWolfe, etta, nexp)

      double precision delta, sigma, epsilon, theta, gamma, rho, tol,
&          eta, fpert, f0, wolfe_hi, wolfe_lo,
&          awolfe_hi, QuadCutOff, zero, feps,
&          psi0, psil, psi2,
&          x (1), xtemp (1), d (1), gtemp (1),

```

```

&          a, dphia, b, dphib, alpha, phi, dphi, c,
&          a0, da0, b0, db0, width, fquad, dphi0,
&          cg_dot, etta

      integer          nrestart, nexpand, nsecant, maxit,
&          n, n5, n6, nf, ng, info,
&          ngrow, nshrink, cg_update, iter, flag

      logical          QuadOK, QuadStep, PrintLevel, PrintFinal,
&          StopRule, ERule, Step, cg_Wolfe,
&          SWolfe, IWolfe, AWolfe

      external         cg_value, cg_grad

      common /cgparms/ delta, sigma, epsilon, theta, gamma, rho, tol,
&          eta, fpert, f0, wolfe_hi, wolfe_lo,
&          awolfe_hi, QuadCutOff, zero, feps,
&          psi0, psil, psi2,
&          n, n5, n6, nf, ng, info,
&          nrestart, nexpand, nsecant, maxit,
&          QuadStep, PrintLevel, PrintFinal, StopRule,
&          ERule, Step, QuadOK

      call cg_step (xtemp, x, d, alpha)
      call cg_grad (gtemp, xtemp, n, nexp)
      ng = ng + 1
      dphi = cg_dot (gtemp, d)
c
c Find initial interval [a,b] such that dphia < 0, dphib >= 0,
c   and phia <= phi0 + tolf*dabs (phi0)
c
      a = zero
      dphia = dphi0
      ngrow = 0
      nshrink = 0
      do while ( dphi .lt. zero )
        call cg_value (phi, xtemp, n, nexp)
        nf = nf + 1
c
c if quadstep in effect and quadratic conditions hold, check wolfe condition
c
      if ( QuadOK ) then
        if ( ngrow .eq. 0 ) fquad = dmin1 (phi, f0)
        if ( phi .le. fquad ) then
          if ( PrintLevel ) then
            write (*, 10) alpha, phi, fquad
10          format ('alpha:', e14.6, ' phi:', e14.6,
&          'fquad:', e14.6)
          endif
        if (cg_Wolfe(alpha, phi, dphi, SWolfe, IWolfe, AWolfe, etta)) return
        endif
      endif
      if ( phi .le. fpert ) then
        a = alpha
        dphia = dphi
      else
c
c contraction phase
c
        b = alpha
        do while ( .true. )
          alpha = .5d0*(a+b)
          nshrink = nshrink + 1

```

```

        if ( nshrink .gt. nexpand ) then
            info = 6
            return
        endif
        call cg_step (xtemp, x, d, alpha)
        call cg_grad (gtemp, xtemp, n, nexp)
        ng = ng + 1
        dphi = cg_dot (gtemp, d)
        if ( dphi .ge. zero ) goto 100
        call cg_value (phi, xtemp, n, nexp)
        nf = nf + 1
        if ( PrintLevel ) then
            write (6, 20) a, b, alpha, phi, dphi
20          format ('contract, a:', e14.6,
&                ' b:', e14.6, ' alpha:', e14.6,
&                ' phi:', e14.6, ' dphi:', e14.6)
        endif
        if ( QuadOK .and. (phi .le. fquad) ) then
            if(cg_Wolfe (alpha, phi, dphi,SWolfe,IWolfe,AWolfe,etta)) return
        endif
        if ( phi .le. fpert ) then
            a = alpha
            dphia = dphi
        else
            b = alpha
        endif
        enddo
    endif
c
c expansion phase
c
        ngrow = ngrow + 1
        if ( ngrow .gt. nexpand ) then
            info = 3
            return
        endif
        alpha = rho*alpha
        call cg_step (xtemp, x, d, alpha)
        call cg_grad (gtemp, xtemp, n, nexp)
        ng = ng + 1
        dphi = cg_dot (gtemp, d)
        if ( PrintLevel ) then
            write (*, 30) a, alpha, phi, dphi
30          format ('expand, a:', e14.6, ' alpha:', e14.6,
&                ' phi:', e14.6, ' dphi:', e14.6)
            write (6, *) "expand, alpha:", alpha, "dphi:", dphi
        endif
        enddo
100 continue
        b = alpha
        dphib = dphi
        if ( QuadOK ) then
            call cg_value (phi, xtemp, n, nexp)
            nf = nf + 1
            if ( ngrow + nshrink .eq. 0 ) fquad = dmin1 (phi, f0)
            if ( phi .le. fquad ) then
                if(cg_Wolfe(alpha, phi, dphi,SWolfe,IWolfe,AWolfe,etta)) return
            endif
        endif
        do iter = 1, nsecant
            if ( PrintLevel ) then
                write (*, 40) a, b, dphia, dphib
40              format ('secant, a:', e14.6, ' b:', e14.6,

```

```

&          ' da:', e14.6, ' db:', e14.6)
endif
width = gamma*(b - a)
if ( -dphia .le. dphib ) then
    alpha = a - (a-b)*(dphia/(dphia-dphib))
else
    alpha = b - (a-b)*(dphib/(dphia-dphib))
endif
c = alpha
a0 = a
b0 = b
da0 = dphia
db0 = dphib
flag = cg_update (a, dphia, b, dphib, alpha, phi,
&                dphi, x, xtemp, d, gtemp, cg_value, cg_grad,
&                SWolfe,IWolfe,AWolfe,etta,nexp)
if ( flag .gt. 0 ) then
    return
else if ( flag .eq. 0 ) then
    if ( c .eq. a ) then
        if ( dphi .gt. da0 ) then
            alpha = c - (c-a0)*(dphi/(dphi-da0))
        else
            alpha = a
        endif
    else
        if ( dphi .lt. db0 ) then
            alpha = c - (c-b0)*(dphi/(dphi-db0))
        else
            alpha = b
        endif
    endif
    if ( (alpha .gt. a) .and. (alpha .lt. b) ) then
        if ( PrintLevel ) write (*, *) "2nd secant"
        flag = cg_update (a, dphia, b, dphib, alpha, phi,
&                        dphi, x, xtemp, d, gtemp, cg_value, cg_grad,
&                        SWolfe,IWolfe,AWolfe,etta,nexp)
        if ( flag .gt. 0 ) return
    endif
endif
endif
c
c  bisection iteration
c
    if ( (b-a) .ge. width ) then
        alpha = .5d0*(b+a)
        if ( PrintLevel ) write (*, *) "bisection"
        flag = cg_update (a, dphia, b, dphib, alpha, phi,
&                        dphi, x, xtemp, d, gtemp, cg_value, cg_grad,
&                        SWolfe,IWolfe,AWolfe,etta,nexp)
        if ( flag .gt. 0 ) return
    else
        if ( b .le. a ) then
            info = 7
            return
        endif
    endif
endif
end do
info = 4
return
end

```

c CG_UPDATE

c-----

```

c
c update returns 1 if Wolfe condition is satisfied or too many iterations
c returns 0 if the interval updated successfully
c returns -1 if search done
c
      integer function cg_update (a, dphia, b, dphib, alpha, phi,
&                                dphi, x, xtemp, d, gtemp, cg_value, cg_grad,
&                                SWolfe,IWolfe,AWolfe,etta,nexp)

      double precision delta, sigma, epsilon, theta, gamma, rho, tol,
&                                eta, fpert, f0, wolfe_hi, wolfe_lo,
&                                awolfe_hi, QuadCutOff, zero, feps,
&                                psi0, psi1, psi2,
&                                a, dphia, b, dphib, alpha, phi, dphi,
&                                x (1), xtemp (1), d (1), gtemp (1),
&                                cg_dot,etta

      integer                    nrestart, nexpand, nsecant, maxit,
&                                n, n5, n6, nf, ng, info,
&                                nshrink

      logical                    QuadOK, QuadStep, PrintLevel, PrintFinal,
&                                StopRule, ERule, Step, cg_Wolfe,
&                                SWolfe,IWolfe,AWolfe

      external                  cg_value, cg_grad

      common /cgparms/delta, sigma, epsilon, theta, gamma, rho, tol,
&                                eta, fpert, f0, wolfe_hi, wolfe_lo,
&                                awolfe_hi, QuadCutOff, zero, feps,
&                                psi0, psi1, psi2,
&                                n, n5, n6, nf, ng, info,
&                                nrestart, nexpand, nsecant, maxit,
&                                QuadStep, PrintLevel, PrintFinal, StopRule,
&                                ERule, Step, QuadOK

      call cg_step (xtemp, x, d, alpha)
      call cg_value (phi, xtemp, n, nexp)
      nf = nf + 1
      call cg_grad (gtemp, xtemp, n, nexp)
      ng = ng + 1
      dphi = cg_dot (gtemp, d)
      if ( PrintLevel ) then
10         write (*, 10) alpha, phi, dphi
&         format ('update alpha:', e14.6, ' phi:', e14.6,
&                 ' dphi:', e14.6)
      endif
      cg_update = 0
      if(cg_Wolfe (alpha, phi, dphi,SWolfe,IWolfe,AWolfe,etta)) then
        cg_update = 1
        goto 110
      endif
      if ( dphi .ge. zero ) then
        b = alpha
        dphib = dphi
        goto 110
      else
        if ( phi .le. fpert ) then
          a = alpha
          dphia = dphi

```

```

        goto 110
    endif
endif
nshrink = 0
b = alpha
do while ( .true. )
    alpha = .5d0*(a+b)
    nshrink = nshrink + 1
    if ( nshrink .gt. nexpanse ) then
        info = 8
        cg_update = 1
        goto 110
    endif
    call cg_step (xtemp, x, d, alpha)
    call cg_grad (gtemp, xtemp, n, nexpanse)
    ng = ng + 1
    dphi = cg_dot (gtemp, d)
    call cg_value (phi, xtemp, n, nexpanse)
    nf = nf + 1
    if ( PrintLevel ) then
        write (6, 20) a, alpha, phi, dphi
20      format ('contract, a:', e14.6, ' alpha:', e14.6,
&            ' phi:', e14.6, ' dphi:', e14.6)
    endif
    if(cg_Wolfe(alpha, phi, dphi,SWolfe,IWolfe,AWolfe,etta)) then
        cg_update = 1
        goto 110
    endif
    if ( dphi .ge. zero ) then
        b = alpha
        dphib = dphi
        goto 100
    endif
    if ( phi .le. fpert ) then
        if ( PrintLevel ) then
            write (6, *) "update a:", alpha, "dphia:", dphi
        endif
        a = alpha
        dphia = dphi
    else
        b = alpha
    endif
enddo
100  continue
    cg_update = -1
110  continue
    if ( PrintLevel ) then
        write (*, 200) a, b, dphia, dphib, cg_update
200  format ('UP a:', e14.6, ' b:', e14.6,
&        ' da:', e14.6, ' db:', e14.6, ' up:', i2)
    endif
    return
end

c
c*****
c Last Line of CG_DESCENT of Hager and Zhang (modified as above)

```



```

        if(i.le.n) go to 93
        return

4      continue
c
        i=1
        Extended Beale
94      x(i) = 1.d0
        x(i+1)= 0.8d0
        i=i+2
        if(i.le.n) go to 94
        return

5      continue
c
        i=1
        Extended Powell
95      x(i) = 3.d0
        x(i+1)= -1.d0
        x(i+2)= 0.d0
        x(i+3)= 1.d0
        i=i+4
        if(i.le.n) go to 95
        return

6      continue
c
        i=1
        Extended Maratos
96      x(i) = 0.1d0
        x(i+1)= 0.1d0
        i=i+2
        if(i.le.n) go to 96
        return

7      continue
c
        i=1
        Extended Cliff
97      x(i) = 0.001d0
        x(i+1)= -0.001d0
        i=i+2
        if(i.le.n) go to 97
        return

8      continue
c
        i=1
        Extended Wood   WOODS (CUTE)
98      x(i) = -3.d0
        x(i+1)= -1.d0
        x(i+2)= -3.d0
        x(i+3)= -1.d0
        i=i+4
        if(i.le.n) go to 98
        return

9      continue
c
        do i=1,n
            x(i) = 5.001d0
        end do
        return

10     continue
c
        i=1
        Extended Rosenbrock  SROSENBR (CUTE)
910    x(i) = -1.2d0

```

```

        x(i+1)= 1.d0
        i=i+2
        if(i.le.n) go to 910
    return

11    continue
c                                     Generalized Risenbrock GENROSNB (CUTE)
        i=1
911    x(i) = -1.2d0
        x(i+1)= 1.1d0
        i=i+2
        if(i.le.n) go to 911
    return

12    continue
c                                     Extended Himmelblau
        do i=1,n
            x(i) = 1.d0
        end do
    return

13    continue
c                                     HIMMELBG (CUTE)
        do i=1,n
            x(i) = 1.5d0
        end do
    return

14    continue
c                                     HIMMELBH (CUTE)
        do i=1,n
            x(i) = 0.8d0
        end do
    return

15    continue
c                                     Extended Trigonometric ET1
        do i=1,n
            x(i) = 0.2d0
        end do
    return

16    continue
c                                     Extended Trigonometric ET2
        do i=1,n
            x(i) = 0.2d0
        end do
    return

17    continue
c                                     Extended Block Diagonal BD1
        do i=1,n
            x(i) = 1.0d0
        end do
    return

18    continue
c                                     Extended Tridiagonal 1
        do i=1,n
            x(i) = 2.d0
        end do
    return

```

19	continue	
c		Extended Three Expo Terms
	do i=1,n	
	x(i) = 0.1d0	
	end do	
	return	
20	continue	
c		Generalized Tridiagonal 1
	do i=1,n	
	x(i) = 2.d0	
	end do	
	return	
21	continue	
c		Generalized Tridiagonal 2
	do i=1,n	
	x(i) = -1.d0	
	end do	
	return	
22	continue	
c		Tridiagonal Double Bordered TR-DB1
	do i=1,n	
	x(i) = -1.d0	
	end do	
	return	
23	continue	
c		Broyden Pentadiagonal (CUTE)
	do i=1,n	
	x(i) = -1.d0	
	end do	
	return	
24	continue	
c		Extended PSC1
	i=1	
924	x(i) = 3.d0	
	x(i+1)= 0.1d0	
	i=i+2	
	if(i.le.n) go to 924	
	return	
25	continue	
c		Perturbed Quadratic PQ1
	do i=1,n	
	x(i) = 1.d0	
	end do	
	return	
26	continue	
c		Perturbed Quadratic PQ2
	do i=1,n	
	x(i) = 0.5d0	
	end do	
	return	
27	continue	
c		Almost Perturbed Quadratic
	do i=1,n	
	x(i) = 0.5d0	
	end do	
	return	

```

28      continue
c
      do i=1,n
        x(i) = 0.5d0
      end do
      return

29      continue
c
      do i=1,n
        x(i) = float(i)/100.d0
      end do
      return

30      continue
c
      do i=1,n
        x(i) = 1.d0
      end do
      return

31      continue
c
      do i=1,n
        x(i) = 0.5d0
      end do
      return

32      continue
*
      FH1
*      Full Hessian FH1 (Summ of Quadratics, Quadratic inside)
*
      do i=1,n
        x(i) = float(i)/float(n)
      end do
      return

33      continue
*
      FH2
*      Full Hessian FH2 (Quadratic, perturbed with sin/cos)
*
      do i=1,n
        x(i) = 1.d0
      end do
      return

34      continue
*
      FH3
*      Full Hessian FH3 (Quartic, perturbed with sin/cos)
*
      do i=1,n
        x(i) = 1.d0
      end do
      return

35      continue
c
      do i=1,n
        x(i) = 0.001d0
      end do
      return

```

```

end do
return

36  continue
c                                     D-DBAUP3
*                               Diagonal Double Bordered Arrow Up
    i=1
936  x(i) = 0.4d0
    x(i+1)= 1.0d0
    i=i+2
    if(i.le.n) go to 936
return

37  continue
c                                     QP1 Extended Quadratic Penalty
    do i=1,n
        x(i) = 1.d0
    end do
return

38  continue
c                                     QP2 Extended Quadratic Penalty
    do i=1,n
        x(i) = 2.d0
    end do
return

39  continue
c                                     QP3 Extended Quadratic Penalty
    do i=1,n
        x(i) = 1.d0
    end do
return

40  continue
c                                     STAIRCASE S1
    do i=1,n
        x(i) = 1.d0
    end do
return

41  continue
c                                     STAIRCASE S2
    do i=1,n
        x(i) = 1.d0
    end do
return

42  continue
c                                     STAIRCASE S3
    do i=1,n
        x(i) = 2.d0
    end do
return

43  continue
c                                     NONDQUAR
*                               Tridiagonal Double Bordered Arrow-Down
*
    i=1
943  x(i) = 1.d0
    x(i+1)= -1.d0

```

```

        i=i+2
        if(i.le.n) go to 943
    return

44      continue
c
*          TRIDIA
*          Tridiagonal
*
        do i=1,n
            x(i) = 1.d0
        end do
        return

45      continue
c
*          ARWHEAD
*          Diagonal Bouble bordered Arrow Down
*
        do i=1,n
            x(i) = 1.d0
        end do
        return

46      continue
c
*          NONDIA (CUTE)
*          Diagonal Bouble bordered Arrow Up
*
        do i=1,n
            x(i) = -0.01d0
        end do
        return

47      continue
c
*          BDQRTIC (CUTE)
*
        do i=1,n
            x(i) = 1.d0
        end do
        return

48      continue
c
*          DQDRTIC (CUTE)
*
        do i=1,n
            x(i) = 3.d0
        end do
        return

49      continue
c
*          EG2 (CUTE)
*
        do i=1,n
            x(i) = 0.001d0
        end do
        return

50      continue
c
*          EG3
*
        do i=1,n
            x(i) = 0.02d0
        end do
        return

51      continue
c
*          EDENSCH (CUTE)
*
        do i=1,n
            x(i) = 0.d0

```

```

        end do
        return

52    continue
c
        do i=1,n
            x(i) = 0.5d0
        end do
        return

53    continue
c
        do i=1,n
            x(i) = 2.d0
        end do
        return

54    continue
c
        do i=1,n
            x(i) = 1.d0
        end do
        return

55    continue
c
        do i=1,n
            x(i) = 10.d0
        end do
        return

56    continue
c
        do i=1,n
            x(i) = 1.d0
        end do
        return

57    continue
c
        i=1
957    x(i) = 100.d0
        x(i+1)= -100.d0
        i=i+2
        if(i.1e.n) go to 957
        return

58    continue
c
        do i=1,n
            x(i) = 0.00000d0
        end do
        return

59    continue
c
        do i=1,n
            x(i) = -0.1d0
        end do
        return

60    continue
c

```

FLETCHCR (CUTE)

ENGVAL1 (CUTE)

DENSCHNA (CUTE)

DENSCHNB (CUTE)

DENSCHNC (CUTE)

DENSCHNF (CUTE)

SINQUAD (CUTE)

DIXON3DQ (CUTE)

BIGGSB1 (CUTE)


```

do i=1,n
  x(i) = 0.1d0
end do
return

61  continue
c                                     PRODSin (m=n-1)
do i=1,n
  x(i) = 0.000001d0
end do
return

62  continue
c                                     PROD1 (m=n)
do i=1,n
  x(i) = 1.d0
end do
return

63  continue
c                                     PRODCos (m=n-1)
do i=1,n
  x(i) = 0.1d0
end do
x(1)=1.d0
return

64  continue
c                                     PROD2 (m=1)
do i=1,n
  x(i) = 0.00001d0
end do
x(n)=1.d0
return

65  continue
c                                     DIXMAANA (CUTE)
do i=1,n
  x(i) = 2.d0
end do
return

66  continue
c                                     DIXMAANB (CUTE)
do i=1,n
  x(i) = 2.d0
end do
return

67  continue
c                                     DIXMAANC (CUTE)
do i=1,n
  x(i) = 2.d0
end do
return

68  continue
c                                     DIXMAAND (CUTE)
do i=1,n
  x(i) = 2.d0
end do
return

```

```

69      continue
c
          DIXMAANL (CUTE)
      do i=1,n
          x(i) = 1.d0
      end do
      return

70      continue
c
          ARGLINB (m=5)
      i=1
970     x(i) = 0.01d0
          x(i+1)= 0.001d0
          i=i+2
          if(i.le.n) go to 970
      return

71      continue
c
          VARDIM (CUTE)
      do i=1,n
          x(i) = 1.d0-float(i)/float(n)/100000.d0
c
          x(i)=1.d0
      end do
      return

72      continue
c
          DIAG-AUP1
      do i=1,n
          x(i) = 4.d0
      end do
      return

73      continue
c
          ENGVAL8
      do i=1,n
          x(i) = 2.d0
      end do
      return

74      continue
c
          QUARTIC (CUTE)
      do i=1,n
          x(i) = 2.d0
      end do
      return

75      continue
c
          LIARWHD
      do i=1,n
          x(i) = 4.d0
      end do
      return

76      continue
c
          NONSCOMP
      do i=1,n
          x(i) = 3.d0
      end do
      return

77      continue
c
          Linear perturbed

```

```

do i=1,n
  x(i) = 2.d0
end do
return

78  continue
c                                     CUBE
  i=1
978  x(i) = -1.2d0
     x(i+1)= 1.1d0
     i=i+2
     if(i.le.n) go to 978
return

79  continue
c                                     HARKERP
do i=1,n
  x(i) = 2.d0
end do
return

80  continue
c                                     QUARTICM
do i=1,n
  x(i) = 2.d0
end do
return

end
c-----Last line INIPOINT

```

```

*****
*                                     Date created: November 26, 2018.
*
*
*   FUNCTIONS FOR UNCONSTRAINED OPTIMIZATION
*   =====
*
*                                     Dr. Neculai Andrei
*****

```

```

*
  subroutine cg_value(f, x, n, nexp)
    real*8 x(n), f

    real*8 t1,t2,t3,t4, c, d
    real*8 s, temp(1000000), temp1, tsum, sum
    real*8 u(1000000), v(1000000), t(1000000)
    real*8 u1, v1, c1, c2
    real*8 alpha, beta, gamma, delta

    integer k1, k2, k3, k4

*
  go to ( 1, 2, 3, 4, 5, 6, 7, 8, 9,10,
*       11,12,13,14,15,16,17,18,19,20,
*       21,22,23,24,25,26,27,28,29,30,
*       31,32,33,34,35,36,37,38,39,40,
*       41,42,43,44,45,46,47,48,49,50,
*       51,52,53,54,55,56,57,58,59,60,

```

```

*          61,62,63,64,65,66,67,68,69,70,
*          71,72,73,74,75,76,77,78,79,80) nexp

cF1                                FREUROTH (CUTE)
*                                Extended Freudenstein & Roth
*
*                                Initial Point: [0.5, -2, ...,0.5, -2].
*

1  continue
   f = 0.d0

   do i=1,n/2
      t1=-13.d0+x(2*i-1)+5.d0*x(2*i)*x(2*i)-x(2*i)**3-2.d0*x(2*i)
      t2=-29.d0+x(2*i-1)+x(2*i)**3+x(2*i)**2-14.d0*x(2*i)

      f = f + t1*t1 + t2*t2
   end do

   return

cF2                                Extended White & Holst function
*
*                                Initial point: [-1.2, 1, -1.2, 1, ....., -1.2, 1]

2  continue
   c=1.d0

   f=0.d0
   do i=1,n/2
      f = f + c*(x(2*i)-x(2*i-1)**3)**2 + (1.d0-x(2*i-1))**2
   end do
   return

cF3                                TR-WHITEHOLST
*                                Tridiagonal. White-Holst (c=4)
*                                Initial point x =[-1.2, 1, ..., -1.2, 1]
*

3  continue
   c = 4.d0
   f = 0.d0

   do i=1,n-1
      f = f + c*(x(i+1)-x(i)**3)**2 + (1.d0-x(i))**2
   end do
   return

cF4                                Extended Beale Function  BEALE (CUTE)
*
*                                Initial Point: [1, 0.8, ....., 1, 0.8]
*

4  continue

   f=0.d0

   do i=1,n/2
      t1=1.5d0 -x(2*i-1)+x(2*i-1)*x(2*i)
      t2=2.25d0 -x(2*i-1)+x(2*i-1)*x(2*i)*x(2*i)
      t3=2.625d0-x(2*i-1)+x(2*i-1)*x(2*i)*x(2*i)*x(2*i)

      f = f + t1*t1 + t2*t2 + t3*t3
   end do

```

```

end do
return

cF5                                Extended Powell
*
*                                Initial Point: [3, -1, 0, 1, .....].
*
5    continue

    f=0.d0

    do i=1,n/4
        t1= x(4*i-3) + 10.d0*x(4*i-2)
        t2= x(4*i-1) - x(4*i)
        t3= x(4*i-2) - 2.d0*x(4*i-1)
        t4= x(4*i-3) - x(4*i)

        f = f + t1*t1 + 5.d0*t2*t2 + t3**4 + 10.d0*t4**4
    end do
    return

cF6                                Extended Maratos Function
*
*                                Initial Point: [1.1, 0.1, ...,1.1, 0.1].
*
6    continue
    c = 1.d0
    f = 0.d0

    do i=1,n/2
        t1 = x(2*i-1)**2 + x(2*i)**2 - 1.d0

        f = f + (x(2*i-1) + c*t1*t1)
    end do
    return

cF7                                Extended CLIFF (CUTE)
*
*                                Initial Point: [0, -0.1, ....., 0, -0.1].
*
7    continue

    f=0.d0

    do i=1,n/2
        temp1 = (x(2*i-1)-3.d0)/100.d0

        f = f+temp1*temp1-(x(2*i-1)-x(2*i))+dexp(2.d0*(x(2*i-1)-x(2*i)))
    end do
    return

cF8                                Extended Wood Function
*                                WOODS (CUTE)
*
*                                Initial Point: [-3,-1,-3,-1,.....]
8    continue

    f=0.d0

    do i=1,n/4
        f = f + 100.d0*(x(4*i-3)**2-x(4*i-2))**2

```

```

*      +      (x(4*i-3)-1.d0)**2
*      + 90.d0*(x(4*i-1)**2-x(4*i))**2
*      +      (1.d0-x(4*i-1))**2
*      + 10.1d0*(x(4*i-2)-1.d0)**2
*      + 10.1d0*(x(4*i) -1.d0)**2
*      + 19.8d0*(x(4*i-2)-1.d0)*(x(4*i)-1.d0)
end do
return

cF9                      Extended Hiebert Function
*
*                      Initial Point: [0,0,...0].
9      continue

      c1 = 10.d0
      c2 = 500.d0

      f = 0.d0

      do i=1,n/2
        f = f + (x(2*i-1)-c1)**2 + (x(2*i-1)*x(2*i)-c2)**2
      end do
      return

cF10                      SROSENBR (CUTE)
*                      Extended Rosenbrock function
*
* Initial point: [-1.2, 1, -1.2, 1, ....., -1.2, 1]

10     continue
      c=1000.d0

      f=0.d0
      do i=1,n/2
        f = f + c*(x(2*i)-x(2*i-1))**2**2 + (1.d0-x(2*i-1))**2
      end do
      return

cF11                      GENROSNB (CUTE)
*                      Generalized Rosenbrock
*                      Initial Point: [-1.2, 1, ... -1.2, 1]

11     continue

      f = (x(1)-1.d0)**2
      do i=2,n
        f = f + 100.d0*(x(i)-x(i-1))**2**2
      end do
      return

cF12                      HIMMELBC (CUTE)
*                      Extended Himmelblau Function
*
*                      Initial Point: [1, 1, ....., 1]

12     continue

      f=0.d0

```

```

do i=1,n/2
  u1 = x(2*i-1)**2 + x(2*i)      - 11.d0
  v1 = x(2*i-1)      + x(2*i)**2 - 7.d0

  f = f + u1*u1 + v1*v1
end do
return

cF13                                HIMMELBG (CUTE)
*
*                                Initial Point: [1.5,1.5,...,1.5]

13  continue

  f=0.d0
  do i=1,n/2
    f = f + (2.d0*x(2*i-1)**2+3.d0*x(2*i)**2)*
*          (dexp(-x(2*i-1)-x(2*i)))
  end do
  return

cF14                                HIMMELBH (CUTE)
*
*                                Initial Point: [1.5,1.5,...,1.5]

14  continue

  f= 0.d0
  do i=1,n/2
    f=f+(-3.d0*x(2*i-1)-2.d0*x(2*i)+2.d0+x(2*i-1)**3 + x(2*i)**2)
  end do
  return

cF15                                Extended Trigonometric ET1
*
*                                Initial Point: [0.2, 0.2, ...,0.2].

15  continue
  s= float(n)
  do i=1,n
    s = s - dcos(x(i))
  end do

  do i=1,n
    temp(i) = s + float(i)*(1.d0-dcos(x(i))) - dsin(x(i))
  end do

  f = 0.d0
  do i=1,n
    f = f + temp(i)**2
  end do
  return

cF16                                Extended Trigonometric ET2
*
*                                Initial Point: [0.2, 0.2, ...,0.2].

16  continue
  s= float(n)

```

```

do i=1,n
  s = s - dsin(x(i))
end do

do i=1,n
  temp(i) = s + float(i)*(1.d0-dsin(x(i))) - dsin(x(i))
end do

f = 0.d0
do i=1,n
  f = f + temp(i)**2
end do
return

cF17                                Extended Block Diagonal BD1 Function
*
*                                Initial Point: [0.1, 0.1, ..., 0.1].
*
17  continue

f = 0.d0

do i=1,n/2
  t1 = x(2*i-1)**2 + x(2*i)**2 - 2.d0
  t2 = dexp(x(2*i-1)) - x(2*i)

  f = f + t1*t1 + t2*t2
end do
return

cF18                                Extended Tridiagonal-1 Function
*
*                                Initial Point: [2,2,...,2]
*
18  continue

f=0.d0
do i=1,n/2
  u(i) = x(2*i-1) + x(2*i) - 3.d0
  v(i) = x(2*i-1) - x(2*i) + 1.d0
end do
do i=1,n/2
  f = f + u(i)**2 + v(i)**4
end do
return

cF19                                Extended Three Exponential Terms
*
*                                Intial Point: [0.1,0.1,.....,0.1].
*
19  continue
f=0.d0

do i=1,n/2
  t1= x(2*i-1) + 3.d0*x(2*i) - 0.1d0
  t2= x(2*i-1) - 3.d0*x(2*i) - 0.1d0
  t3=-x(2*i-1) - 0.1d0

  f = f + dexp(t1) + dexp(t2) + dexp(t3)
end do
return

```



```

cF20                                Generalized Tridiagonal-1 Function
*
*                                Initial Point: [2,2,...,2]
20  continue

    f=0.d0
    do i=1,n-1
        u(i) = x(i) + x(i+1) - 3.d0
        v(i) = x(i) - x(i+1) + 1.d0
    end do

    do i=1,n-1
        f = f + u(i)**2 + v(i)**4
    end do
    return

cF21                                Generalized Tridiagonal-2
*                                Penta Diagonal
*                                Initial point: [-1, -1, ....., -1., -1]
21  continue
    f = 0.d0
    u(1) = 5.d0*x(1)-3.d0*x(1)**2-x(1)**3-3.d0*x(2)+1.d0

    do i=2,n-1
        u(i)=5.d0*x(i)-3.d0*x(i)**2-x(i)**3-x(i-1)-3.d0*x(i+1)+1.d0
    end do

    u(n)=5.d0*x(n)-3.d0*x(n)**2-x(n)**3-x(n-1)+1.d0

    do i=1,n
        f = f + u(i)**2
        v(i) = 5.d0 -6.d0*x(i) -3.d0*x(i)**2
    end do
    return

cF22                                TR-DB1
*                                Tridiagonal Double Bordered
*                                Initial Point: [-1, -1, ....., -1]
*
22  continue
    f = (x(1)-1.d0)**2

    do i=1,n-1
        temp(i) = x(1) - 0.5d0*x(i)**2 - 0.5d0*x(i+1)**2
        f = f + temp(i)*temp(i)
    end do
    return

cF23                                Broyden Pentadiagonal
*
*                                Initial point x0=[-1., -1., ..., -1.].
*
23  continue
*

    temp(1) = 3.d0*x(1) - 2.d0*x(1)*x(1)
    do i=2,n-1
        temp(i) = 3.d0*x(i)-2.d0*x(i)*x(i)-x(i-1)-2.d0*x(i+1)+1.d0
    end do

```

```

end do

temp(n) = 3.d0*x(n)-2.d0*x(n)*x(n)-x(n-1)+1.d0

f = 0.d0

do i=1,n
    f = f + temp(i)*temp(i)
end do
return

cF24                                Extended PSC1 Function
*
*                                Initial point: [3, 0.1, ..., 3, 0.1]

24    continue

    f = 0.d0
    do i=1,n/2
        f = f + (x(2*i-1)**2 +x(2*i)**2 +x(2*i-1)*x(2*i))**2
*          + (dsin(x(2*i-1)))**2 + (dcos(x(2*i)))**2
    end do
    return

cF25                                Perturbed Quadratic function PQ1
*
*                                Initial Point:  [1, 1, .....,1].
*

25    continue

    temp1 = 0.d0
    do i=1,n
        temp1 = temp1 + x(i)
    end do

    f = temp1*temp1/100.d0

    do i=1,n
        f = f + float(i)*x(i)**2
    end do

    return

cF26                                Perturbed Quadratic function PQ2
*
*                                Initial Point:  [0.5, 0.5, ....., 0.5].
*

26    continue

    temp1 = 0.d0
    do i=1,n
        temp1 = temp1 + float(i)*x(i)
    end do

    f = temp1*temp1

    do i=1,n
        f = f + float(i)*x(i)**2
    end do
    return

```

```

cF27                      Almost Perturbed Quadratic
*
*                      Initial point x0=[0.5, 0.5, ...,0.5].
*
27      continue
*
      f = ((x(1)+x(n))**2)/100.d0

      do i=1,n
        f = f + float(i)*x(i)*x(i)
      end do
      return

cF28                      Almost Perturbed Quartic
*
*                      Initial point x0=[0.5, 0.5, ...,0.5].
*
28      continue
*

      f = ((x(1)+x(n))**2)/100.d0

      do i=1,n
        f = f + float(i)*x(i)**4
      end do
      return

cF29                      Extended Penalty Function  U52 (MatrixRom)
*
*                      Intial Point: [1,2,3,.....,n].
*
29      continue
      temp1=0.d0
      do i=1,n
        temp1 = temp1 + x(i)**2
      end do
*
      f = (temp1 - 0.25d0)**2

      do i=1,n-1
        f = f + (x(i)-1.d0)**2
      end do
      return

cF30                      TR-Summ of quadratics Function
*
*                      Initial Point: [1, 1, ....., 1]
*
30      continue

      c = 100000.d0
      f = 0.d0

      do i=1,n-1
        f = f + x(i)*x(i) + c*(x(i+1)+x(i)*x(i))**2
      end do
      return

```

```

cF31                                Quadratic Diagonal Perturbed Function
*
*                                Initial Point:  [0.5, 0.5, ....., 0.5].
*
31  continue

    temp1 = 0.d0
    do i=1,n
        temp1 = temp1 + x(i)
    end do

    f = temp1*temp1

    do i=1,n
        f = f + (float(i)/100.d0) * x(i)**2
    end do
    return

cF32                                FH1 (m=50)
*                                Full Hessian FH1 (Summ of Quadratics, Quadratic inside)
*
32  continue
    m=50
    f=0.d0

    do i=1,m
        u(i)=0.d0
        do j=1,n
            u(i) = u(i) + float(i)*float(j)*x(j)*x(j)
        end do

        f = f + (u(i)-1.d0)**2
    end do
    return

cF33                                FH2
*                                Full Hessian FH2 (Quadratic, perturbed with sin/cos)
*                                Initial Point:  [1, 1, ....., 1].
*
33  continue
    s = 0.d0
    do i=1,n
        s = s + x(i)
    end do

    f = s*s

    do i=1,n
        f = f + float(i)*(dsin(x(i)) + dcos(x(i)))/1000.d0
    end do
    return

cF34                                FH3
*                                Full Hessian FH3 (Quartic, perturbed with sin/cos)
*                                Initial Point:  [1, 1, ....., 1].
*
34  continue
    s = 0.d0
    do i=1,n

```

```

        s = s + x(i)**2
    end do

    f = s*s

    do i=1,n
        f = f + float(i)*(dsin(x(i)) + dcos(x(i)))/1000.d0
    end do
    return

cF35                                Diagonal Full Bordered
*
*                                Initial point: [0.1, 0.1, ....., 0.1]

35    continue
    f=(x(1)-1.d0)**4 + (x(n)**2-x(1)**2)**2

    do i=1,n-2
        temp(i) = sin(x(i+1)-x(n)) - x(1)**2 - x(i+1)**2
        f = f + temp(i)*temp(i)
    end do
    return

cF36                                D-DBAUP3
*                                Diagonal Double Bordered Arrow Up
*                                Initial point: x0=[4, 0, .....,4,0]
*

36    continue
    f=0.d0

    do i=1,n
        f = f + 4.d0*(x(i)*x(i) - x(1))**2 + (x(i)-1.d0)**2
    end do
    return

cF37                                QP1 Extended Quadratic Penalty
*
*                                Initial Point: [1, 1, .....,1].
*

37    continue

    t1=0.d0
    do i=1,n
        t1 = t1 + x(i)*x(i)
    end do
    t1 = t1 - 0.5d0

    f = 0.d0
    do i=1,n-1
        f = f + (x(i)*x(i) - 2.d0)**2
    end do

    f = f + t1*t1
    return

cF38                                QP2 Extended Quadratic Penalty Function
*
*                                Initial Point: [1, 1, .....,1].
*

```

```

38      continue

      t1=0.d0
      do i=1,n
         t1 = t1 + x(i)*x(i)
      end do
      t1 = t1 - 100.d0

      f = 0.d0
      do i=1,n-1
         f = f + (x(i)*x(i) - dsin(x(i)))**2
      end do

      f = f + t1*t1
      return

cF39                                QP3 Extended Quadratic Penalty
*
*                                Initial Point: [1., 1., ...,1.].

39      continue

      t1=0.d0
      do i=1,n
         t1 = t1 + x(i)*x(i)
      end do
      t1 = t1 - 0.25d0

      f = t1*t1

      do i=1,n-1
         f = f - (x(i)*x(i) - 1.d0)**2
      end do
      return

cF40                                STAIRCASE S1
*
*                                Initial point x0=[1,1,...,1].
*

40      continue

      f=0.d0
      do i=1,n-1
         f = f + (x(i)+x(i+1)-float(i))**2
      end do
      return

cF41                                STAIRCASE S2
*
*                                Initial point x0=[1,1,...,1].
*

41      continue
      f = 0.d0
      do i=2,n
         f = f + (x(i-1)+x(i)-float(i))**2
      end do
      return

cF42                                STAIRCASE S3

```

```

*
*           Initial point x0=[2,2,...,2].
*
42  continue
    f = 0.d0
    do i=2,n
        f = f + (x(i-1)+x(i)+float(i))**2
    end do
    return

cF43           NONDQUAR
*           Tridiagonal Double Bordered Arrow-Down
*
43  continue

    f = (x(1)-x(2))**2 + (x(n-1)+x(n))**2

    do i=1,n-2
        f = f + (x(i)+x(i+1)+x(n))**4
    end do
    return

cF44           TRIDIA (CUTE)
*
*           Initial point x0=[1,1,...,1].
*
44  continue
*
    alpha=5.d0
    beta =1.d0
    gamma=1.d0
    delta=1.d0

    f=gamma*(delta*x(1)-1.d0)**2

    do i=2,n
        f = f + float(i)*(alpha*x(i)-beta*x(i-1))**2
    end do
    return

cF45           ARWHEAD (CUTE)
*
*           Initial point x0=[1,1,...,1].
*
45  continue

    f=0.d0
    do i=1,n-1
        f = f + (-4.d0*x(i)+3.d0) + (x(i)**2+x(n)**2)**2
    end do
    return

cF46           NONDIA (Shanno-78) (CUTE)
*
*           Initial point x0=[-1,-1,...,-1].
*
*
46  continue

```

```

c=100.d0

f=(x(1)-1.d0)**2 + c*(x(1)-x(1)**2)**2

do i=2,n
  f = f + c*(x(1)-x(i)**2)**2
end do
return

cF47                                BDQRTIC (CUTE)
*
*                                Initial point x0=[1.,1.,...,1.].
*
*
47  continue
*
  n4=n-4
  f=0.d0

  do i=1,n4
    temp(i) = x(i)**2 + 2.d0*x(i+1)**2 + 3.d0*x(i+2)**2
    *                                + 4.d0*x(i+3)**2 + 5.d0*x(n)**2
  end do

  do i=1,n4
    f = f + (-4.d0*x(i)+3.d0)**2 + temp(i)**2
  end do
  return

cF48                                DQDRTIC (CUTE)
*
*                                Initial point x0=[3,3,3...,3].
*
*
48  continue

  c=1000.d0
  d=1000.d0

  f=0.d0
  do i=1,n-2
    f = f + (x(i)**2 + c*x(i+1)**2 + d*x(i+2)**2)
  end do
  return

cF49                                EG2 (CUTE)
*
*                                Initial point x0=[1,1,1...,1].
*
*
49  continue

  f=0.5d0*dsin(x(n)*x(n))
  do i=1,n-1
    f = f + dsin(x(1)+x(i)*x(i)-1.d0)
  end do
  return

```



```

cF50                                EG3
*
*                                Initial point x0=[1,1,1...,1].
*
50    continue

    f=0.5d0*dcos(x(n)*x(n))

    do i=1,n-1
        f = f + dcos(x(1)+x(i)*x(i)-1.d0)
    end do
    return

cF51                                EDENSCH Function (CUTE)
*
*                                Initial Point: [0., 0., ..., 0.].
51    continue

    f = 16.d0

    do i=1,n-1
        f = f + (x(i)-2.d0)**4 +
*              (x(i)*x(i+1)-2.d0*x(i+1))**2 +
*              (x(i+1)+1.d0)**2
    end do
    return

cF52                                FLETCHCR (CUTE)
*
*                                Initial Point: [0.5,0.5,...0.5]
52    continue

    f=0.d0
    do i=1,n-1
        f = f + 100.d0*(x(i+1)-x(i)+1.d0-x(i)*x(i))**2
    end do
    return

cF53                                ENGVAL1 (CUTE)
*
*                                Initial point x0=[2.,2.,2...,2.].
*
53    continue

    do i=1,n-1
        t(i) = x(i)*x(i) + x(i+1)*x(i+1)
    end do

    f = 0.d0

    do i=1,n-1
        f = f + t(i)*t(i) + (-4.d0*x(i) + 3.d0)
    end do
    return

cF54                                DENSCHNA (CUTE)
*
*                                Initial point: [8, 8,...,8]

```

```

*
54   continue

      f=0.d0
      do i=1,n/2
        f = f + x(2*i-1)**4 +
*           (x(2*i-1)+x(2*i))**2 +
*           (-1.d0+dexp(x(2*i)))**2
      end do
      return

cF55                                DENSCHNB  (CUTE)
*
*           Initial point: [0.1, 0.1,...,0.1]

55   continue

      f=0.d0
      do i=1,n/2
        f = f + (x(2*i-1)-2.d0)**2 +
*           ((x(2*i-1)-2.d0)**2)*(x(2*i)**2) +
*           (x(2*i)+1.d0)**2
      end do
      return

cF56                                DENSCHNC  (CUTE)
*
*           Initial point: [8, 8,...,8]

56   continue

      f=0.d0
      do i=1,n/2
        f = f + (-2.d0+x(2*i-1)**2+x(2*i)**2)**2 +
*           (-2.d0+dexp(x(2*i-1)-1.d0)+x(2*i)**3)**2
      end do
      return

cF57                                DENSCHNF  (CUTE)
*
*           Initial point: [2,0,2,0,...,2,0]

57   continue

      f=0.d0
      do i=1,n/2
        f=f+(2.d0*(x(2*i-1)+x(2*i))**2+(x(2*i-1)-x(2*i))**2-8.d0)**2+
*           (5.d0*x(2*i-1)**2+(x(2*i)-3.d0)**2-9.d0)**2
      end do
      return

cF58                                SINQUAD  (CUTE)
*
*           Initial Point: [0.1, 0.1, ..., 0.1]

58   continue

      f=(x(1)-1.d0)**4 + (x(n)**2-x(1)**2)**2

```

```

do i=1,n-2
  t(i) = dsin(x(i+1)-x(n)) - x(1)**2 + x(i+1)**2
  f = f + t(i)*t(i)
end do
return

cF59                                DIXON3DQ  (CUTE)
*
*                                Initial Point x0=[-1, -1,..., -1]
*
59  continue

f=(x(1)-2.d0)**2

do i=1,n-1
  f = f + (x(i)-x(i+1))**2
end do

f = f + (x(n)-1.d0)**2
return

cF60                                BIGGSB1  (CUTE)
*
*                                Initial Point: [0., 0., ...,0.]
*
60  continue

f=(x(1)-1.d0)**2 + (1.d0-x(n))**2
do i=2,n
  f = f + (x(i)-x(i-1))**2
end do
return

cF61                                PRODSin  (m=n-1)
*
*                                Initial point x0=[5. 5, 5, 5,...,5].
*
61  continue

m = n-1
t1=0.d0
t2=0.d0

do i=1,m
  t1 = t1 + x(i)*x(i)
end do

do i=1,n
  t2 = t2 + dsin(x(i))
end do

f = t1*t2
return

cF62                                PROD1  (m=n)
*
*                                Initial point x0=[1. 1, 1, 1,...,1].
*
62  continue

```

```

m = n
t1=0.d0
t2=0.d0

do i=1,m
    t1 = t1 + x(i)
end do

do i=1,n
    t2 = t2 + x(i)
end do

f = t1*t2
return

cF63                                PRODcos (m=n-1)
*
*                                Initial point x0=[5. 5, 5, 5,...,5].
*
63    continue

c    m = n-1
    m=n/2
    t1=0.d0
    t2=0.d0

    do i=1,m
        t1 = t1 + x(i)*x(i)
    end do

    do i=1,n
        t2 = t2 + dcos(x(i))
    end do

    f = t1*t2
    return

cF64                                PROD2 (m=1)
*
*                                Initial point x0=[15. 15, 15, 15,...,15].
*
64    continue

    m = 1
    t1=0.d0
    t2=0.d0

    do i=1,m
        t1 = t1 + x(i)**4
    end do

    do i=1,n
        t2 = t2 + float(i)*x(i)
    end do

    f = t1*t2
    return

cF65                                DIXMAANA (CUTE)
*
```

```

*               Initial point x0=[2.,2.,2...,2.].
*               Modified m=n/4
65  continue
*
    alpha = 1.d0
    beta  = 0.d0
    gamma = 0.125d0
    delta = 0.125d0

    k1 = 0
    k2 = 0
    k3 = 0
    k4 = 0

    m = n/4

    f = 1.d0

    do i=1,n
        f = f + alpha * x(i)*x(i)*((float(i)/float(n))**k1)
    end do

    do i=1,n-1
        f = f + beta * x(i)*x(i)*((x(i+1)+x(i+1)*x(i+1))**2) *
*          ((float(i)/float(n))**k2)
    end do

    do i=1,2*m
        f = f + gamma * x(i)*x(i) * (x(i+m)**4) *
*          ((float(i)/float(n))**k3)
    end do

    do i=1,m
        f = f + delta * x(i) * x(i+2*m) *
*          ((float(i)/float(n))**k4)
    end do
    return

```

```

cF66               DIXMAANB (CUTE)
*
*               Initial point x0=[2.,2.,2...,2.].
*               Modified m=n/4
66  continue
*
    alpha = 1.d0
    beta  = 0.0625d0
    gamma = 0.0625d0
    delta = 0.0625d0

    k1 = 0
    k2 = 0
    k3 = 0
    k4 = 1

    m = n/4
    f = 1.d0

    do i=1,n
        f = f + alpha * x(i)*x(i)*((float(i)/float(n))**k1)
    end do

    do i=1,n-1

```

```

      f = f + beta * x(i)*x(i)*((x(i+1)+x(i+1)*x(i+1))**2) *
*      ((float(i)/float(n))**k2)
    end do

    do i=1,2*m
      f = f + gamma * x(i)*x(i) * (x(i+m)**4) *
*      ((float(i)/float(n))**k3)
    end do

    do i=1,m
      f = f + delta * x(i) * x(i+2*m) *
*      ((float(i)/float(n))**k4)
    end do
    return

```

```

cF67                                DIXMAANC (CUTE)
*
*                                Initial point x0=[2.,2.,2...,2.].
*                                Modified m=n/4
67  continue
*
      alpha = 1.d0
      beta  = 0.125d0
      gamma = 0.125d0
      delta = 0.125d0

      k1 = 0
      k2 = 0
      k3 = 0
      k4 = 0

      m = n/4
      f = 1.d0

      do i=1,n
        f = f + alpha * x(i)*x(i)*((float(i)/float(n))**k1)
      end do

      do i=1,n-1
        f = f + beta * x(i)*x(i)*((x(i+1)+x(i+1)*x(i+1))**2) *
*        ((float(i)/float(n))**k2)
      end do

      do i=1,2*m
        f = f + gamma * x(i)*x(i) * (x(i+m)**4) *
*        ((float(i)/float(n))**k3)
      end do

      do i=1,m
        f = f + delta * x(i) * x(i+2*m) *
*        ((float(i)/float(n))**k4)
      end do
    return

```

```

cF68                                DIXMAAND (CUTE)
*
*                                Initial point x0=[2.,2.,2...,2.].
*                                Modified m=n/4
68  continue
*
      alpha = 1.d0
      beta  = 0.26d0

```

```

gamma = 0.26d0
delta = 0.26d0

k1 = 0
k2 = 0
k3 = 0
k4 = 0

m = n/4
f = 1.d0

do i=1,n
  f = f + alpha * x(i)*x(i)*((float(i)/float(n))**k1)
end do

do i=1,n-1
  f = f + beta * x(i)*x(i)*((x(i+1)+x(i+1)*x(i+1))**2) *
* ((float(i)/float(n))**k2)
end do

do i=1,2*m
  f = f + gamma * x(i)*x(i) * (x(i+m)**4) *
* ((float(i)/float(n))**k3)
end do

do i=1,m
  f = f + delta * x(i) * x(i+2*m) *
* ((float(i)/float(n))**k4)
end do
return

```

```

cF69                                DIXMAANL (CUTE)
*
*                                Initial point x0=[2.,2.,2...,2.].
*                                Modified m=n/4
69  continue
*
  alpha = 1.d0
  beta  = 0.26d0
  gamma = 0.26d0
  delta = 0.26d0

  k1 = 2
  k2 = 0
  k3 = 0
  k4 = 2

  m = n/4
  f = 1.d0

  do i=1,n
    f = f + alpha * x(i)*x(i)*((float(i)/float(n))**k1)
  end do

  do i=1,n-1
    f = f + beta * x(i)*x(i)*((x(i+1)+x(i+1)*x(i+1))**2) *
* ((float(i)/float(n))**k2)
  end do

  do i=1,2*m
    f = f + gamma * x(i)*x(i) * (x(i+m)**4) *
* ((float(i)/float(n))**k3)

```

```

end do

do i=1,m
  f = f + delta * x(i) * x(i+2*m) *
*      ((float(i)/float(n))**k4)
end do
return

cF70                                ARGLINB (m=5)
*
*      Initial point x0=[0.01  0.001, .... ,0.01  0.001].
*
*
70  continue

m=5
f=0.d0

do i=1,m
  u(i)=0.d0
  do j=1,n
    u(i) = u(i) + float(i)*float(j)*x(j)
  end do

  f = f + (u(i)-1.d0)**2
end do
return

cF71                                VARDIM (CUTE)
*
*      Initial point x0=[1-1/n, 1-2/n,...,1-n/n.].
*      Modified m=n/4
71  continue

s = float(n)*float(n+1)/2.d0

t1=0.d0
do i=1,n
  t1 = t1 + float(i)*x(i)
end do
t1 = t1-s

f = 0.d0
do i=1,n
  f = f + (x(i)-1.d0)**2
end do

f = f + t1**2 + t1**4
return

cF72                                DIAG-AUP1
*
*      Initial point x0=[4., 4., ....4.].
*
72  continue

```



```

f=0.d0
do i=1,n
  f = f + 4.d0*(x(i)*x(i) - x(1))**2 + (x(i)**2-1.d0)**2
end do
return

cF73                                ENGVAl8
*
*                                Initial point x0=[2., 2., ....2.].
*
73      continue

      f = 0.d0
      do i=1,n-1
        f = f + (x(i)**2+x(i+1)**2)**2 - (7.d0-8.d0*x(i))
      end do
      return

cF74                                QUARTIC    (CUTE)
*
*                                Initial point x0=[2., 2., ....2.].
*
74      continue

      f = 0.d0
      do i=1,n
        f = f + (x(i)-1.d0)**4
      end do
      return

cF75                                LIARWHD    (CUTE)
*
*                                Initial point x0=[4., 4., ....4.].
*
75      continue

      f = 0.d0
      do i=1,n
        f = f + 4.d0*(x(i)**2-x(1))**2 + (x(i)-1.d0)**2
      end do

      return

cF76                                NONSCOMP (CUTE)
*
*                                Initial point x0=[3., 3., ..., 3.].
*
76      continue

      f = (x(1)-1.d0)**2
      do i=2,n
        f = f + 4.d0*(x(i)-x(i-1)**2)**2
      end do
      return

cF77                                Linear Perturbed
*

```

```

*               Initial point x0=[2., ...,2.]
*
77  continue

    f = 0.d0
    do i=1,n
        f = f + float(i)*x(i)**2 + x(i)/100.d0
    end do
    return

cF78               CUBE
*
*               Initial point x0=[-1.2, 1, -1.2, 1.,..., -1.2, 1]
*
78  continue

    f = (x(1)-1.d0)**2
    do i=2,n
        f = f + 100.d0*(x(i)-x(i-1)**3)**2
    end do
    return

cF79               HARKERP
*
*               Initial point x0=[1,2,...,n]
*
79  continue

    s = 0.d0
    do i=1,n
        s = s + x(i)
    end do

    f = s*s
    do i=1,n
        f = f - (x(i) + 0.5d0*x(i)*x(i))
    end do
    return

cF80               QUARTICM
*
*               Initial point x0=[2,2,...,2]
*
80  continue
    f = 0.d0
    do i=1,n
        f = f + (x(i)-float(i))**4
    end do
    return

    end
* -----Last line CG_VALUE

```

```

*****
*                               Date created:  November 26, 2018
*
*                               GRADIENT OF FUNCTIONS
*                               =====
*
*                               Dr. Neculai Andrei
*****
*
  subroutine cg_grad(g, x, n, nexp)
    real*8 x(n), g(n)

    real*8 t1,t2,t3,t4, c, d
    real*8 s, temp(1000000), templ, tsum, sum
    real*8 u(1000000), v(1000000), t(1000000)
    real*8 u1, v1, c1, c2
    real*8 alpha, beta, gamma, delta

    integer k1, k2, k3, k4

*
    go to ( 1, 2, 3, 4, 5, 6, 7, 8, 9,10,
*       11,12,13,14,15,16,17,18,19,20,
*       21,22,23,24,25,26,27,28,29,30,
*       31,32,33,34,35,36,37,38,39,40,
*       41,42,43,44,45,46,47,48,49,50,
*       51,52,53,54,55,56,57,58,59,60,
*       61,62,63,64,65,66,67,68,69,70,
*       71,72,73,74,75,76,77,78,79,80) nexp

cF1                               FREUROTH (CUTE)
*                               Extended Freudenstein & Roth
*
*                               Initial Point: [0.5, -2, ...,0.5, -2].
*
1    continue
    j=1

    do i=1,n/2
      t1=-13.d0+x(2*i-1)+5.d0*x(2*i)*x(2*i)-x(2*i)**3-2.d0*x(2*i)
      t2=-29.d0+x(2*i-1)+x(2*i)**3+x(2*i)**2-14.d0*x(2*i)

      g(j)  =2.d0*(t1+t2)
      g(j+1)=2.d0*t1*(10.d0*x(2*i)-3.d0*x(2*i)*x(2*i)-2.d0) +
*          2.d0*t2*(3.d0*x(2*i)*x(2*i)+2.d0*x(2*i)-14.d0)
      j=j+2
    end do
    return

cF2                               Extended White & Holst function
*
*                               Initial point: [-1.2, 1, -1.2, 1, ....., -1.2, 1]

2    continue
    c=1.d0

    j=1
    do i=1,n/2
      g(j)  = -6.d0*c*x(2*i-1)*x(2*i-1)*(x(2*i)-x(2*i-1)**3) -
*          2.d0*(1.d0-x(2*i-1))

```

```

        g(j+1) = 2.d0*c*(x(2*i)-x(2*i-1)**3)
        j = j + 2
    end do
    return

cF3                                TR-WHITEHOLST
*                                Tridiagonal. White-Holst (c=4)
*                                Initial point x =[-1.2, 1, ..., -1.2, 1]
*
3    continue
    c = 4.d0

    g(1) = -6.d0*c*(x(2)-x(1)**3)*x(1)*x(1) - 2.d0*(1.d0-x(1))

    do i=2,n-1
        g(i) = 2.d0*c*(x(i)-x(i-1)**3) -
*           6.d0*c*(x(i+1)-x(i)**3)*x(i)*x(i) -
*           2.d0*(1.d0-x(i))
    end do

    g(n) = 2.d0*c*(x(n)-x(n-1)**3)
    return

cF4                                Extended Beale Function  BEALE (CUTE)
*
*                                Initial Point: [1, 0.8, ....., 1, 0.8]
*
4    continue
*
    j=1
    do i=1,n/2
        t1=1.5d0 -x(2*i-1)+x(2*i-1)*x(2*i)
        t2=2.25d0 -x(2*i-1)+x(2*i-1)*x(2*i)*x(2*i)
        t3=2.625d0-x(2*i-1)+x(2*i-1)*x(2*i)*x(2*i)*x(2*i)

        g(j) =2.d0*t1*(-1.d0+x(2*i)) +
*           2.d0*t2*(-1.d0+x(2*i)**2) +
*           2.d0*t3*(-1.d0+x(2*i)**3)
        g(j+1)=2.d0*t1*x(2*i-1) +
*           2.d0*t2*2.d0*x(2*i-1)*x(2*i) +
*           2.d0*t3*3.d0*x(2*i-1)*x(2*i)*x(2*i)
        j=j+2
    end do
    return

cF5                                Extended Powell
*
*                                Initial Point: [3, -1, 0, 1, .....].
*
5    continue
    j=1
    do i=1,n/4
        t1= x(4*i-3) + 10.d0*x(4*i-2)
        t2= x(4*i-1) - x(4*i)
        t3= x(4*i-2) - 2.d0*x(4*i-1)
        t4= x(4*i-3) - x(4*i)

        g(j) = 2.d0*t1 + 40.d0*t4**3
        g(j+1)= 20.d0*t1 + 4.d0*t3**3
        g(j+2)= 10.d0*t2 - 8.d0*t3**3

```

```

        g(j+3)= -10.d0*t2 - 40.d0*t4**3

        j=j+4
    end do
    return

cF6                                Extended Maratos Function
*
*                                Initial Point: [1.1, 0.1, ...,1.1, 0.1].
*
6    continue
    c = 1.d0

    j=1
    do i=1,n/2
        t1 = x(2*i-1)**2 + x(2*i)**2 - 1.d0

        g(j)    = 1.d0 + 4.d0 * c * t1 * x(2*i-1)
        g(j+1) =      4.d0 * c * t1 * x(2*i)
        j=j+2
    end do
    return

cF7                                Extended CLIFF (CUTE)
*
*                                Initial Point: [0, -0.1, ....., 0, -0.1].
*
7    continue

    j=1
    do i=1,n/2
        temp1 = (x(2*i-1)-3.d0)/100.d0

        g(j)    = temp1/50.d0 - 1.d0 + 2.d0*dexp(2.d0*(x(2*i-1)-x(2*i)))
        g(j+1) = 1.d0 - 2.d0*dexp(2.d0*(x(2*i-1)-x(2*i)))
        j=j+2
    end do
    return

cF8                                Extended Wood Function
*
*                                WOODS (CUTE)
*
*                                Initial Point: [-3,-1,-3,-1,.....]
8    continue

    j=1
    do i=1,n/4
        g(j)    = 400.d0*(x(4*i-3)**2-x(4*i-2))*x(4*i-3)
        *      + 2.d0*(x(4*i-3)-1.d0)
        g(j+1) = -200.d0*(x(4*i-3)**2-x(4*i-2))
        *      + 20.2d0*(x(4*i-2)-1.d0)
        *      + 19.8d0*(x(4*i)-1.d0)
        g(j+2) = 360.d0*(x(4*i-1)**2-x(4*i))*x(4*i-1)
        *      - 2.d0*(1.d0-x(4*i-1))
        g(j+3) = -180.d0*(x(4*i-1)**2-x(4*i))
        *      + 20.2d0*(x(4*i)-1.d0)
        *      + 19.8d0*(x(4*i-2)-1.d0)
        j=j+4
    end do
    return

```

```

cF9                                     Extended Hiebert Function
*
*                                     Initial Point: [0,0,...0].
9      continue

      c1 = 10.d0
      c2 = 500.d0

      j=1
      do i=1,n/2
        g(j) = 2.d0*(x(2*i-1)-c1)
*      + 2.d0*(x(2*i-1)*x(2*i)-c2)*x(2*i)
        g(j+1) = 2.d0*(x(2*i-1)*x(2*i)-c2)*x(2*i-1)
        j=j+2
      end do
      return

cF10                                     SROSENR (CUTE)
*                                     Extended Rosenbrock function
*
* Initial point: [-1.2, 1, -1.2, 1, ....., -1.2, 1]

10     continue
      c=1000.d0

      j=1
      do i=1,n/2
        g(j) = -4.d0*c*x(2*i-1)*(x(2*i)-x(2*i-1)**2) -
*      2.d0*(1.d0-x(2*i-1))
        g(j+1) = 2.d0*c*(x(2*i)-x(2*i-1)**2)
        j = j + 2
      end do
      return

cF11                                     GENROSNB (CUTE)
*                                     Generalized Rosenbrock
*                                     Initial Point: [-1.2, 1, ... -1.2, 1]

11     continue

      g(1) = 2.d0*(x(1)-1.d0)-400.d0*x(1)*(x(2)-x(1)**2)
      do i=2,n-1
        g(i) = 200.d0*(x(i)-x(i-1)**2)-400.d0*x(i)*(x(i+1)-x(i)**2)
      end do

      g(n) = 200.d0*(x(n)-x(n-1)**2)
      return

cF12                                     HIMMELBC (CUTE)
*                                     Extended Himmelblau Function
*
*                                     Initial Point: [1, 1, ....., 1]

12     continue

      j=1
      do i=1,n/2
        u1 = x(2*i-1)**2 + x(2*i) - 11.d0
        v1 = x(2*i-1) + x(2*i)**2 - 7.d0

```

```

      g(j)    = 4.d0*u1*x(2*i-1) + 2.d0*v1
      g(j+1) = 2.d0*u1          + 4.d0*v1*x(2*i)
      j=j+2
end do
return

```

```

cF13                                HIMMELBG (CUTE)
*
*                                Initial Point: [1.5,1.5,...,1.5]

13  continue

      j=1
      do i=1,n/2
        t1 = 2.d0*x(2*i-1)**2+3.d0*x(2*i)**2
        t2 = dexp(-x(2*i-1)-x(2*i))

        g(j)    = 4.d0*x(2*i-1)*t2 - t1*t2

        g(j+1) = 6.d0*x(2*i)*t2   - t1*t2

        j=j+2
      end do
return

```

```

cF14                                HIMMELBH (CUTE)
*
*                                Initial Point: [1.5,1.5,...,1.5]

14  continue

      j=1
      do i=1,n/2

        g(j)    = -3.d0 + 3.d0*x(2*i-1)**2

        g(j+1) = -2.d0 + 2.d0*x(2*i)

        j=j+2
      end do
return

```

```

cF15                                Extended Trigonometric ET1
*
*                                Initial Point: [0.2, 0.2, ...,0.2].

15  continue
      s= float(n)
      do i=1,n
        s = s - dcos(x(i))
      end do

      do i=1,n
        temp(i) = s + float(i)*(1.d0-dcos(x(i))) - dsin(x(i))
      end do

      s=0.d0
      do i=1,n

```

```

        s = s + temp(i)
    end do

    do i=1,n
        g(i) = 2.d0*s*dsin(x(i)) +
+          2.d0*temp(i)*(float(i)*dsin(x(i))-dcos(x(i)))
    end do
    return

cF16                                Extended Trigonometric ET2
*
*                                Initial Point: [0.2, 0.2, ...,0.2].

16    continue
    s= float(n)
    do i=1,n
        s = s - dsin(x(i))
    end do

    do i=1,n
        temp(i) = s + float(i)*(1.d0-dsin(x(i))) - dsin(x(i))
    end do

    s=0.d0
    do i=1,n
        s = s + temp(i)
    end do

    do i=1,n
        g(i) = -2.d0*s*dcos(x(i)) +
+          2.d0*temp(i)*(-float(i)*dcos(x(i))-dcos(x(i)))
    end do
    return

cF17                                Extended Block Diagonal BD1 Function
*
*                                Initial Point: [0.1, 0.1, ..., 0.1].
*

17    continue

    j=1
    do i=1,n/2
        t1 = x(2*i-1)**2 + x(2*i)**2 - 2.d0
        t2 = dexp(x(2*i-1)) - x(2*i)

        g(j)  = 4.d0*t1*x(2*i-1) + 2.d0*t2*dexp(x(2*i-1))
        g(j+1) = 4.d0*t1*x(2*i) - 2.d0*t2
        j=j+2
    end do
    return

cF18                                Extended Tridiagonal-1 Function
*
*                                Initial Point: [2,2,...,2]

18    continue

    do i=1,n/2
        u(i) = x(2*i-1) + x(2*i) - 3.d0
        v(i) = x(2*i-1) - x(2*i) + 1.d0
    end do

```



```

j=1
do i=1,n/2
  g(j) = 2.d0*u(i) + 4.d0*v(i)**3
  g(j+1) = 2.d0*u(i) - 4.d0*v(i)**3
  j=j+2
end do
return

cF19                                Extended Three Exponential Terms
*
*                                Initial Point: [0.1,0.1,.....,0.1].
*
19  continue

j=1
do i=1,n/2
  t1= x(2*i-1) + 3.d0*x(2*i) - 0.1d0
  t2= x(2*i-1) - 3.d0*x(2*i) - 0.1d0
  t3=-x(2*i-1) - 0.1d0

  g(j) = dexp(t1) + dexp(t2) - dexp(t3)
  g(j+1) = 3.d0*dexp(t1) - 3.d0*dexp(t2)
  j=j+2
end do
return

cF20                                Generalized Tridiagonal-1 Function
*
*                                Initial Point: [2,2,...,2]
20  continue

do i=1,n-1
  u(i) = x(i) + x(i+1) - 3.d0
  v(i) = x(i) - x(i+1) + 1.d0
end do

g(1) = 2.d0*u(1) + 4.d0*v(1)**3

do i=2,n-1
  g(i) = 2.d0*u(i-1) - 4.d0*v(i-1)**3 + 2.d0*u(i) + 4.d0*v(i)**3
end do

g(n) = 2.d0*u(n-1) - 4.d0*v(n-1)**3
return

cF21                                Generalized Tridiagonal-2
*                                Penta Diagonal
*                                Initial point: [-1, -1, ....., -1., -1]
21  continue
u(1) = 5.d0*x(1)-3.d0*x(1)**2-x(1)**3-3.d0*x(2)+1.d0

do i=2,n-1
  u(i)=5.d0*x(i)-3.d0*x(i)**2-x(i)**3-x(i-1)-3.d0*x(i+1)+1.d0
end do

u(n)=5.d0*x(n)-3.d0*x(n)**2-x(n)**3-x(n-1)+1.d0
*

```

```

do i=1,n
  v(i) = 5.d0 -6.d0*x(i) -3.d0*x(i)**2
end do
*
g(1) = 2.d0*u(1)*v(1) - 2.d0*u(2)

do i=2,n-1
  g(i) = -6.d0*u(i-1) + 2.d0*u(i)*v(i) - 2.d0*u(i+1)
end do

g(n) = -6.d0*u(n-1) + 2.d0*u(n)*v(n)
return

cF22                                TR-DB1
*                                Tridiagonal Double Bordered
*                                Initial Point: [-1, -1, ..., -1]
*
22  continue

do i=1,n-1
  temp(i) = x(1) - 0.5d0*x(i)**2 - 0.5d0*x(i+1)**2
end do
*--
g(1) = 2.d0*(x(1)-1.d0) + 2.d0*temp(1)*(1.d0-x(1))

do i=2,n-1
  g(1) = g(1) + 2.d0*temp(i)
end do

do i=2,n-1
  g(i) = -2.d0*x(i)*(temp(i-1) + temp(i))
end do

g(n) = -2.d0*x(n)*temp(n-1)
return

cF23                                Broyden Pentadiagonal
*
*                                Initial point x0=[-1., -1., ..., -1.].
*
23  continue
*

temp(1) = 3.d0*x(1) - 2.d0*x(1)*x(1)
do i=2,n-1
  temp(i) = 3.d0*x(i)-2.d0*x(i)*x(i)-x(i-1)-2.d0*x(i+1)+1.d0
end do

temp(n) = 3.d0*x(n)-2.d0*x(n)*x(n)-x(n-1)+1.d0

g(1) = 2.d0*temp(1)*(3.d0-4.d0*x(1)) - 2.d0*temp(2)

g(2) = 2.d0*temp(2)*(3.d0-4.d0*x(2)) - 2.d0*temp(3)

do i=3,n-1
  g(i) = -4.d0*temp(i-1)
*      +2.d0*temp(i)*(3.d0-4.d0*x(i))
*      -2.d0*temp(i+1)
end do

```

```

g(n) = -4.d0*temp(n-1) + 2.d0*temp(n)*(3.d0-4.d0*x(n))
return

cF24                                Extended PSC1 Function
*
*                                Initial point: [3, 0.1, ..., 3, 0.1]

24  continue

    j=1
    do i=1,n/2
      g(j) = 2.d0*(x(2*i-1)**2+x(2*i)**2+x(2*i-1)*x(2*i)) *
+          (2.d0*x(2*i-1)+x(2*i)) +
+          2.d0*(dsin(x(2*i-1)))*(dcos(x(2*i-1)))

      g(j+1) = 2.d0*(x(2*i-1)**2+x(2*i)**2+x(2*i-1)*x(2*i)) *
+          (2.d0*x(2*i)+x(2*i-1)) -
+          2.d0*(dcos(x(2*i)))*(dsin(x(2*i)))
      j=j+2
    end do
    return

cF25                                Perturbed Quadratic function PQ1
*
*                                Initial Point:  [1, 1, .....,1].
*

25  continue

    temp1 = 0.d0
    do i=1,n
      temp1 = temp1 + x(i)
    end do

    do i=1,n
      g(i) = float(i) * 2.d0 * x(i) + temp1/50.d0
    end do
    return

cF26                                Perturbed Quadratic function PQ2
*
*                                Initial Point:  [0.5, 0.5, ....., 0.5].
*

26  continue

    temp1 = 0.d0
    do i=1,n
      temp1 = temp1 + float(i)*x(i)
    end do

    do i=1,n
      g(i) = float(i)*2.d0*x(i) + 2.d0*temp1*float(i)
    end do
    return

cF27                                Almost Perturbed Quadratic
*
*                                Initial point x0=[0.5, 0.5, ...,0.5].
*

27  continue

```

```

*
g(1) = 2.d0*x(1) + (x(1)+x(n))/50.d0

do i=2,n-1
  g(i) = 2.d0*float(i)*x(i)
end do

g(n) = 2.d0*float(n)*x(n) + (x(1)+x(n))/50.d0
return

cF28                      Almost Perturbed Quartic
*
*                      Initial point x0=[0.5, 0.5, ...,0.5].
*
28  continue
*
g(1) = 4.d0*x(1)**3 + (x(1)+x(n))/50.d0

do i=2,n-1
  g(i) = 4.d0*float(i)*x(i)**3
end do

g(n) = 4.d0*float(n)*x(n)**3 + (x(1)+x(n))/50.d0
return

cF29                      Extended Penalty Function  U52 (MatrixRom)
*
*                      Intial Point: [1,2,3,.....,n].
*
29  continue
temp1=0.d0
do i=1,n
  temp1 = temp1 + x(i)**2
end do

do i=1,n-1
  g(i) = 2.d0*(x(i)-1.d0) + 4.d0*x(i)*(temp1-0.25d0)
end do

g(n) = 4.d0*x(n)*(temp1-0.25d0)
return

cF30                      TR-Summ of quadratics Function
*
*                      Initial Point: [1, 1, ....., 1]
*
30  continue

c = 100000.d0

g(1) = 2.d0*x(1) + 4.d0*c*(x(2)+x(1)*x(1))*x(1)

do i=2,n-1
  g(i) = 2.d0*c*(x(i)+x(i-1)**2) + 2.d0*x(i) +
*      4.d0*c*(x(i+1)+x(i)*x(i))*x(i)
end do

g(n) = 2.d0*c*(x(n)+x(n-1)**2)
return

```

```

cF31                                Quadratic Diagonal Perturbed Function
*
*                                Initial Point:  [0.5, 0.5, ....., 0.5].
*
31  continue

    temp1 = 0.d0
    do i=1,n
        temp1 = temp1 + x(i)
    end do

    do i=1,n
        g(i) = float(i) * x(i) / 50.d0 + 2.d0*temp1
    end do
    return

cF32                                FH1 (m=50)
*                                Full Hessian FH1 (Summ of Quadratics, Quadratic inside)
*
32  continue
    m=50

    do i=1,m
        u(i)=0.d0
        do j=1,n
            u(i) = u(i) + float(i)*float(j)*x(j)*x(j)
        end do
    end do

*--
    do j=1,n
        g(j) = 0.d0
        do i=1,m
            g(j) = g(j) + 4.d0*(u(i)-1.d0)*float(i)*float(j)*x(j)
        end do
    end do
    return

cF33                                FH2
*                                Full Hessian FH2 (Quadratic, perturbed with sin/cos)
*                                Initial Point:  [1, 1, ....., 1].
*
33  continue
    s = 0.d0
    do i=1,n
        s = s + x(i)
    end do

    do i=1,n
        g(i) = 2.d0*s + float(i)*(dcos(x(i)) - dsin(x(i)))/1000.d0
    end do
    return

cF34                                FH3
*                                Full Hessian FH3 (Quartic, perturbed with sin/cos)
*                                Initial Point:  [1, 1, ....., 1].
*
34  continue
    s = 0.d0
    do i=1,n

```

```

        s = s + x(i)**2
    end do

    do i=1,n
        g(i) = 4.d0*s*x(i) + float(i)*(dcos(x(i)) - dsin(x(i)))/1000.d0
    end do
    return

cF35                                Diagonal Full Bordered
*
*                                Initial point: [0.1, 0.1, ....., 0.1]

35    continue

    do i=1,n-2
        temp(i) = sin(x(i+1)-x(n)) - x(1)**2 - x(i+1)**2
    end do
*--
    g(1) = 4.d0*(x(1)-1.d0)**3 - 4.d0*x(1)*(x(n)**2-x(1)**2)
    do i=1,n-2
        g(1) = g(1) - 4.d0*temp(i)*x(1)
    end do

    do i=2,n-1
        g(i) = 2.d0*temp(i-1)*(cos(x(i)-x(n))-2.d0*x(i))
    end do

    g(n) = 4.d0*x(n)*(x(n)**2-x(1)**2)
    do i=1,n-2
        g(n) = g(n) - 2.d0*temp(i)*cos(x(i+1)-x(n))
    end do
    return

cF36                                D-DBAUP3
*                                Diagonal Double Bordered Arrow Up
*                                Initial point: x0=[4, 0, .....,4,0]
*
36    continue

    g(1) = 2.d0*(x(1)-1.d0) + 8.d0*(x(1)*x(1)-x(1))*(2.d0*x(1)-1.d0)
    do i=2,n
        g(1) = g(1) - 8.d0*(x(i)*x(i)-x(1))
    end do

    do i=2,n
        g(i) = 16.d0*x(i)*(x(i)*x(i)-x(1)) + 2.d0*(x(i)-1.d0)
    end do
    return

cF37                                QP1 Extended Quadratic Penalty
*
*                                Initial Point: [1, 1, .....,1].
*
37    continue

    t1=0.d0
    do i=1,n
        t1 = t1 + x(i)*x(i)
    end do
    t1 = t1 - 0.5d0

```

```

do i=1,n-1
  g(i) = 4.d0*(x(i)*x(i)-2.d0)*x(i) + 4.d0*t1*x(i)
end do

g(n) = 4.d0*t1*x(n)
return

cF38                                QP2 Extended Quadratic Penalty Function
*
*                                Initial Point: [1, 1, .....,1].
*
38  continue

t1=0.d0
do i=1,n
  t1 = t1 + x(i)*x(i)
end do
t1 = t1 - 100.d0

do i=1,n-1
  g(i) = 2.d0*(x(i)*x(i)-dsin(x(i)))*(2.d0*x(i)-dcos(x(i)))
*      + 4.d0*t1*x(i)
end do

g(n) = 4.d0*t1*x(n)
return

cF39                                QP3 Extended Quadratic Penalty
*
*                                Initial Point: [1., 1., .....,1.].

39  continue

t1=0.d0
do i=1,n
  t1 = t1 + x(i)*x(i)
end do
t1 = t1 - 0.25d0

do i=1,n-1
  g(i) = -4.d0*(x(i)*x(i)-1.d0)*x(i) + 4.d0*t1*x(i)
end do

g(n) = 4.d0*t1*x(n)
return

cF40                                STAIRCASE S1
*
*                                Initial point x0=[1,1,...,1].
*
40  continue

  g(1) = 2.d0*(x(1)+x(2)-1.d0)
do i=2,n-1
  g(i) = 2.d0*(x(i-1)+x(i)-float(i-1)) +
*      2.d0*(x(i)+x(i+1)-float(i))
end do
g(n) = 2.d0*(x(n-1)+x(n)-float(n-1))
return

```

```

cF41                                STAIRCASE S2
*
*                                Initial point x0=[1,1,...,1].
*
41  continue

    g(1)=2.d0*(x(1)+x(2)-2.d0)
    do i=2,n-1
      g(i) = 2.d0*(x(i-1)+x(i)-float(i)) +
*          2.d0*(x(i)+x(i+1)-float(i+1))
    end do
    g(n) = 2.d0*(x(n-1)+x(n)-float(n))
    return

cF42                                STAIRCASE S3
*
*                                Initial point x0=[2,2,...,2].
*
42  continue

    g(1) = 2.d0*(x(1)+x(2)+2.d0)

    do i=2,n-1
      g(i) = 2.d0*(x(i-1)+x(i)+float(i))+
*          2.d0*(x(i)+x(i+1)+float(i+1))
    end do

    g(n) = 2.d0*(x(n-1)+x(n)+float(n))
    return

cF43                                NONDQUAR
*                                Tridiagonal Double Bordered Arrow-Down
*
43  continue

    g(1) = 2.d0*(x(1)-x(2))+4.d0*(x(1)+x(2)+x(n))**3
    g(2) =-2.d0*(x(1)-x(2))+4.d0*(x(1)+x(2)+x(n))**3 +
*          4.d0*(x(2)+x(3)+x(n))**3

    do i=3,n-2
      g(i) = 4.d0*(x(i-1)+x(i)+x(n))**3 +
*          4.d0*(x(i)+x(i+1)+x(n))**3
    end do

    g(n-1) = 4.d0*(x(n-2)+x(n-1)+x(n))**3 +
*          2.d0*(x(n-1)+x(n))

    g(n) = 2.d0*(x(n-1)+x(n))
    do i=1,n-2
      g(n) = g(n) + 4.d0*(x(i)+x(i+1)+x(n))**3
    end do
    return

cF44                                TRIDIA (CUTE)
*
*                                Initial point x0=[1,1,...,1].
*
44  continue

```



```

*
  alpha=5.d0
  beta =1.d0
  gamma=1.d0
  delta=1.d0

  g(1) = 2.d0*gamma*(delta*x(1)-1.d0)*delta -
*       4.d0*(alpha*x(2)-beta*x(1))*beta

  do i=2,n-1
    g(i) = 2.d0*float(i)*(alpha*x(i)-beta*x(i-1))*alpha -
*       2.d0*float(i+1)*(alpha*x(i+1)-beta*x(i))*beta
  end do

  g(n) = 2.d0*float(n)*(alpha*x(n)-beta*x(n-1))*alpha
  return

cF45                                ARWHEAD  (CUTE)
*
*                                Initial point x0=[1,1,...,1].
*
45  continue

  do i=1,n-1
    g(i) = -4.d0 + 4.d0*x(i)*(x(i)**2+x(n)**2)
  end do

  g(n) = 0.d0
  do i=1,n-1
    g(n) = g(n) + 4.d0*x(n)*(x(i)**2+x(n)**2)
  end do
  return

cF46                                NONDIA  (Shanno-78)  (CUTE)
*
*                                Initial point x0=[-1,-1,...,-1].
*
*
46  continue

  c=100.d0

  g(1)=2.d0*(x(1)-1.d0) + 2.d0*c*(x(1)-x(1)**2)*(1.d0-2.d0*x(1))
  do i=2,n
    g(1) = g(1) + 2.d0*c*(x(1)-x(i)**2)
  end do

  do i=2,n
    g(i) = -4.d0*c*x(i)*(x(1)-x(i)**2)
  end do
  return

cF47                                BDQRTIC (CUTE)
*
*                                Initial point x0=[1.,1.,...,1.].
*
*
47  continue
*

```

```

n4=n-4

do i=1,n4
  temp(i) = x(i)**2 + 2.d0*x(i+1)**2 + 3.d0*x(i+2)**2
*          + 4.d0*x(i+3)**2 + 5.d0*x(n)**2
end do

g(1) = -8.d0*(-4.d0*x(1)+3.d0) +
*      (4.d0*temp(1))*x(1)
g(2) = -8.d0*(-4.d0*x(2)+3.d0) +
*      (8.d0*temp(1)+ 4.d0*temp(2))*x(2)
g(3) = -8.d0*(-4.d0*x(3)+3.d0) +
*      (12.d0*temp(1)+ 8.d0*temp(2)+ 4.d0*temp(3))*x(3)
g(4) = -8.d0*(-4.d0*x(4)+3.d0) +
*      (16.d0*temp(1)+12.d0*temp(2) +8.d0*temp(3)+
*      4.d0*temp(4))*x(4)

do i=5,n4
  g(i) = -8.d0*(-4.d0*x(i)+3.d0) +
*        (16.d0*temp(i-3)+12.d0*temp(i-2)+
*        8.d0*temp(i-1)+4.d0*temp(i))*x(i)
end do

g(n4+1) = (16.d0*temp(n4-2)+12.d0*temp(n4-1)+8.d0*temp(n4))*x(n4+1)
g(n4+2) = (16.d0*temp(n4-1)+12.d0*temp(n4))*x(n4+2)
g(n4+3) = (16.d0*temp(n4))*x(n4+3)

tsum=0.d0
do i=1,n4
  tsum = tsum + temp(i)
end do
g(n) = 20.d0*tsum*x(n)
return

cF48                                DQDRTIC  (CUTE)
*
*          Initial point x0=[3,3,3...,3].
*
*
48  continue

c=1000.d0
d=1000.d0

g(1) = 2.d0*x(1)
g(2) = 2.d0*c*x(2) + 2.d0*x(2)

do i=3,n-2
  g(i) = 2.d0*(1.d0+d+c)*x(i)
end do

g(n-1) = 2.d0*(c+d)*x(n-1)
g(n) = 2.d0*d*x(n)
return

cF49                                EG2  (CUTE)
*
*          Initial point x0=[1,1,1...,1].
*
*
49  continue

```

```

g(1)=(1.d0+2.d0*x(1))*dcos(x(1)+x(1)*x(1)-1.d0)
do i=2,n-1
  g(1) = g(1) + dcos(x(1)+x(i)*x(i)-1.d0)
end do

do i=2,n-1
  g(i) = 2.d0*x(i)*dcos(x(1)+x(i)*x(i)-1.d0)
end do

g(n) = x(n)*dcos(x(n)*x(n))
return

cF50                                EG3
*
*                                Initial point x0=[1,1,1...,1].
*
*
50  continue

g(1)=-(1.d0+2.d0*x(1))*dsin(x(1)+x(1)*x(1)-1.d0)
do i=2,n-1
  g(1) = g(1) - dsin(x(1)+x(i)*x(i)-1.d0)
end do

do i=2,n-1
  g(i) = -2.d0*x(i)*dsin(x(1)+x(i)*x(i)-1.d0)
end do

g(n) = -x(n)*dsin(x(n)*x(n))
return

cF51                                EDENSCH Function (CUTE)
*
*                                Initial Point: [0., 0., ..., 0.].
*
51  continue

g(1) = 4.d0*(x(1)-2.d0)**3 + 2.d0*x(2)*(x(1)*x(2)-2.d0*x(2))
*
do i=2,n-1
  g(i) = 2.d0*(x(i-1)*x(i)-2.d0*x(i))*(x(i-1)-2.d0) +
*       2.d0*(x(i)+1.d0) +
*       4.d0*(x(i)-2.d0)**3 +
*       2.d0*x(i+1)*(x(i)*x(i+1)-2.d0*x(i+1))
end do

g(n) = 2.d0*(x(n-1)*x(n)-2.d0*x(n))*(x(n-1)-2.d0) +
*       2.d0*(x(n)+1.d0)
return

cF52                                FLETCHCR (CUTE)
*
*                                Initial Point: [0.5,0.5,...0.5]
*
52  continue

g(1) = 200.d0*(x(2)-x(1)+1.d0-x(1)*x(1))*(-1.d0-2.d0*x(1))

do i=2,n-1
  g(i) = 200.d0*(x(i)-x(i-1)+1.d0-x(i-1)*x(i-1))+
*       200.d0*(x(i+1)-x(i)+1.d0-x(i)*x(i))*(-1.d0-2.d0*x(i))

```

```

end do

g(n) = 200.d0*(x(n)-x(n-1)+1.d0-x(n-1)**2)
return

cF53                                ENGVAL1 (CUTE)
*
*                                Initial point x0=[2.,2.,2...,2.].
*
53  continue

do i=1,n-1
  t(i) = x(i)*x(i) + x(i+1)*x(i+1)
end do

g(1) = 4.d0*x(1)*t(1) - 4.d0

do i=2,n-1
  g(i) = 4.d0*x(i)*t(i-1) + 4.d0*x(i)*t(i) - 4.d0
end do

g(n) = 4.d0*x(n)*t(n-1)
return

cF54                                DENSCHNA (CUTE)
*
*                                Initial point: [8, 8,...,8]
*
54  continue

j=1
do i=1,n/2
  g(j) = 4.d0*x(2*i-1)**3 + 2.d0*(x(2*i-1)+x(2*i))
  g(j+1) = 2.d0*(x(2*i-1)+x(2*i)) +
*      2.d0*(dexp(x(2*i)))*(-1.d0+dexp(x(2*i)))
  j=j+2
end do
return

cF55                                DENSCHNB (CUTE)
*
*                                Initial point: [0.1, 0.1,...,0.1]
*
55  continue

j=1
do i=1,n/2
  g(j) = 2.d0*(x(2*i-1)-2.d0) + 2.d0*(x(2*i-1)-2.d0)*x(2*i)*x(2*i)
  g(j+1) = ((x(2*i-1)-2.d0)**2)*2.d0*x(2*i) + 2.d0*(x(2*i)+1.d0)
  j=j+2
end do
return

cF56                                DENSCHNC (CUTE)
*
*                                Initial point: [8, 8,...,8]
*
56  continue

```

```

j=1
do i=1,n/2
  g(j) = 4.d0*x(2*i-1)*(-2.d0+x(2*i-1)**2+x(2*i)**2)+
* 2.d0*(dexp(x(2*i-1)-1.d0))*(-2.d0+dexp(x(2*i-1)-1.d0)+x(2*i)**3)
  g(j+1) = 4.d0*x(2*i)*(-2.d0+x(2*i-1)**2+x(2*i)**2)+
* 6.d0*(x(2*i)**2)*(-2.d0+dexp(x(2*i-1)-1.d0)+x(2*i)**3)
  j=j+2
end do
return

cF57                                DENSCHNF (CUTE)
*
*      Initial point: [2,0,2,0,...,2,0]

57  continue

j=1
do i=1,n/2
  g(j)=2.d0*(2.d0*(x(2*i-1)+x(2*i))**2+(x(2*i-1)-x(2*i))**2-8.d0)*
* (4.d0*(x(2*i-1)+x(2*i))+2.d0*(x(2*i-1)-x(2*i))) +
* 2.d0*(5.d0*x(2*i-1)**2+(x(2*i)-3.d0)**2-9.d0)*10.d0*x(2*i-1)
  g(j+1)=2.d0*(2.d0*(x(2*i-1)+x(2*i))**2+(x(2*i-1)-x(2*i))**2-8.d0)*
* (4.d0*(x(2*i-1)+x(2*i))-2.d0*(x(2*i-1)-x(2*i))) +
* 2.d0*(5.d0*x(2*i-1)**2+(x(2*i)-3.d0)**2-9.d0)*2.d0*(x(2*i)-3.d0)
  j=j+2
end do
return

cF58                                SINGUAD (CUTE)
*
*      Initial Point: [0.1, 0.1, ..., 0.1]

58  continue

do i=1,n-2
  t(i) = dsin(x(i+1)-x(n)) - x(1)**2 + x(i+1)**2
end do

c
g(1) = 4.d0*(x(1)-1.d0)**3 - 4.d0*x(1)*(x(n)**2-x(1)**2)
do i=1,n-2
  g(1) = g(1) - 4.d0*t(i)*x(1)
end do

do i=2,n-1
  g(i) = 2.d0*t(i-1)*(dcos(x(i)-x(n))+2.d0*x(i))
end do

g(n) = 4.d0*x(n)*(x(n)**2-x(1)**2)
do i=1,n-2
  g(n) = g(n) - 2.d0*t(i)*dcos(x(i+1)-x(n))
end do
return

cF59                                DIXON3DQ (CUTE)
*
*      Initial Point x0=[-1, -1,..., -1]

59  continue

g(1) = 2.d0*(x(1)-2.d0) + 2.d0*(x(1)-x(2))

```

```

do i=2,n-1
  g(i) = -2.d0*(x(i-1)-x(i)) + 2.d0*(x(i)-x(i+1))
end do

g(n) = -2.d0*(x(n-1)-x(n)) + 2.d0*(x(n)-1.d0)
return

cF60                                BIGGSB1 (CUTE)
*
*          Initial Point: [0., 0., ...,0.]

60  continue

g(1) = 4.d0*x(1) - 2.d0*x(2) - 2.d0

do i=2,n-1
  g(i) = 4.d0*x(i) - 2.d0*x(i-1) - 2.d0*x(i+1)
end do

g(n) = 4.d0*x(n) - 2.d0*x(n-1) - 2.d0
return

cF61                                PRODSin (m=n-1)
*
*          Initial point x0=[5. 5, 5, 5,...,5].
*
61  continue

m = n-1
t1=0.d0
t2=0.d0

do i=1,m
  t1 = t1 + x(i)*x(i)
end do

do i=1,n
  t2 = t2 + dsin(x(i))
end do

do i=1,m
  g(i) = 2.d0*x(i)*t2 + t1*dcos(x(i))
end do

do i=m+1,n
  g(i) = t1*dcos(x(i))
end do
return

cF62                                PROD1 (m=n)
*
*          Initial point x0=[1. 1, 1, 1,...,1].
*
62  continue

m = n
t1=0.d0
t2=0.d0

```

```

do i=1,m
  t1 = t1 + x(i)
end do

do i=1,n
  t2 = t2 + x(i)
end do

do i=1,m
  g(i) = t1+t2
end do

do i=m+1,n
  g(i) = t1
end do
return

cF63                                PRODcos (m=n-1)
*
*          Initial point x0=[5. 5, 5, 5,...,5].
*
63  continue

c    m = n-1
    m=n/2
    t1=0.d0
    t2=0.d0

do i=1,m
  t1 = t1 + x(i)*x(i)
end do

do i=1,n
  t2 = t2 + dcos(x(i))
end do

do i=1,m
  g(i) = 2.d0*x(i)*t2 - t1*dsin(x(i))
end do

do i=m+1,n
  g(i) = -t1*dsin(x(i))
end do
return

cF64                                PROD2 (m=1)
*
*          Initial point x0=[15. 15, 15, 15,...,15].
*
64  continue

    m = 1
    t1=0.d0
    t2=0.d0

do i=1,m
  t1 = t1 + x(i)**4
end do

do i=1,n
  t2 = t2 + float(i)*x(i)

```

```

end do

do i=1,m
  g(i) = 4.d0*t2*x(i)**3 + float(i)*t1
end do

do i=m+1,n
  g(i) = float(i)*t1
end do
return

cF65                                DIXMAANA (CUTE)
*
*                                Initial point x0=[2.,2.,2...,2.].
*                                Modified m=n/4
65  continue
*
  alpha = 1.d0
  beta  = 0.d0
  gamma = 0.125d0
  delta = 0.125d0

  k1 = 0
  k2 = 0
  k3 = 0
  k4 = 0

  m = n/4

do i=1,n
  g(i) = 0.d0
end do
c1

do i=1,n
  g(i) = g(i) + 2.d0*alpha*x(i)*((float(i)/float(n))**k1)
end do
c2

  g(1) = g(1) + 2.d0*beta*x(1)*((x(2)+x(2)*x(2))**2)*
*      ((float(1)/float(n))**k2)
do i=2,n-1
  g(i) = g(i) + 2.d0*beta*(x(i-1)**2)*(x(i)+x(i)**2)*
*      (1.d0+2.d0*x(i))*((float(i-1)/float(n))**k2)+
*      2.d0*beta*x(i)*((x(i+1)+x(i+1)**2)**2)*
*      ((float(i)/float(n))**k2)
end do
  g(n) = g(n) + 2.d0*beta*(x(n-1)**2)*(x(n)+x(n)**2)*
*      (1.d0+2.d0*x(n))
c3

do i=1,2*m
  g(i) = g(i) + 2.d0*gamma*x(i)*(x(i+m)**4)*
*      ((float(i)/float(n))**k3)
  g(i+m) = g(i+m) + gamma*(x(i)**2)*4.d0*(x(i+m)**3)*
*      ((float(i)/float(n))**k3)
end do
c4

do i=1,m
  g(i) = g(i) + delta*x(i+2*m)*((float(i)/float(n))**k4)
  g(i+2*m) = g(i+2*m) + delta*x(i)*((float(i)/float(n))**k4)

```



```

end do
return

cF66                                DIXMAANB (CUTE)
*
*                                Initial point x0=[2.,2.,2...,2.].
*                                Modified m=n/4
66  continue
*
    alpha = 1.d0
    beta  = 0.0625d0
    gamma = 0.0625d0
    delta = 0.0625d0

    k1 = 0
    k2 = 0
    k3 = 0
    k4 = 1

    m = n/4

    do i=1,n
        g(i) =0.d0
    end do
c1

    do i=1,n
        g(i) = g(i) + 2.d0*alpha*x(i)*((float(i)/float(n))**k1)
    end do
c2

    g(1) = g(1) + 2.d0*beta*x(1)*((x(2)+x(2)*x(2))**2)*
*          ((float(1)/float(n))**k2)
    do i=2,n-1
        g(i) = g(i) + 2.d0*beta*(x(i-1)**2)*(x(i)+x(i)**2)*
*          (1.d0+2.d0*x(i))*((float(i-1)/float(n))**k2)+
*          2.d0*beta*x(i)*((x(i+1)+x(i+1)**2)**2)*
*          ((float(i)/float(n))**k2)
    end do
    g(n) = g(n) + 2.d0*beta*(x(n-1)**2)*(x(n)+x(n)**2)*
*          (1.d0+2.d0*x(n))
c3

    do i=1,2*m
        g(i) = g(i) + 2.d0*gamma*x(i)*(x(i+m)**4)*
*          ((float(i)/float(n))**k3)
        g(i+m) = g(i+m) + gamma*(x(i)**2)*4.d0*(x(i+m)**3)*
*          ((float(i)/float(n))**k3)
    end do
c4

    do i=1,m
        g(i) = g(i) + delta*x(i+2*m)*((float(i)/float(n))**k4)
        g(i+2*m) = g(i+2*m) + delta*x(i)*((float(i)/float(n))**k4)
    end do
    return

cF67                                DIXMAANC (CUTE)
*
*                                Initial point x0=[2.,2.,2...,2.].
*                                Modified m=n/4

```

```

67      continue
*
      alpha = 1.d0
      beta  = 0.125d0
      gamma = 0.125d0
      delta = 0.125d0

      k1 = 0
      k2 = 0
      k3 = 0
      k4 = 0

      m = n/4

      do i=1,n
        g(i) =0.d0
      end do
c1

      do i=1,n
        g(i) = g(i) + 2.d0*alpha*x(i)*((float(i)/float(n))**k1)
      end do
c2

      g(1) = g(1) + 2.d0*beta*x(1)*((x(2)+x(2)*x(2))**2)*
*          ((float(1)/float(n))**k2)
      do i=2,n-1
        g(i) = g(i) + 2.d0*beta*(x(i-1)**2)*(x(i)+x(i)**2)*
*          (1.d0+2.d0*x(i))*((float(i-1)/float(n))**k2)+
*          2.d0*beta*x(i)*((x(i+1)+x(i+1)**2)**2)*
*          ((float(i)/float(n))**k2)
      end do
      g(n) = g(n) + 2.d0*beta*(x(n-1)**2)*(x(n)+x(n)**2)*
*          (1.d0+2.d0*x(n))
c3

      do i=1,2*m
        g(i) = g(i) + 2.d0*gamma*x(i)*(x(i+m)**4)*
*          ((float(i)/float(n))**k3)
        g(i+m) = g(i+m) + gamma*(x(i)**2)*4.d0*(x(i+m)**3)*
*          ((float(i)/float(n))**k3)
      end do
c4

      do i=1,m
        g(i) = g(i) + delta*x(i+2*m)*((float(i)/float(n))**k4)
        g(i+2*m) = g(i+2*m) + delta*x(i)*((float(i)/float(n))**k4)
      end do
      return

cF68                                DIXMAAND (CUTE)
*
*                                Initial point x0=[2.,2.,2...,2.].
*                                Modified m=n/4
68      continue
*
      alpha = 1.d0
      beta  = 0.26d0
      gamma = 0.26d0
      delta = 0.26d0

      k1 = 0

```

```

        k2 = 0
        k3 = 0
        k4 = 0

        m = n/4

        do i=1,n
            g(i) =0.d0
        end do
c1

        do i=1,n
            g(i) = g(i) + 2.d0*alpha*x(i)*((float(i)/float(n))**k1)
        end do
c2

        g(1) = g(1) + 2.d0*beta*x(1)*((x(2)+x(2)*x(2))**2)*
            ((float(1)/float(n))**k2)
        do i=2,n-1
            g(i) = g(i) + 2.d0*beta*(x(i-1)**2)*(x(i)+x(i)**2)*
            * (1.d0+2.d0*x(i))*((float(i-1)/float(n))**k2)+
            * 2.d0*beta*x(i)*((x(i+1)+x(i+1)**2)**2)*
            * ((float(i)/float(n))**k2)
        end do
        g(n) = g(n) + 2.d0*beta*(x(n-1)**2)*(x(n)+x(n)**2)*
        * (1.d0+2.d0*x(n))
c3

        do i=1,2*m
            g(i) = g(i) + 2.d0*gamma*x(i)*(x(i+m)**4)*
            * ((float(i)/float(n))**k3)
            g(i+m) = g(i+m) + gamma*(x(i)**2)*4.d0*(x(i+m)**3)*
            * ((float(i)/float(n))**k3)
        end do
c4

        do i=1,m
            g(i) = g(i) + delta*x(i+2*m)*((float(i)/float(n))**k4)
            g(i+2*m) = g(i+2*m) + delta*x(i)*((float(i)/float(n))**k4)
        end do
        return

cF69                                DIXMAANL (CUTE)
*
*                                Initial point x0=[2.,2.,2...,2.].
*                                Modified m=n/4
69  continue
*

        alpha = 1.d0
        beta  = 0.26d0
        gamma = 0.26d0
        delta = 0.26d0

        k1 = 2
        k2 = 0
        k3 = 0
        k4 = 2

        m = n/4

        do i=1,n
            g(i) =0.d0
        end do

```

```

c1
    do i=1,n
        g(i) = g(i) + 2.d0*alpha*x(i)*((float(i)/float(n))**k1)
    end do

c2
    g(1) = g(1) + 2.d0*beta*x(1)*((x(2)+x(2)*x(2))**2)*
    * ((float(1)/float(n))**k2)
    do i=2,n-1
        g(i) = g(i) + 2.d0*beta*(x(i-1)**2)*(x(i)+x(i)**2)*
        * (1.d0+2.d0*x(i))*((float(i-1)/float(n))**k2)+
        * 2.d0*beta*x(i)*((x(i+1)+x(i+1)**2)**2)*
        * ((float(i)/float(n))**k2)
    end do
    g(n) = g(n) + 2.d0*beta*(x(n-1)**2)*(x(n)+x(n)**2)*
    * (1.d0+2.d0*x(n))

c3
    do i=1,2*m
        g(i) = g(i) + 2.d0*gamma*x(i)*(x(i+m)**4)*
        * ((float(i)/float(n))**k3)
        g(i+m) = g(i+m) + gamma*(x(i)**2)*4.d0*(x(i+m)**3)*
        * ((float(i)/float(n))**k3)
    end do

c4
    do i=1,m
        g(i) = g(i) + delta*x(i+2*m)*((float(i)/float(n))**k4)
        g(i+2*m) = g(i+2*m) + delta*x(i)*((float(i)/float(n))**k4)
    end do
    return

cF70
                                ARGLINB (m=5)
*
*      Initial point x0=[0.01   0.001, .... ,0.01   0.001].
*
70  continue

    m=5

    do i=1,m
        u(i)=0.d0
        do j=1,n
            u(i) = u(i) + float(i)*float(j)*x(j)
        end do
    end do

c
    do j=1,n
        g(j) = 0.d0
        do i=1,m
            g(j) = g(j) + 2.d0*(u(i)-1.d0)*float(i)*float(j)
        end do
    end do
    return

cF71
                                VARDIM (CUTE)
*
*      Initial point x0=[1-1/n, 1-2/n,...,1-n/n.].
*      Modified m=n/4
71  continue

```

```

s = float(n)*float(n+1)/2.d0

t1=0.d0
do i=1,n
    t1 = t1 + float(i)*x(i)
end do
t1 = t1-s

do i=1,n
    g(i) = 2.d0*(x(i)-1.d0) + 2.d0*t1*float(i) + 4.d0*float(i)*t1**3
end do
return

cF72                                DIAG-AUP1
*
*                                Initial point x0=[4., 4., ....4.].
*

72    continue

g(1) = 4.d0*(x(1)**2-1.d0)*x(1) +
*      8.d0*(x(1)*x(1)-x(1))*(2.d0*x(1)-1.d0)
do i=2,n
    g(1) = g(1) - 8.d0*(x(i)*x(i)-x(1))
end do

do i=2,n
    g(i) = 16.d0*x(i)*(x(i)*x(i)-x(1)) + 4.d0*(x(i)**2-1.d0)*x(i)
end do
return

cF73                                ENGVAL8
*
*                                Initial point x0=[2., 2., ....2.].
*

73    continue

g(1) = 4.d0*(x(1)**2+x(2)**2)*x(1) + 8.d0

do i=2,n-1
    g(i)=4.d0*(x(i-1)**2+x(i)**2)*x(i) +
*      4.d0*(x(i)**2+x(i+1)**2)*x(i) + 8.d0
end do

g(n) = 4.d0*(x(n-1)**2+x(n)**2)*x(n)
return

cF74                                QUARTIC    (CUTE)
*
*                                Initial point x0=[2., 2., ....2.].
*

74    continue

do i=1,n
    g(i) = 4.d0*((x(i)-1.d0)**3)
end do
return

```

```

cF75                                LIARWHD    (CUTE)
*
*                                Initial point x0=[4., 4., ....4.].
*
75      continue

      g(1) = 8.d0*(x(1)**2-x(1))*(2.d0*x(1)-1.d0) + 2.d0*(x(1)-1.d0)
      do i=2,n
        g(1) = g(1) - 8.d0*(x(i)**2-x(1))
      end do

      do i=2,n
        g(i) = 8.d0*(x(i)**2-x(1))*(2.d0*x(i)) + 2.d0*(x(i)-1.d0)
      end do
      return

cF76                                NONSCOMP (CUTE)
*
*                                Initial point x0=[3., 3., ..., 3.].
*
76      continue

      g(1) = 2.d0*(x(1)-1.d0) - 8.d0*(x(2)-x(1)**2)*(2.d0*x(1))

      do i=2,n-1
        g(i) = 8.d0*(x(i)-x(i-1)**2) - 8.d0*(x(i+1)-x(i)**2)*(2.d0*x(i))
      end do

      g(n) = 8.d0*(x(n)-x(n-1)**2)
      return

cF77                                Linear Perturbed
*
*                                Initial point x0=[2., ...,2.]
*
77      continue

      do i=1,n
        g(i) = float(i)*2.d0*x(i) + 1.d0/100.d0
      end do
      return

cF78                                CUBE
*
*                                Initial point x0=[-1.2, 1, -1.2, 1.,..., -1.2, 1]
*
78      continue

      g(1) = 2.d0*(x(1)-1.d0) - 600.d0*(x(2)-x(1)**3)*(x(1)**2)
      do i=2,n-1
        g(i) = 200.d0*(x(i)-x(i-1)**3) - 600.0*(x(i+1)-x(i)**3)*(x(i)**2)
      end do
      g(n) = 200.d0*(x(n)-x(n-1)**3)
      return

cF79                                HARKERP
*

```

```

*               Initial point x0=[1,2,...,n]
*
79  continue

    s = 0.d0
    do i=1,n
        s = s + x(i)
    end do

    do i=1,n
        g(i) = 2.d0*s - 1.d0 - x(i)
    end do
    return

cF80               QUARTICM
*
*               Initial point x0=[2,2,...,2]
*
80  continue

    do i=1,n
        g(i) = 4.d0*(x(i)-float(i))**3
    end do
    return
end

c ===== Last line CG_GRAD
c
c
c
c
c

c
c ===== Last line CG3x8.FOR package =====
c
c
c               Dr. Neculai Andrei
c       Center for Advanced Modeling and optimization,
c       Academy of Romanian Scientists,
c       Bucharest, Romania
c
c
c=====

               ---ooooOoooo---

```