NONCONVEX MINIMIZATION CALCULATIONS AND THE CONJUGATE GRADIENT METHOD

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Abstract We consider the global convergence of conjugate gradient methods without restarts, assuming exact arithmetic and exact line searches, when the objective function is twice continuously differentiable and has bounded level sets. Most of our attention is given to the Polak-Ribière algorithm, and unfortunately we find examples that show that the calculated gradients can remain bounded away from zero. The examples that have only two variables show also that some variable metric algorithms for unconstrained optimization need not converge. However, a global convergence theorem is proved for the Fletcher-Reeves version of the conjugate gradient method.

1. Introduction

The conjugate gradient method is highly useful for calculating local unconstrained minima of differentiable functions of many variables because it does not require the storage of any matrices. We consider a Polak-Ribière version of the method with exact line searches, which is as follows. We let $F(.)$ from $\mathbb{R}^n$ to $\mathbb{R}$ be the objective function, we let $\underline{x}\in\mathbb{R}^n$ be the vector of variables, we let $\{\underline{x}_k;\ k=1,2,3,\ldots\}$ be the sequence of points that is generated by the algorithm, and $\underline{g}_k$ denotes the gradient $\underline{\nabla}F(\underline{x}_k)$.

Step 0 $\underline{x}_1\in\mathbb{R}^n$ is chosen by the user and $k=1$ is set.

Step 1 Calculate $\underline{g}_k=\underline{\nabla}F(\underline{x}_k)$. If $\underline{g}_k=0$ then end.

Step 2 If $k=1$ then set $\underline{d}_k=-\underline{g}_k$.

Step 3 If $k>1$ then set $\underline{d}_k=-\underline{g}_k+\beta_k\underline{d}_{k-1}$ where

$$\beta_k=\underline{g}_k^T(\underline{g}_k-\underline{g}_{k-1})/\|\underline{g}_{k-1}\|^2 . \tag{1.1}$$

Step 4 Find the least positive number α_k such that the function of one variable

$$\phi_k(\alpha)=F(\underline{x}_k+\alpha\underline{d}_k),\qquad \alpha\in\mathbb{R}, \tag{1.2}$$

has a local minimum at $\alpha=\alpha_k$, or make an error return if the search for α_k is unsuccessful.

Step 5 Set $\underline{x}_{k+1}=\underline{x}_k+\alpha_k\underline{d}_k$, increase k by one, and branch back to Step 1.

Due to the choice of $\underline{d}_k$, this algorithm finds the exact minimum of a convex quadratic function in at most n steps (see Fletcher, 1980), and it is generally far more efficient than the method of steepest descents. Of course in practice one relaxes the condition on the step-length α_k, and also a restart procedure is often used (Powell, 1977, for example). Further, the definition of $\underline{d}_{k+1}$ may be modified when α_k is not a local minimum of the function (1.2) (Buckley, 1982). Thus one can develop some very useful procedures, but the purpose of this paper is to answer a fundamental question about the convergence of the given basic method.

In order that the required value of α_k is well-defined for all k , we assume that the level set

$$L=\{\underline{x} : F(\underline{x}) \leq F(\underline{x}_1)\}\subset\mathbb{R}^n \tag{1.3}$$

is bounded. We assume also that $F(.)$ is twice continuously differentiable. We ask whether these conditions are sufficient for the given method to provide the limit

$$\lim_{k\to\infty} \inf \|\underline{g}_k\| = 0 . \tag{1.4}$$

It is well-known that this limit is obtained if the directional derivatives

$$\rho_k=\underline{d}_k^T\underline{g}_k/(\|\underline{d}_k\| \; \|\underline{g}_k\|) < 0 , \qquad k=1,2,3,..., \tag{1.5}$$

are bounded away from zero. Specifically, letting all vector norms be Euclidean, and letting Ω be an upper bound on the induced matrix norms $\{\|\nabla^2F(\underline{x})\| ; \underline{x}\varepsilon L\}$, we have the relation

$$F(\underline{x})\leq F(\underline{x}_k)+(\underline{x}-\underline{x}_k)^T\underline{g}_k+\tfrac{1}{2}\Omega\|\underline{x}-\underline{x}_k\|^2 , \qquad \underline{x}\varepsilon L , \tag{1.6}$$

which, after some consideration of rates of change of first derivatives, gives the inequality

$$\begin{aligned} F(\underline{x}_{k+1})&\leq \min_{\alpha}[F(\underline{x}_k)+\alpha\underline{d}_k^T\underline{g}_k+\tfrac{1}{2}\Omega\alpha^2\|\underline{d}_k\|^2] \\ &= F(\underline{x}_k)-\rho_k^2\|\underline{g}_k\|^2/(2\Omega) . \end{aligned} \tag{1.7}$$

Thus, because $F(.)$ is bounded below, $\Sigma\rho_k^2\|\underline{g}_k\|^2$ is convergent. Hence condition (1.4) fails only if $\Sigma\rho_k^2$ is finite (Zoutendijk, 1970).

Therefore, noting that the definitions of α_{k-1} and $\underline{d}_k$ imply the value $\rho_k=-\|\underline{g}_k\|/\|\underline{d}_k\|$, the gradient norms $\{\|\underline{g}_k\| ; k=1,2,3,...\}$ are bounded away from zero only if the sequence $\{\|\underline{d}_k\| ; k=1,2,3,...\}$ is divergent. In this case, due to Step 3 and the existence of an upper bound on $\{\|\underline{\nabla}F(\underline{x})\| ; \underline{x}\varepsilon L\}$, the direction $\underline{d}_k$ tends to be parallel to $\underline{d}_{k-1}$. Therefore, if one is seeking counter-examples to the limit (1.4), it is suitable to consider cases when the points $\{\underline{x}_k;\ k=1,2,3,\ldots\}$ tend to lie on a straight line, which we take as the first co-ordinate direction in $\mathbb{R}^n$. There are no counter-examples in which the sequence $\{\underline{x}_k;\ k=1,2,3,\ldots\}$ converges, because in this case, due to first derivative continuity, the numbers $\{\beta_k;\ k=1,2,3,\ldots\}$ would tend to zero, which would keep $\{\|\underline{d}_k\|;\ k=1,2,3,\ldots\}$ uniformly bounded.

For many finite sequences of distinct points $\{\underline{x}_k;\ k=1,2,\ldots,\ell\}$ one can find gradients $\{\underline{g}_k;\ k=1,2,\ldots,\ell-1\}$ such that the points can be generated by the conjugate gradient method. Specifically, we let $\underline{g}_1=\underline{x}_1-\underline{x}_2$, and, for $k\geq 2$, because of the definition of α_{k-1} and $\underline{d}_k$, $\underline{g}_k$ has to be a multiple of the vector in the space spanned by $(\underline{x}_{k+1}-\underline{x}_k)$ and $(\underline{x}_k-\underline{x}_{k-1})$ that is orthogonal to $(\underline{x}_k-\underline{x}_{k-1})$. In order to determine the sign and length of $\underline{g}_k$, we note that the value (1.1) implies the conjugacy condition

$$(\underline{x}_{k+1}-\underline{x}_k)^T(\underline{g}_k-\underline{g}_{k-1})=0, \qquad k\geq 2. \tag{1.8}$$

Thus, starting with $\underline{g}_1=\underline{x}_1-\underline{x}_2$, the gradients $\{\underline{g}_k;\ k=1,2,3,\ldots\}$ can usually be found recursively, but the descent conditions $\{\underline{g}_k^T(\underline{x}_{k+1}-\underline{x}_k)<0;\ k=2,3,\ldots,\ell-1\}$ may not hold. Thus not all sequences $\{\underline{x}_k;\ k=1,2,\ldots,\ell\}$ are admissible. Further restrictions on the sequences occur if one lets $\ell\to\infty$, in particular from the aim of keeping the gradient norms $\{\|\underline{g}_k\|;\ k=1,2,3,\ldots\}$ bounded and bounded away from zero.

In spite of these difficulties, we seek sequences that provide counter-examples to the limit (1.4). To simplify the analysis we impose the conditions

$$\left.\begin{aligned}(\underline{x}_{k+m})_1&=(\underline{x}_k)_1\\ \hat{\underline{x}}_{k+m}&=\theta\hat{\underline{x}}_k\end{aligned}\right\}, \qquad k=1,2,3,\ldots, \tag{1.9}$$

where m is a small positive integer, where $(\underline{x})_1$ denotes the first component of $\underline{x}$, where $\hat{\underline{x}}$ is the vector in $\mathbb{R}^{n-1}$ whose components are the last $(n-1)$ components of $\underline{x}$, and where θ is a constant from $(0,1)$. Thus the distance from $\underline{x}_k$ to the first co-ordinate direction tends to zero as $k\to\infty$. Having chosen m and n, there are only a finite number of parameters in the sequence $\{\underline{x}_k;\ k=1,2,3,\ldots\}$. One can express the conditions for consistency with the conjugate gradient method as inequality constraints on the parameters, and one can investigate whether the inequalities have a solution. Some interesting cases for $n=2$ and $n=3$ are reported in Sections 2 and 3 respectively.

Two examples are given for $n=2$. For $m=3$ we find that gradients can stay bounded away from zero if one gives up the second derivative continuity of the objective function. Secondly, by letting $m=8$, it is shown that one can preserve the second derivative continuity if one modifies Step 4 of the algorithm by allowing α_k

to be any local minimum of the function (1.2) that satisfies $\phi_k(\alpha_k) < \phi_k(0)$. This is an important case because in practice one can usually accept any local minimum that reduces the objective function. However, the constraints on α_k in Step 4 are present because in this example the choice of α_k is so contrived that it is unlikely to occur.

For $n=3$ and $m=4$ we give an example that has properties that are similar to the $n=2$ and $m=8$ case of Section 2, and, by letting $n=3$ and $m=6$, we answer the main question of this paper. We find the gradients $\{\underline{g}_k;\ k=1,2,3,\ldots\}$ can remain bounded away from zero when all the conditions that have been stated are satisfied.

Section 4 includes a brief discussion of the examples and their implications. Further, we ask whether it is helpful to replace the multiplier (1.1) by the value

$$\beta_k = \|\underline{g}_k\|^2 / \|\underline{g}_{k-1}\|^2 , \tag{1.10}$$

which is suggested by Fletcher and Reeves (1964). It is proved that this version of the conjugate gradient algorithm has the strong advantage over the Polak-Ribière version that it always provides the limit (1.4), assuming that $F(.)$ is twice continuously differentiable and that the level set (1.3) is bounded.

2. Two variable examples

Let $n=2$, and let the sequence $\{\underline{x}_k;\ k=1,2,3,\ldots\}$ satisfy expression (1.9) for $m=3$, where θ is a constant from $(0,1)$. Then there exist real parameters a_i and b_i $(i=1,2,3)$ such that, for each non-negative integer j, we have

$$\underline{\delta}_{3j+1} = a_1\begin{pmatrix} 1 \\ b_1\theta^j \end{pmatrix}, \quad \underline{\delta}_{3j+2} = a_2\begin{pmatrix} 1 \\ b_2\theta^j \end{pmatrix}, \quad \underline{\delta}_{3j+3} = a_3\begin{pmatrix} 1 \\ b_3\theta^j \end{pmatrix},$$

where $\{\underline{\delta}_k = \underline{x}_{k+1} - \underline{x}_k;\ k=1,2,3,\ldots\}$ and where $a_1 + a_2 + a_3 = 0$. Thus, due to the line searches, the gradients have the form

$$\underline{g}_{3j+1} = c_{3j+1}\begin{pmatrix} b_3\theta^{j-1} \\ -1 \end{pmatrix}, \quad \underline{g}_{3j+2} = c_{3j+2}\begin{pmatrix} b_1\theta^j \\ -1 \end{pmatrix}, \quad \underline{g}_{3j+3} = c_{3j+3}\begin{pmatrix} b_2\theta^j \\ -1 \end{pmatrix},$$

where $\{c_k;\ k=1,2,3,\ldots\}$ are real multipliers. Therefore the conjugacy condition (1.8) implies the equations

$$\left.\begin{aligned} c_{3j+1}(b_3\theta^{j-1} - b_1\theta^j) &= c_{3j}(b_2\theta^{j-1} - b_1\theta^j) \\ c_{3j+2}(b_1\theta^j - b_2\theta^j) &= c_{3j+1}(b_3\theta^{j-1} - b_2\theta^j) \\ c_{3j+3}(b_2\theta^j - b_3\theta^j) &= c_{3j+2}(b_1\theta^j - b_3\theta^j) \end{aligned}\right\} , \tag{2.1}$$

which gives the ratio

$$\frac{c_{3j+3}}{c_{3j}} = \frac{b_2 - b_1\theta}{b_3 - b_1\theta} \; \frac{b_3 - b_2\theta}{\theta(b_1 - b_2)} \quad \frac{b_1 - b_3}{b_2 - b_3} = 1 , \tag{2.2}$$

where the right hand side is set to one because otherwise the gradients $\{\underline{g}_k;\ k=1,2,3,\ldots\}$ either diverge or tend to zero.

We assume without loss of generality that $a_1 > 0$, $a_2 > 0$ and $a_3 = -a_1 - a_2$. Therefore all the search directions are downhill if and only if the inequalities

$$\left.\begin{aligned} c_{3j+1}(b_3 - b_1\theta) &< 0 \\ c_{3j+2}(b_1 - b_2) &< 0 \\ c_{3j+3}(b_2 - b_3) &> 0 \end{aligned}\right\} \tag{2.3}$$

hold. Thus, remembering $c_{3j+3} = c_{3j}$, the equations (2.1) imply the conditions

$$\left.\begin{aligned} (b_2 - b_3)(b_2 - b_1\theta) &< 0 \\ (b_3 - b_1\theta)(b_3 - b_2\theta) &> 0 \\ (b_1 - b_2)(b_1 - b_3) &< 0 \end{aligned}\right\} . \tag{2.4}$$

We consider values of b_1, b_2 and b_3 that satisfy expressions (2.2) and (2.4).

In particular the values $b_1 = 3$, $b_2 = 2$, $b_3 = 2 + \sqrt{2}$ and $\theta = 1/3$ are suitable. In this case, from the relation

$$\underline{x}_{3j+4} - \underline{x}_{3j+1} = \begin{pmatrix} 0 \\ (a_1b_1 + a_2b_2 + a_3b_3)\theta^j \end{pmatrix} , \tag{2.5}$$

and from the fact that the second component of $\underline{x}_{3j+1}$ tends to zero as $j \to \infty$, we deduce the vector

$$\underline{x}_{3j+1} = \begin{pmatrix} 0 \\ -[3a_1 + 2a_2 - (2+\sqrt{2})(a_1 + a_2)]\,\theta^j/(1-\theta) \end{pmatrix} , \tag{2.6}$$

assuming without loss of generality that $(\underline{x}_{3j+1})_1 = 0$. Similarly $\underline{x}_{3j+2}$ and $\underline{x}_{3j+3}$ can be calculated, and we note the value

$$(\underline{x}_{3j+2})_2 = -[3\theta a_1 + 2a_2 - (2+\sqrt{2})(a_1+a_2)]\theta^j/(1-\theta) \quad . \tag{2.7}$$

Letting a_1 and a_2 be any positive constants, and letting ℓ be any positive integer, one can apply this procedure to find sequences $\{\underline{x}_k;\ k=1,2,\ldots,\ell\}$ and $\{\underline{g}_k;\ k=1,2,\ldots,\ell\}$ that are consistent with the conjugate gradient method, that satisfy condition (1.9) for $m=3$, and there exist upper bounds on $\|\underline{g}_k\|$ and $\|\underline{g}_k\|^{-1}$ that are independent of k and ℓ. However, if we let $\ell\to\infty$, we violate the continuity of $\{\underline{\nabla}F(\underline{x});\ \underline{x}\varepsilon\mathbb{R}^2\}$.

Specifically, if we have first derivative continuity, and if we let $c_{3j+1}=-1$ for definiteness, its sign being determined by condition (2.3), then equation (2.6) and the form of $\underline{g}_{3j+1}$ imply the relation

$$F(\underline{x}_{3j+1}) - F(\underline{x}^*) = [(\sqrt{2}-1)a_1 + \sqrt{2}a_2]\theta^j/(1-\theta) + o(\theta^j) \quad , \tag{2.8}$$

where $F(\underline{x}^*)$ is the limit of the sequence $\{F(\underline{x}_k);\ k=1,2,3,\ldots\}$. However, expression (2.7) and the ratio

$$c_{3j+2}/c_{3j+1} = (b_3 - b_2\theta)/(b_1\theta - b_2\theta) = 4+3\sqrt{2} \tag{2.9}$$

show that the dominant part of $F(\underline{x}_{3j+2}) - F(\underline{x}^*)$ has the value

$$(4+3\sqrt{2})[(\sqrt{2}+1)a_1 + \sqrt{2}a_2]\theta^j/(1-\theta) \quad , \tag{2.10}$$

which is greater than expression (2.8) for sufficiently large j. Thus we violate the condition that the sequence of function values $\{F(\underline{x}_k);\ k=1,2,3,\ldots\}$ must decrease monotonically. It can be shown that it is not possible to overcome this defect by using other feasible values of b_1, b_2 and b_3.

This example illustrates quite well the method that is used to construct all the given examples. In particular we note that the parameters θ and $\{b_i;\ i=1,2,\ldots,m\}$ in the differences $\{\underline{\delta}_k = \underline{x}_{k+1} - \underline{x}_k;\ k=1,2,3,\ldots\}$ define the gradients $\{\underline{g}_k;\ k=1,2,3,\ldots\}$, except for the scaling factors $\{c_k;\ k=1,2,3,\ldots\}$, whose ratios are fixed by the conjugacy condition (1.8). For any choice of θ and $\{b_i;\ i=1,2,\ldots,m\}$, the points $\{\underline{x}_k;\ k=1,2,3,\ldots\}$ are found by the construction that gives the vector (2.6). At this stage the parameters $\{a_i;\ i=1,2,\ldots,m\}$ are available to help the sequence $\{F(\underline{x}_k);\ k=1,2,3,\ldots\}$ to decrease monotonically.

The following example with $n=2$ and $m=8$ shows that decreasing function values do not always conflict with second derivative continuity. Let the steps of the algorithm have the form

$$\underline{\delta}_{8j+i} = a_i \begin{pmatrix} 1 \\ b_i\phi^{2j} \end{pmatrix}, \quad \underline{\delta}_{8j+i+4} = a_i \begin{pmatrix} -1 \\ b_i\phi^{2j+1} \end{pmatrix}, \quad i=1,2,3,4, \tag{2.11}$$

where the numbers $\{a_i;\ i=1,2,3,4\}$ are all positive, and consider the values $\phi=\frac{1}{2}$, $b_1=-2$, $b_2=1$, $b_3=-1$ and $b_4=-2$. Thus, if equation (1.9) holds, we have $\theta=\phi^2=1/4$. The gradients

$$\left.\begin{array}{ll} \underline{g}_{8j+1}=\begin{pmatrix}-8\phi^{2j}\\ 2\end{pmatrix}, & \underline{g}_{8j+2}=\begin{pmatrix}-4\phi^{2j}\\ -2\end{pmatrix} \\ \underline{g}_{8j+3}=\begin{pmatrix}-\phi^{2j}\\ 1\end{pmatrix}, & \underline{g}_{8j+4}=\begin{pmatrix}3\phi^{2j}\\ 3\end{pmatrix} \end{array}\right\} \tag{2.12}$$

and the relations

$$\left.\begin{array}{l} (\underline{g}_{k+4})_1 = -\phi(\underline{g}_k)_1 \\ (\underline{g}_{k+4})_2 = (\underline{g}_k)_2 \end{array}\right\} \quad k=1,2,3,\ldots, \tag{2.13}$$

satisfy all the line search and conjugacy conditions.

Due to symmetry, we can reduce the objective function on every iteration if we achieve the relations

$$F(\underline{x}_{8j+1}) > F(\underline{x}_{8j+2}) > F(\underline{x}_{8j+3}) > F(\underline{x}_{8j+4}) > F(\underline{x}_{8j+5}) . \tag{2.14}$$

Now, when the first component of $\underline{x}$ is equal to the first component of $\underline{x}_k$, where k is any positive integer, then the values (2.12) allow the second component of $\underline{\nabla}F(\underline{x})$ to be constant, provided that the first components of the points $\{\underline{x}_{8j+i};\ i=1,2,\ldots 8\}$ are all different. Thus we satisfy the equation

$$F(\underline{x}_k) - F(\underline{x}^*) = (\underline{x}_k)_2(\underline{g}_k)_2, \quad k=1,2,3,\ldots . \tag{2.15}$$

It follows that expression (2.14) is equivalent to the inequalities

$$\begin{aligned} &-2(a_1b_1+a_2b_2+a_3b_3+a_4b_4) \\ &\quad > 2(\phi a_1b_1+a_2b_2+a_3b_3+a_4b_4) \\ &\quad > -(\phi a_1b_1+\phi a_2b_2+a_3b_3+a_4b_4) \\ &\quad > -3(\phi a_1b_1+\phi a_2b_2+\phi a_3b_3+a_4b_4) \\ &\quad > -2\phi(a_1b_1+a_2b_2+a_3b_3+a_4b_4) . \end{aligned} \tag{2.16}$$

These inequalities are consistent because, if $a_1=336$, $a_2=864$, $a_3=364$ and $a_4=1$, then the five lines of this expression take the values 348, 324, 270, 264 and 174 respectively. Further, if we let $(\underline{x}_1)_1=0$, then the first components of the vectors $\{\underline{x}_{8j+i}; i=1,2,\ldots,8\}$ have the values 0, 336, 1200, 1564, 1565, 1229, 365 and 1, which are all different.

It is straightforward to construct a twice continuously differentiable function $\{F(\underline{x}); x\in\mathbb{R}^2\}$ that satisfies the gradient conditions (2.12) and (2.13). In order to describe a suitable construction, we note that the required value

$$\underline{g}_{8j+2} = \underline{\nabla}F \begin{pmatrix} 336 \\ -324\phi^{2j} \end{pmatrix} = \begin{pmatrix} -4\phi^{2j} \\ -2 \end{pmatrix} \tag{2.17}$$

is obtained if $F(.)$ has the form

$$F(x_1,x_2) = \frac{1}{81}(x_1 - 336)x_2 - 2x_2 + e_2(x_1 - 336)^2 \tag{2.18}$$

whenever $|x_1 - 336| \leq 0.1$, where e_2 is any constant. By choosing e_2 to be sufficiently large, we ensure that $\underline{x}_{8j+2}$ is a local minimum of the objective function on the line through $\underline{x}_{8j+1}$ and $\underline{x}_{8j+2}$ for all j. The remaining gradient conditions are satisfied similarly, which defines $F(x_1,x_2)$ whenever $|x_1 - (\underline{x}_k)_1| \leq 0.1$ for some integer k. Intermediate values of $F(\underline{x})$ may then be chosen in a way that gives second derivative continuity.

To show the main disadvantage of this example we consider the line search from

$$\underline{x}_{8j+7} = \begin{pmatrix} 365 \\ 540\phi^{2j+1} \end{pmatrix} \quad \text{to} \quad \underline{x}_{8j+8} = \begin{pmatrix} 1 \\ 176\phi^{2j+1} \end{pmatrix} .$$

The point $(336, 511\phi^{2j+1})$ is on this line segment, and, due to expression (2.18), we have the value

$$F(336, 511\phi^{2j+1}) = F(\underline{x}^*) - 1022\phi^{2j+1} . \tag{2.19}$$

Therefore a smaller step-length in the line search would make the objective function much less than $F(\underline{x}^*)$, which shows that we have not satisfied the conditions of Step 4 of the algorithm of Section 1. Perhaps this algorithm always gives the limit (1.4) when $F(.)$ is twice continuously differentiable, when L is bounded, and when there are only two variables.

3. Three variable examples

First we let $n = 3$ and $m = 4$, and we consider a cycle of the form

$$\underline{\delta}_{4j+1} = a_1 \begin{pmatrix} 1 \\ b_1\phi^{2j} \\ h_1\phi^{2j} \end{pmatrix}, \qquad \underline{\delta}_{4j+2} = a_2 \begin{pmatrix} 1 \\ b_2\phi^{2j} \\ h_2\phi^{2j} \end{pmatrix},$$

$$\underline{\delta}_{4j+3} = a_1 \begin{pmatrix} -1 \\ b_1\phi^{2j+1} \\ h_1\phi^{2j+1} \end{pmatrix}, \qquad \underline{\delta}_{4j+4} = a_2 \begin{pmatrix} -1 \\ b_2\phi^{2j+1} \\ h_2\phi^{2j+1} \end{pmatrix},$$

where $j = 0,1,2,\ldots$. In this case, applying the construction that is described in Section 1, we find that $\underline{g}_{4j+2}$, for example, is a multiple of the vector

$$\begin{pmatrix} b_1(b_1 - b_2)\phi^{2j} + h_1(h_1 - h_2)\phi^{2j} \\ (b_2 - b_1) + h_1(b_2h_1 - b_1h_2)\phi^{4j} \\ (h_2 - h_1) + b_1(b_1h_2 - b_2h_1)\phi^{4j} \end{pmatrix}.$$

We avoid complicated expressions by substituting the parameter values $b_1 = 9$, $b_2 = 55$, $h_1 = h_2 = 45$ and $\phi = 5/18$, which gives the gradients

$$\underline{g}_{4j+1} = c_{4j+1} \begin{pmatrix} 360\phi^{2j} \\ 1 - 5832\phi^{4j} \\ 1 + 7128\phi^{4j} \end{pmatrix}, \quad \underline{g}_{4j+2} = c_{4j+2} \begin{pmatrix} -9\phi^{2j} \\ 1 + 2025\phi^{4j} \\ -405\phi^{4j} \end{pmatrix},$$

$$\underline{g}_{4j+3} = c_{4j+3} \begin{pmatrix} -360\phi^{2j+1} \\ 1 - 5832\phi^{4j+2} \\ 1 + 7128\phi^{4j+2} \end{pmatrix}, \quad \underline{g}_{4j+4} = c_{4j+4} \begin{pmatrix} 9\phi^{2j+1} \\ 1 + 2025\phi^{4j+2} \\ -405\phi^{4j+2} \end{pmatrix},$$

where the conjugacy condition (1.8) is obtained by forcing the multipliers $\{c_k;\ k=2, 3,4,\ldots\}$ to satisfy the equations

$$\left.\begin{aligned} c_{4j}(9 + 9\phi) &= c_{4j+1}(414\phi + 268272\phi^{4j+1}) \\ c_{4j+1}(460) &= c_{4j+2}(46 + 93150\phi^{4j}) \\ c_{4j+2}(9 + 9\phi) &= c_{4j+3}(414\phi + 268272\phi^{4j+3}) \\ c_{4j+3}(460) &= c_{4j+4}(46 + 93150\phi^{4j+2}) \end{aligned}\right\} \qquad (3.1)$$

Thus we deduce the ratios

$$\left.\begin{aligned} c_k/c_{k+2} &= (1+648\phi^k)(1+2025\phi^k),\ k \text{ even} \\ c_k/c_{k+2} &= (1+648\phi^{k+1})(1+2025\phi^{k-1}),\ k \text{ odd} \end{aligned}\right\} ,\qquad (3.2)$$

so the gradient norms $\{\|\underline{g}_k\|;\ k=1,2,3,\ldots\}$ are uniformly bounded and bounded away from zero. Moreover, equations (3.1)-(3.2) allow $c_k < 0$ for all k, so we can satisfy the descent conditions $\{\underline{\delta}_k^T\underline{g}_k < 0;\ k=1,2,3,\ldots\}$.

Because terms of order ϕ^{4j} may be ignored, the condition for monotonically decreasing function values that corresponds to expression (2.16) is the relation

$$\begin{aligned} -c_{4j+1}[(a_1b_1+a_2b_2)+(a_1h_1+a_2h_2)] &> -c_{4j+2}(\phi a_1b_1+a_2b_2) \\ &> -c_{4j+3}\phi[(a_1b_1+a_2b_2)+(a_1h_1+a_2h_2)] \quad . \end{aligned} \qquad (3.3)$$

Therefore, remembering $c_k < 0$, and noting that expression (3.1) gives the approximate ratios

$$c_{4j+1} : c_{4j+2} : c_{4j+3} \approx 1 : 10 : 1 \ , \qquad (3.4)$$

we require a_1 and a_2 to satisfy the inequalities

$$\begin{aligned} 54a_1 + 100a_2 &> 25a_1 + 550a_2 \\ &> \phi(54a_1 + 100a_2) \ . \end{aligned} \qquad (3.5)$$

The values $a_1 = 20$ and $a_2 = 1$ are suitable.

In this case, however, if we let $(\underline{x}_{4j+1})_1 = 0$, then we have the points

$$\underline{x}_{4j+1} = \begin{pmatrix} 0 \\ -235\phi^{2j}/(1-\phi) \\ -945\phi^{2j}/(1-\phi) \end{pmatrix}, \qquad \underline{x}_{4j+2} = \begin{pmatrix} 20 \\ -105\phi^{2j}/(1-\phi) \\ -295\phi^{2j}/(1-\phi) \end{pmatrix} .$$

Thus the vector

$$\hat{\underline{x}}_j = \begin{pmatrix} 1 \\ -228.5\phi^{2j}/(1-\phi) \\ -912.5\phi^{2j}/(1-\phi) \end{pmatrix} \qquad (3.6)$$

is the point on the line segment from $\underline{x}_{4j+1}$ to $\underline{x}_{4j+2}$ whose first component is $(\underline{x}_{4j+4})_1$. Thus, using the given gradients, we deduce the values

$$\left.\begin{aligned} F(\underline{x}_{4j+1}) &= F(\underline{x}^*) - 1180c_{4j+1}\phi^{2j}/(1-\phi) + o(\phi^{2j}) \\ F(\hat{\underline{x}}_j) &= F(\underline{x}^*) - 228.5c_{4j+4}\phi^{2j}/(1-\phi) + o(\phi^{2j}) \end{aligned}\right\} . \qquad (3.7)$$

Because $c_{4j+1} < 0$ and because $c_{4j+4} \approx 10c_{4j+1}$, it follows that $F(\hat{\underline{x}}_j)$ is larger than $F(\underline{x}_{4j+1})$. Therefore again the conditions of Step 4 of the algorithm of Section 1 are not satisfied. It seems that it is not possible to satisfy these conditions by adjusting the parameters a_i, b_i and h_i $(i=1,2)$.

For $n=3$ and $m=6$ we consider steps of the form

$$\underline{\delta}_{6j+i} = a_i \begin{pmatrix} 1 \\ b_i\phi^{2j} \\ h_i\phi^{2j} \end{pmatrix}, \qquad \underline{\delta}_{6j+i+3} = a_i \begin{pmatrix} -1 \\ b_i\phi^{2j+1} \\ h_i\phi^{2j+1} \end{pmatrix}, \qquad i=1,2,3. \qquad (3.8)$$

In fact it is suitable if the parameters have the values $b_1 = 1$, $b_2 = -12$, $b_3 = -0.3$, $h_1 = h_2 = 117$, $h_3 = 120.9$, $\phi = 0.3$, $a_1 = 42$, $a_2 = 21$, $a_3 = 28$ and $(\underline{x}_1)_1 = 0$, which gives the points and gradients

$$\underline{x}_{6j+1} = \begin{pmatrix} 0 \\ 312\phi^{2j} \\ -15366\phi^{2j} \end{pmatrix}, \qquad \underline{g}_{6j+1} = c_{6j+1} \begin{pmatrix} -403\phi^{2j} \\ -403\phi^{4j} \\ -1-\phi^{4j} \end{pmatrix},$$

$$\underline{x}_{6j+2} = \begin{pmatrix} 42 \\ 354\phi^{2j} \\ -10452\phi^{2j} \end{pmatrix}, \qquad \underline{g}_{6j+2} = c_{6j+2} \begin{pmatrix} -\phi^{2j} \\ 1+13689\phi^{4j} \\ -117\phi^{4j} \end{pmatrix},$$

$$\underline{x}_{6j+3} = \begin{pmatrix} 63 \\ 102\phi^{2j} \\ -7995\phi^{2j} \end{pmatrix}, \qquad \underline{g}_{6j+3} = c_{6j+3} \begin{pmatrix} 81\phi^{2j} \\ -3-42471\phi^{4j} \\ -1-4356\phi^{4j} \end{pmatrix},$$

$$\underline{x}_{6j+4} = \begin{pmatrix} 91 \\ 312\phi^{2j+1} \\ -15366\phi^{2j+1} \end{pmatrix}, \qquad \underline{g}_{6j+4} = c_{6j+4} \begin{pmatrix} 403\phi^{2j+1} \\ -403\phi^{4j+2} \\ -1-\phi^{4j+2} \end{pmatrix},$$

$$\underline{x}_{6j+5} = \begin{pmatrix} 49 \\ 354\phi^{2j+1} \\ -10452\phi^{2j+1} \end{pmatrix}, \qquad \underline{g}_{6j+5} = c_{6j+5} \begin{pmatrix} \phi^{2j+1} \\ 1+13689\phi^{4j+2} \\ -117\phi^{4j+2} \end{pmatrix},$$

$$\underline{x}_{6j+6} = \begin{pmatrix} 28 \\ 102\phi^{2j+1} \\ -7995\phi^{2j+1} \end{pmatrix}, \qquad \underline{g}_{6j+6} = c_{6j+6} \begin{pmatrix} -81\phi^{2j+1} \\ -3-42471\phi^{4j+2} \\ -1-4356\phi^{4j+2} \end{pmatrix}.$$

The signs of the gradients have been chosen so that the downhill conditions $\{\underline{\delta}_k^T \underline{g}_k < 0\,;\ k=2,3,4,\ldots\}$ are satisfied if and only if $\{c_k > 0\,;\ k=2,3,4,\ldots\}$. Further, the conjugacy condition (1.8) implies the equations

$$\left.\begin{aligned} c_{6j}(3+471900\phi^{4j}) &= c_{6j+1}(4+4\phi^{4j}) \\ c_{6j+1}(40-363\phi^{4j}) &= c_{6j+2}(1+136890\phi^{4j}) \\ c_{6j+2}(1+140400\phi^{4j}) &= c_{6j+3}(30+3953070\phi^{4j}) \end{aligned}\right\} . \tag{3.9}$$

Thus as $k \to \infty$ we have $c_{k+3}/c_k = 1 + O(\phi^{2k/3})$, which ensures that the sequences $\{\|\underline{g}_k\|\,,\ k=1,2,3,\ldots\}$ and $\{\|\underline{g}_k\|^{-1}\,;\ k=1,2,3,\ldots\}$ are uniformly bounded. We show that the required gradients allow $\{F(\underline{x})\,;\ \underline{x}\in\mathbb{R}^3\}$ to be twice continuously differentiable, and to decrease monotonically on the line segment from $\underline{x}_k$ to $\underline{x}_{k+1}$ for each k.

We begin by assuming that all terms of order ϕ^{4j} are negligible. Therefore we seek a function $\{\bar{F}(\underline{x});\ \underline{x}\in\mathbb{R}^3\}$ that satisfies the required monotonicity conditions and that has the derivative values

$$\underline{\nabla}\bar{F}\begin{pmatrix} 0 \\ 312\psi \\ -15366\psi \end{pmatrix} = \begin{pmatrix} -1209\psi \\ 0 \\ -3 \end{pmatrix}, \qquad \underline{\nabla}\bar{F}\begin{pmatrix} 42 \\ 354\psi \\ -10452\psi \end{pmatrix} = \begin{pmatrix} -120\psi \\ 120 \\ 0 \end{pmatrix},$$

$$\underline{\nabla}\bar{F}\begin{pmatrix} 63 \\ 102\psi \\ -7995\psi \end{pmatrix} = \begin{pmatrix} 324\psi \\ -12 \\ -4 \end{pmatrix}, \qquad \underline{\nabla}\bar{F}\begin{pmatrix} 91 \\ 312\psi \\ -15366\psi \end{pmatrix} = \begin{pmatrix} 1209\psi \\ 0 \\ -3 \end{pmatrix}$$

$$\underline{\nabla}\bar{F}\begin{pmatrix} 49 \\ 354\psi \\ -10452\psi \end{pmatrix} = \begin{pmatrix} 120\psi \\ 120 \\ 0 \end{pmatrix}, \qquad \underline{\nabla}\bar{F}\begin{pmatrix} 28 \\ 102\psi \\ -7995\psi \end{pmatrix} = \begin{pmatrix} -324\psi \\ -12 \\ -4 \end{pmatrix}.$$

We let $\bar{F}(.)$ have the form

$$\bar{F}(x_1,x_2,x_3) = \lambda(x_1)x_2 + \mu(x_1)x_3 \quad , \tag{3.10}$$

where x_1, x_2 and x_3 are the components of $\underline{x}$, and where $\lambda(.)$ and $\mu(.)$ are twice continuously differentiable functions of one variable such that $\lambda(x_1) = \lambda(91 - x_1)$ and $\mu(x_1) = \mu(91 - x_1)$ for $0 \le x_1 \le 91$. Further, for $0 \le x_1 \le 91$, we let $\sigma(x_1)\psi$ be the value of $\bar{F}(\underline{x})$ at the point $\underline{x}$ whose first component is x_1, and whose last two components are defined by the property that $\underline{x}$ is on the piecewise linear curve that joins

$$\begin{pmatrix} 0 \\ 312\psi \\ -15366\psi \end{pmatrix}, \quad \begin{pmatrix} 42 \\ 354\psi \\ -10452\psi \end{pmatrix}, \quad \begin{pmatrix} 63 \\ 102\psi \\ -7995\psi \end{pmatrix} \text{ and } \begin{pmatrix} 91 \\ 312\phi\psi \\ -15366\phi\psi \end{pmatrix}.$$

Therefore we require $\{\sigma(x_1);\ 0 \le x_1 \le 91\}$ to decrease strictly monotonically.

We consider in sequence the values of $\nabla\bar{F}(.)$ that are given in the previous paragraph. The first value implies $\sigma(0) = 46098$, because $\lambda(0) = 0$ and $\mu(0) = -3$, and $\sigma'(0+) = -1560$. Similarly we find $\sigma(42) = 42480$, $\sigma'(42-) = 0$, $\sigma'(42+) = -1560$, $\sigma(63) = 30756$, $\sigma'(63-) = 0$, $\sigma'(63+) = -156$, $\sigma(91) = 13829.4$, $\sigma'(91-) = 0$, $\sigma(49) = 32400$ and $\sigma(28) = 44280$, so our parameters allow $\{\sigma(x_1);\ 0 \le x_1 \le 91\}$ to be monotonic.

We let $\{\sigma(x);\ 0 \le x \le 91\}$ be any real valued function that is three times continuously differentiable on each of the intervals $[0,42]$, $[42,63]$ and $[63,91]$, that satisfies the conditions of the previous paragraph, whose first derivative is negative on $(0,42)$, $(42,63)$ and $(63,91)$, that has the second derivative values $\sigma''(42-) = \sigma''(63-) = \sigma''(91-) = M$, where M is a parameter, and, in order that $\{\bar{F}(\underline{x});\ \underline{x}\in\mathbb{R}^3\}$ is twice continuously differentiable when $x_1 = 42$ and 63, we require particular values of $\sigma''(42+)$ and $\sigma''(63+)$ that are discussed later. Of course M is positive, in order that, for $i = 1,2,3$, $\underline{x}_{6j+i+1}$ is a local minimum of $\bar{F}(.)$ on the line through $\underline{x}_{6j+i}$ and $\underline{x}_{6j+i+1}$.

The choice of $\sigma(.)$ imposes a constraint on the functions $\lambda(.)$ and $\mu(.)$ of expression (3.10). Further, due to the symmetry of $\lambda(x_1)$ and $\mu(x_1)$ about $x_1 = 45.5$, we must have that $\{\tau(x_1) \equiv \sigma(91 - x_1);\ 0 \le x_1 \le 91\}$ is the value of $\bar{F}(\underline{x})/\psi$ at the point $\underline{x}$ whose first component is x_1, and whose last two components are defined by the property that $\underline{x}$ is on the piecewise linear curve that joins

$$\begin{pmatrix} 91 \\ 312\psi \\ -15366\psi \end{pmatrix}, \quad \begin{pmatrix} 49 \\ 354\psi \\ -10452\psi \end{pmatrix}, \quad \begin{pmatrix} 28 \\ 102\psi \\ -7995\psi \end{pmatrix} \text{ and } \begin{pmatrix} 0 \\ 312\phi\psi \\ -15366\phi\psi \end{pmatrix}.$$

Thus, for each x_1, $\lambda(x_1)$ and $\mu(x_1)$ have to satisfy two equations. We claim that, having chosen $\sigma(.)$, these equations define the twice continuously differentiable functions $\lambda(.)$ and $\mu(.)$ uniquely.

For example, on the interval [63,91] we have the equations

$$\left.\begin{aligned} \sigma(x_1) &= (120.9 - 0.3x_1)\lambda(x_1) + (-15611.7 + 120.9x_1)\mu(x_1) \\ \tau(x_1) &= (403 - x_1)\lambda(x_1) + (-4719 - 117x_1)\mu(x_1) \end{aligned}\right\} , \qquad (3.11)$$

which imply the values

$$\left.\begin{aligned} \lambda(x_1) &= \frac{-(121 + 3x_1)\sigma(x_1) + (400.3 - 3.1x_1)\tau(x_1)}{4(x_1 - 91)(x_1 - 403)} \\ \mu(x_1) &= \frac{(-403 + x_1)\sigma(x_1) + (120.9 - 0.3x_1)\tau(x_1)}{156(x_1 - 91)(x_1 - 403)} \end{aligned}\right\} \qquad (3.12)$$

for $63 \le x_1 < 91$. Both $\lambda(.)$ and $\mu(.)$ are bounded near $x_1 = 91$ because, due to $\sigma(91) = 0.3\tau(91)$, the numerators of expression (3.12) are zero at $x_1 = 91$. Further, the required value of $\underline{\nabla}\bar{F}(\underline{x}_{6j+4})$ is given by continuity and by the conditions $\sigma(91) = 13829.4$, $\sigma'(91-) = 0$, $\tau(91) = 46098$ and $\tau'(91-) = 1560$. Both $\lambda(.)$ and $\mu(.)$ are twice continuously differentiable at $x_1 = 91$ because we have chosen each piece of $\sigma(.)$ to be three times continuously differentiable.

By considering the equations that correspond to expression (3.11) on each of the intervals [0,28], [28,42], [42,49] and [49,63], one can verify that $\lambda(.)$ and $\mu(.)$ are well-defined by $\sigma(.)$ and $\tau(.)$ throughout the range $0 \le x_1 \le 91$, but one has to give careful attention to the boundedness of $\lambda(.)$ and $\mu(.)$ near $x_1 = 45.5$, because it depends on the condition $\tau(45.5) = \sigma(45.5)$.

We now turn to the question of choosing $\sigma''(63+)$, for example, so that $\bar{F}(\underline{x})$ is twice continuously differentiable at $x_1 = 63$. Because $\tau(.)$ has no derivative discontinuities at $x_1 = 63$, it is sufficient if the value of $\sigma''(63+)$ allows $\lambda''(.)$ and $\mu''(.)$ to be continuous at $x_1 = 63$. Therefore we note that expression (3.11) implies the second derivative

$$\begin{aligned} \sigma''(63+) &= -0.6\lambda'(63) + 102\lambda''(63+) \\ &\quad + 241.8\mu'(63) - 7995\mu''(63+) . \end{aligned} \qquad (3.13)$$

A similar calculation on the interval [42,63] gives the identity

$$\begin{aligned} \sigma''(63-) &= -24\lambda'(63) + 102\lambda''(63-) \\ &\quad + 234\mu'(63) - 7995\mu''(63-) . \end{aligned} \qquad (3.14)$$

It follows that we must choose the value

$$\sigma''(63+) = M + 23.4\lambda'(63) + 7.8\mu'(63) \quad . \qquad (3.15)$$

The derivatives $\lambda'(63)$ and $\mu'(63)$ may be determined from equation (3.11) if

$\sigma'(63+)$ and $\tau'(63)$ are known. The derivative $\sigma'(63+)=-156$ has been specified already, and $\tau'(63)=-\sigma'(28)$ may be set to any positive number before $\sigma''(63+)$ is calculated. Thus it is straightforward to achieve second derivative continuity and the value $\sigma''(63-)=M$, where M is a positive parameter. Of course a similar technique may be used at $x_1=42$.

Having established the existence of $\bar{F}(.)$, we now modify it in order to take account of the $O(\phi^{4j})$ terms that have been ignored so far. For each integer k the required derivative $\underline{g}_k=\underline{\nabla}F(\underline{x}_k)$ is obtained by altering $\bar{F}(\underline{x})$ only for values of $\underline{x}$ that satisfy $|x_1-(\underline{x}_k)_1|<1$, where x_1 and $(\underline{x}_k)_1$ are still the first components of $\underline{x}$ and $\underline{x}_k$ respectively. Therefore it is sufficient to describe the modification for only one of the points $\{\underline{x}_{6j+i};\ i=1,2,\dots,6\}$. We give our attention to the vectors

$$\underline{x}_{6j+3}=\begin{pmatrix}63\\ 102\phi^{2j}\\ -7995\phi^{2j}\end{pmatrix},\qquad \underline{g}_{6j+3}=c_{6j+3}\begin{pmatrix}81\phi^{2j}\\ -3\text{-}42471\phi^{4j}\\ -1\text{-}4356\phi^{4j}\end{pmatrix},$$

remembering the equation

$$\underline{\nabla}\bar{F}(\underline{x}_{6j+3})=4\begin{pmatrix}81\phi^{2j}\\ -3\\ -1\end{pmatrix},$$

and that the overall scaling of the gradients provides $c_{6j+3}=4+O(\phi^{4j})$.

First we seek a function $\{\hat{F}(\underline{x})\ ;\ \underline{x}\in\mathbb{R}^3\}$ that has the gradient

$$\underline{\nabla}\hat{F}(\underline{x}_{6j+3})=4\begin{pmatrix}81\phi^{2j}\\ -3\text{-}42471\phi^{4j}\\ -1\text{-}4356\phi^{4j}\end{pmatrix}, \tag{3.16}$$

and that satisfies all the monotonicity and continuity conditions. Therefore we let $\{\eta(x_1)\ ;\ x_1\in\mathbb{R}\}$ be a twice continuously differentiable function that has the properties

$$\left.\begin{array}{ll}\eta(x_1)=0, & |x_1|\ge 1\\ \eta(0)=1\ , & \\ \eta(-x_1)=\eta(x_1)\ , & \text{all } x_1\\ \eta'(x_1)\ge 0\ , & x_1\le 0\\ \eta'(0)=0 & \end{array}\right\}, \tag{3.17}$$

and we consider the form

$$\hat{F}(x_1,x_2,x_3) = \bar{F}(x_1,x_2,x_3) + 4\,\eta(x_1 - 63)\;\hat{G}(x_2,x_3) \quad , \tag{3.18}$$

where $\hat{G}(.)$ is a homogeneous cubic function of two variables that satisfies the equation

$$\begin{pmatrix} \partial\hat{G}/\partial x_2 \\ \partial\hat{G}/\partial x_3 \end{pmatrix} = \begin{pmatrix} -42471\psi^2 \\ -4356\psi^2 \end{pmatrix} \text{ at } \begin{pmatrix} x_2 \\ x_3 \end{pmatrix} = \begin{pmatrix} 102\psi \\ -7995\psi \end{pmatrix}. \tag{3.19}$$

Thus the derivative (3.16) is obtained, and continuous second derivatives are preserved.

Let $\{\hat{\sigma}_j(x_1)\;;\; 42 \le x_1 \le 63\}$ be the value of $\hat{F}(\underline{x})$ at the point on the line segment from $\underline{x}_{6j+2}$ to $\underline{x}_{6j+3}$ whose first component is x_1. We have $\hat{\sigma}_j'(63) = 0$, and, because the contributions from $\bar{F}(.)$ and $\hat{G}(.)$ to $\sigma_j''(63)$ are both $O(\phi^{2j})$, we may choose the parameter M of $\bar{F}(.)$ so that $\hat{\sigma}_j''(63)$ is positive. Thus, not only is $\underline{x}_{6j+3}$ a local minimum on the line through $\underline{x}_{6j+2}$ and $\underline{x}_{6j+3}$, but also there exists a positive constant ε such that $\hat{\sigma}_j(x_1)$ decreases strictly monotonically for $63 - \varepsilon \le x_1 \le 63$. Now the contribution from $\bar{F}(.)$ to $\{\sigma_j'(x_1)\;;\; 42 \le x_1 \le 63 - \varepsilon\}$ is bounded above by a negative multiple of ϕ^{2j}, while the contribution to this derivative from $\hat{G}(.)$ is only $O(\phi^{4j})$. It follows that $\{\hat{\sigma}_j(x_1)\;;\; 42 \le x_1 \le 63\}$ decreases strictly monotonically for all sufficiently large values of j. Therefore, by arranging for the iterations of the conjugate gradient method to start at a later stage if necessary, we preserve the required conditions on the line search from $\underline{x}_{6j+2}$ to $\underline{x}_{6j+3}$. The same technique is also used to ensure that $\hat{F}(.)$ decreases monotonically from $\underline{x}_{6j+3}$ to $\underline{x}_{6j+4}$ and from $\underline{x}_{6j+4}$ to $\underline{x}_{6j+5}$.

In order to make a further modification to the objective function to allow for the factor c_{6j+3} in $\underline{g}_{6j+3}$, we apply the following construction. Let $u(.)$ be a twice continuously differentiable function from $\mathbb{R}$ to $\mathbb{R}$ such that $|u(t)| = O(|t|^3)$, and, in addition to the conditions (3.17), let $\eta(.)$ satisfy the equation $\{\eta(x_1) = 1\;;\; |x_1| \le \tfrac{1}{2}\}$. We choose $F(.)$ to have the form

$$F(\underline{x}) = \hat{F}(\underline{x}) + \eta(x_1 - 63)\, u(\hat{F}(\underline{x})), \quad \underline{x}\in\mathbb{R}^3 \quad . \tag{3.20}$$

Then $\underline{\nabla}F(\underline{x}) = \underline{\nabla}\hat{F}(\underline{x})$ for $|x_1 - 63| \ge 1$, and we have the gradient

$$\underline{\nabla}F(\underline{x}) = [1 + u'(\hat{F}(\underline{x}))]\underline{\nabla}\hat{F}(\underline{x}) \quad , \quad |x_1 - 63| \le \tfrac{1}{2} \;. \tag{3.21}$$

Further, for $\tfrac{1}{2} \le |x_1 - 63| \le 1$, the directional derivatives of $[F(.) - \hat{F}(.)]$ along the lines from $\underline{x}_{6j+2}$ to $\underline{x}_{6j+3}$, from $\underline{x}_{6j+3}$ to $\underline{x}_{6j+4}$, and from $\underline{x}_{6j+4}$ to $\underline{x}_{6j+5}$ are only $O(\phi^{4j})$. Therefore we apply the technique of the previous paragraph to ensure that $F(.)$ inherits the required monotonicity properties of $\hat{F}(.)$ for

$|x_1 - 63| \geq \frac{1}{2}$. Because the remaining monotonicity conditions are satisfied if the factor $[1 + u'(\hat{F}(\underline{x}))]$ in equation (3.21) is positive, we make a further postponement of the start of the conjugate gradient iterations if necessary to ensure $u'(\hat{F}(\underline{x})) < 1$ for all $\hat{F}(\underline{x})$ in $[0, \hat{F}(\underline{x}_1)]$.

Expressions (3.16) and (3.21) imply that we require $u(.)$ to satisfy the conditic

$$1 + u'(\hat{F}(\underline{x}_{6j+3})) = \tfrac{1}{4}c_{6j+3} \ , \tag{3.22}$$

and equation (3.9) and the scaling of gradients give the value

$$\tfrac{1}{4}c_{6j+3} = \prod_{\ell=1}^{\infty} \frac{(4 + 4\phi^{4j+2\ell})(1 + 13689\phi^{4j+2\ell})(30 + 395307\phi^{4j+2\ell})}{(3 + 471900\phi^{4j+2\ell})(40 - 363\phi^{4j+2\ell})(1 + 14040\phi^{4j+2\ell})} \ . \tag{3.23}$$

Thus $\tfrac{1}{4}c_{6j+3} = v(\phi^{2j})$, where $v(.)$ is the function

$$v(t) = \prod_{\ell=1}^{\infty} \frac{(1 + t^2\phi^{2\ell})(1 + 13689t^2\phi^{2\ell})(1 + 13176.9t^2\phi^{2\ell})}{(1 + 15730t^2\phi^{2\ell})(1 - 9.075t^2\phi^{2\ell})(1 + 14040t^2\phi^{2\ell})} \ , \tag{3.24}$$

which is analytic for small t and satisfies $v(t) = 1 + O(t^2)$. Moreover, by integrating $\underline{\nabla}\hat{F}(.)$ along the straight line from $(63,0,0)$ to $\underline{x}_{6j+3}$, we find the value

$$\hat{F}(\underline{x}_{6j+3}) = 30756\phi^{2j} + 40658904\phi^{6j} \ . \tag{3.25}$$

Therefore we define $u(.)$ by the equations

$$\left.\begin{aligned} u'(30756t + 40658904t^3) &= v(t) - 1 \\ u(0) &= 0 \end{aligned}\right\} , \tag{3.26}$$

which gives $|u(t)| = O(|t^3|)$. The definition of $F(\underline{x})$ for $|x_1 - 63| \leq 1$ is now complete. Similar constructions are used to form $F(\underline{x})$ when x_1 is close to other values of $(\underline{x}_k)_1$.

4. Discussion

Because Sections 2 and 3 only describe successful or partially successful attempts to construct counter-examples to the global convergence of the conjugate gradient method, we mention now some other sequences that were tried that satisfy the periodicity conditions (1.9).

When $m=2$, $\underline{d}_k^T\underline{d}_{k-1}$ must be negative for all sufficiently large k, and in this case, by Step 3 of the algorithm of Section 1, we have $\beta_k<0$. However, $\beta_k<0$ and equation (1.1) imply the condition

$$\begin{aligned}|\beta_k| &= (\underline{g}_k^T\underline{g}_{k-1} - \|\underline{g}_k\|^2)/\|\underline{g}_{k-1}\|^2 \\ &\leq (\|\underline{g}_k\|/\|\underline{g}_{k-1}\|) - (\|\underline{g}_k\|/\|\underline{g}_{k-1}\|)^2 \\ &\leq \tfrac{1}{4}, \qquad\qquad \beta_k<0, \end{aligned} \tag{4.1}$$

where the last line is just the maximum value of the function $\{t-t^2\ ;\ t\in\mathbb{R}\}$. Therefore, for $m=2$, the numbers $\{\|\underline{d}_k\|\ ;\ k=1,2,3,\ldots\}$ remain bounded, which implies the limit (1.4).

Further, in every complete cycle of the form (1.9) we have $\underline{d}_k^T\underline{d}_{k-1}<0$ at least twice for sufficiently large k, so, if $\|\underline{d}_k\|\to\infty$, which is necessary in a counter-example, some mechanism has to combat the regular small values of the ratio $\|\underline{d}_k\|/\|\underline{d}_{k-1}\|$ that are implied by inequality (4.1). It is therefore a little surprising that the first example of Section 2 shows that a suitable mechanism can exist when $m=3$. The mechanism is that, due to equation (1.1), a large positive value of β_k occurs when $\|\underline{g}_k\| >> \|\underline{g}_{k-1}\|$, but in this case for $n=2$, due to the fact that $(\underline{g}_k)_1\to 0$, we have $F(\underline{x}^*)<F(\underline{x}_k)<F(\underline{x}_{k-1})$ only if $|(\underline{x}_k)_2|$ is much smaller than $|(\underline{x}_{k-1})_2|$, which is why the first example of Section 2 is unsatisfactory. In three dimensions, however, the relations $\|\underline{g}_k\| >> \|\underline{g}_{k-1}\|$ and $F(\underline{x}^*)<F(\underline{x}_k)<F(\underline{x}_{k-1})$ imply only that the projection of $(\underline{x}_k-\underline{x}_{k-m})$ in the direction of $\underline{g}_k$ must be small, which allows enough freedom for the first example of Section 3, but it seems that the nice properties of the given $n=3$, $m=4$ case cannot be achieved when $n=m=3$.

The success of the $n=2$, $m=8$ example of Section 2 was not expected by the author, because attempts to make the function values $\{F(\underline{x}_k)\ ;\ k=1,2,3,\ldots\}$ decrease strictly monotonically, $F(.)$ being twice continuously differentiable, had failed for the form of symmetry of expression (2.11) using $n=2$, $m=4$ and $n=2$, $m=6$. The numbers that occur in the second example of Section 3 were found in the way that is suggested in Section 1, namely the conditions for consistency with the conjugate gradient method were expressed as inequality constraints on the parameters, and then a search was made for feasible values.

The examples of Section 2 are relevant not only to the conjugate gradient method, but also to all variable metric algorithms in Broyden's linear family that make exact line searches (see Fletcher, 1980, for instance). The reason is well-known, namely that condition (1.8) and $\underline{d}_k^T \underline{g}_k < 0$ define the direction of $(\underline{x}_{k+1} - \underline{x}_k)$ when there are only two variables. Therefore the DFP and BFGS algorithms may fail to converge, if the condition on the step-length α_k is only that it be a local minimum of the function $\{F(\underline{x}_k + \alpha \underline{d}_k)\ ;\ \alpha \geq 0\}$ that satisfies $F(\underline{x}_k + \alpha_k \underline{d}_k) < F(\underline{x}_k)$. An important consequence of this remark is that if a proof of convergence of one of these algorithms for general twice continuously differentiable objective functions could be found, which now seems unlikely, then the proof would depend on line search conditions that are stronger than one usually assumes. Examples where the DFP algorithm fails to converge are also given by Thompson (1977), but he allows the objective function to have first derivative discontinuities.

The last example of Section 3 shows that the Polak-Ribière version of the conjugate gradient algorithm without restarts, described in Section 1, may fail to find small values of $\|\underline{\nabla} F(\underline{x})\|$ in exact arithmetic. The given objective function may be modified so that it is ℓ times continuously differentiable, where ℓ is any positive integer.

Finally we turn our attention to the Fletcher-Reeves version of the conjugate gradient algorithm, although it is sometimes much less efficient than the Polak-Ribière version (Powell, 1977). Therefore we let the parameter β_k of the algorithm of Section 1 have the value

$$\beta_k = \|\underline{g}_k\|^2 / \|\underline{g}_{k-1}\|^2 \ , \tag{4.2}$$

instead of expression (1.1). Because β_k is now positive for all k, it is no longer possible for $\|\underline{d}_{k-1}\|$ and $\|\underline{d}_k\|$ to be very large and for $\underline{d}_k^T \underline{d}_{k-1}$ to be negative, which rules out examples of the form that are given in Sections 2 and 3. In fact, assuming the conditions that are stated in Section 1, it can be proved as follows that the Fletcher-Reeves algorithm gives the limit (1.4).

From the definition of $\underline{d}_k$ and exact line searches we deduce the equation

$$\begin{aligned} \|\underline{d}_k\|^2 &= \|\underline{g}_k\|^2 + \beta_k^2 \|\underline{d}_{k-1}\|^2 \\ &= \|\underline{g}_k\|^2 + \beta_k^2 [\|\underline{g}_{k-1}\|^2 + \beta_{k-1}^2 \|\underline{d}_{k-2}\|^2] = \dots \\ &= \sum_{\ell=1}^{k} \{ \prod_{j=\ell+1}^{k} \beta_j^2 \} \|\underline{g}_\ell\|^2 = \sum_{\ell=1}^{k} \|\underline{g}_k\|^4 / \|\underline{g}_\ell\|^2 \ , \end{aligned} \tag{4.3}$$

where the product is defined to be one if $\ell = k$, and where the last line depends on the value (4.2). Further, we recall that $\|\underline{g}_k\|$ is bounded above because $\underline{x}_k$ is in the level set (1.3). Therefore, if the gradients were bounded away from zero, we would have $\|\underline{d}_k\|^2 \leq kc$, where c is a positive constant. Thus the sum

$$\sum_k \rho_k^2 = \sum_k \|\underline{g}_k\|^2 / \|\underline{d}_k\|^2 \tag{4.4}$$

would be divergent, which would contradict the remarks that follow inequality (1.7). Hence the Fletcher-Reeves version of the conjugate gradient algorithm achieves the limit (1.4).

Our results suggest that further attention should be given to the choice of the parameters $\{\beta_k;\ k=1,2,3,\ldots\}$ in the conjugate gradient method.

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