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A STUDY OF CONJUGATE GRADIENT METHODS.(U)
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(6) A STUDY OF CONJUGATE GRADIENT METHODS.

by

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Abstract

We prove a number of new properties of algorithms of the Conjugate Gradient type, paying particular attention to methods which utilize variable metric information in determining the conjugate gradient search directions. We attempt a comprehensive discussion of conjugate gradient methods, and present each algorithm within the context of other existing algorithms, an approach which provides fresh insights and some new algorithms.

A STUDY OF CONJUGATE GRADIENT METHODS

L. Nazareth and J. Nocedal

1. Introduction

In 1964 Fletcher and Reeves [1] showed how the conjugate gradient method of Hestenes and Stiefel [2] for solving systems of linear equations could be extended and used to find local minima of non-linear functions. Since then many variants of this algorithm have appeared in the literature. Methods belonging to the conjugate gradient family are particularly valuable when the number of variables is large.

In this paper we prove a number of new properties of conjugate gradient type algorithms, paying particular attention to methods which utilize variable metric information in determining the conjugate gradient steps. We attempt a comprehensive discussion of conjugate gradient methods, and present each algorithm within the context of existing algorithms, an approach which yields dividends by providing fresh insights and some new algorithms. Our concern is with conjugate gradient methods for non-linear unconstrained optimization. Extensive work on conjugate gradient methods for linear systems, e.g. Concus, Golub and O'Leary [3] is not discussed here, though we believe our work also has applications in this area.

Our paper is organized as follows:

Basic conjugate gradient methods are discussed in Section 2.

An important generalization of conjugate gradient methods in which the metric is varied, are discussed in Section 3.

In Section 4 we discuss conjugate gradient methods which relax the requirement that line searches be exact.

Finally in Section 5, we look at extensions of algorithms in Section 4 to the case when the metric is varied.

Within each of the above sections, we discuss one or more of the following:

a) basics--algorithms, properties and interpretations

b) generalizations--in particular to arbitrary metrics and to arbitrary starting directions

c) strategies--scaling, and when and how often to restart.

Subsequent parts of this research deal with convergence analysis [4] and we hope eventually to develop a documented and distributable FORTRAN implementation.

2. Conjugate Gradient Methods

We summarize in this section some known results about the conjugate gradient method. We are concerned with the problems of finding a local minima of a function $f(x)$, $x \in \mathbb{R}^n$. We denote this gradient of f at x_k by $g(x_k)$ or g_k. Let $y_k \triangleq g_{k+1} - g_k$ and $s_k \triangleq x_{k+1} - x_k$.

2.1. Basics

2.1.1. Algorithms

The conjugate gradient method, originally developed by Hestenes and Stiefel [2] to solve systems of linear equations, was adapted to the non-linear unconstrained optimization problem by Fletcher and Reeves [1] in the following way:

Given x_0, let $d_0 = -g(x_0)$.

For $k = 1, 2, \ldots$, let

$$d_k = -g_k + \beta_k d_{k-1} \tag{2.1}$$

where $\beta_k \triangleq \|g_k\|^2 / \|g_{k-1}\|^2$ and $\|\cdot\|$ is the Euclidean norm.

$$x_{k+1} = x_k + \lambda_k d_k \tag{2.2}$$

where λ_k is chosen to minimize f along d_k.

This algorithm is restarted every n or $(n+1)$ iteration.

2.1.2. Properties and Interpretations

a) Several alternate forms of (2.1) have been proposed. The two most popular are

$$\beta_k = \begin{cases} g_k^T y_{k-1} / \|g_{k-1}\|^2 & \text{Polak-Ribiere [5]} \\ g_k^T y_{k-1} / d_{k-1}^T y_{k-1} & \text{Hestenes-Stiefel} \end{cases} \qquad (2.3)$$

When applied to the quadratic function $\psi(x) = \frac{1}{2}(x-x^*)^T A(x-x^*)$, $x \in \mathbb{R}^n$, when A is a positive definite and symmetric matrix, each of the above three algorithms has the following properties (i) finite termination in, at most, n steps; (ii) $g_i^T g_j = 0$, $\forall i > j$, and (iii) $d_i^T y_j = 0$, $i \neq j$ (i.e. directions are conjugate). As long as $g_k \neq 0$, g_k will be linearly independent of $g_1, \ldots, g_{k-1}$ and a new conjugate direction d_k can be developed. If $g_k = 0$, for some $k \leq n$, then the minimum is located in fewer then n steps.

Let $G \triangleq [g_0, \ldots, g_{k-1}]$, $D \triangleq [d_0, \ldots, d_{k-1}]$. Then for quadratics

(i) Each direction lies in the space spanned by previous gradients, i.e. $-G = DR$ when R is upper triangular--called the direction-gradient relation.

(ii) $D^T A D = \alpha$, where α denotes a diagonal matrix

(iii) $A(x_i - x_{i-1}) = (g_i - g_{i-1})$, $i = 1,2,\ldots,k$. These can be written as $AD\lambda = GH$ where $\lambda = \text{diag}(\lambda_0 \cdots \lambda_{k-1})$, λ_i is given by (2.2) and H is a particular upper Hessenberg matrix

$$\begin{bmatrix} -1 & & & & & & \\ 1 & -1 & & & & & \\ & 1 & . & & & & \\ & & . & . & & & \\ & & & . & . & & \\ & & & & . & -1 & \\ & & & & & 1 & -1 \end{bmatrix}$$

(iv) $G^TG = \beta$, β is also diagonal

In summary

$$\left.\begin{aligned} -G &= DR \\ D^TAD &= \alpha \\ AD\lambda &= GH \\ G^TG &= \beta \end{aligned}\right\} \qquad (2.3a)$$

These relations can be manipulated as discussed in Nazareth [6].

All three algorithms mentioned above are the same for quadratics. For arbitrary functions, even when line searches are not exact, successive search directions in the Hestenes-Stiefel algorithm are "conjugate," i.e. $d_k^T y_{k-1} = 0$. For arbitrary functions, the Hestenes-Stiefel and Polak-Ribiere algorithms are the same when line searches are exact. When applied to arbitrary functions and line searches are inexact, the algorithms differ, and Powell [7] has explained why the Polak-Ribiere variant is to be preferred. The reason is that if poor search directions are being generated, and successive iterates are close, so $g_k \tilde{=} g_{k-1}$, then $\beta_k \to 0$; hence the search direction reverts to the negative gradient direction, permitting the algorithm to recover.

It has been shown that all the above algorithms have an n-step quadratic rate of convergence when line searches are exact, Daniel [8], Cohen [9], Polak [10]. This condition on accuracy of the line search can be relaxed to "asymptotically exact," see Kawamura and Volz [11], Lenard [12].

b) If the starting search direction is not along the negative gradient direction $(-g_1)$, then the above algorithms do not usually have finite termination on a quadratic. Indeed, Powell [13] has shown that either termination occurs, or this rate of convergence is linear, the second being more usual. The algorithms can be modified to retain the quadratic termination property as described in Section 2.2.

c) There are three interpretations of the conjugate gradient method (2.1), as applied to quadratic functions, which are of value in explaining some of its properties. Each interpretation also serves as a good staging ground for extending the conjugate gradient method and analyzing the resulting algorithms, as we shall see later.

(1) Interpretation I: Relationship to BFGS method

The BFGS method [14] is currently considered to be the most effective member of the Broyden β-class [14] of Variable Metric updates (see Appendix 1 for a definition of the β-class and d_j^{β}). When the c.g. method or any method of the β-class is applied to a quadratic function, with $d_1^{cg} = d_1^{\beta} = -g_1$ and line searches are exact, it is well known that there is

no flexibility in the choice of subsequent search directions up to multiplication by a scalar; d_j^{cg} and d_j^{β} are, in consequence, linearly dependent. In Nazareth [15], it is shown that the member of the β-class for which these vectors are precisely the same (i.e. equal in magnitude and direction) is the BFGS update. The result is also taken a step further in [15], where it is shown that for arbitrary functions the BFGS algorithm may be interpreted as a conjugate gradient method in which the metric is updated at each step, using any member of the β-class. This observation leads to the generalized conjugate gradient methods of Section 3, where we shall elaborate further upon these brief remarks.

(ii) Interpretation II: Specialized Gram-Schmidt

Given any vector g_j, and a set of search directions $d_1,\ldots,d_{j-1}$, which are conjugate w.r.t A (orthogonal in the inner product defined by A), then vector d_j which lies in the subspace $g_j, d_1,\ldots,d_{j-1}$ and is conjugate to $d_1,\ldots,d_{j-1}$, will have a component in each of the directions $d_1,\ldots,d_{j-1}$. However when g_j is the gradient vector at x_j, then g_j is itself conjugate to $d_1,\ldots,d_{j-2}$. Thus the conjugate gradient method can be viewed as a specialized version of Gram-Schmidt where the vector d_j is chosen to lie in the space spanned by g_j and d_{j-1} which is conjugate to d_{j-1}. Note that these statements require that line searches be exact. Later we show that when line searches are not exact, another specialized version of Gram-Schmidt arises, and this in turn leads to a very natural extension of the conjugate-gradient method.

(iii) Interpretation III: Implicit Lanczos

This Lanczos process is a particular generalized Hessenberg process, the latter being defined as follows:

Given a matrix A and a set of n linearly independent vectors x_i which are columns of X, and an arbitrary initial vector g_0, develop vectors $g_1, g_2, \ldots, g_k$ with $G \triangleq (g_0, g_1, \ldots, g_{n-1})$ s.t.

$$\left.\begin{aligned} AG &= GH \\ G^T X &= U \end{aligned}\right\} \tag{2.4}$$

where H is upper Hessenberg and U is upper triangular. x_i need not be specified beforehand. If they are taken to be the same as g_i and if A is a symmetric matrix, then (2.4) becomes Arnold's method or the symmetric Lanczos method, (see Wilkinson [16]) for tridiagonalizing a symmetric matrix, the latter two methods being equivalent. This is given by

$$\left.\begin{aligned} AG &= GT \\ G^T G &= \alpha \end{aligned}\right\} \tag{2.5}$$

T tridiagonal, α diagonal.

Note in particular that $g_k \in [g_0, Ag_0, \ldots, A^k g_0]$ and is orthogonal to $[g_0, g_1, \ldots, g_{k-1}]$, where $[u_0, \ldots, u_k]$ denotes the subspace spanned by $u_0, \ldots, u_k$. It is not difficult to see that the c.g. method implicitly carries out the above process, where G is identified with the matrix of gradients.

If, for some k, $Ag_k \in [g_0, g_1, \ldots, g_k] = [g_0, Ag_0, \ldots, A^k g_0]$ then the successive gradients $g_0, \ldots, g_{k+1}$ are linearly dependent. In this case the minimum lies in the subspace spanned by $d_0, \ldots, d_k$ (see Nazareth [17]) and $g_{k+1} = 0$. When A has only $m < n$ distinct eigenvalues, it is easy to show that the Krylov sequence $g_0, Ag_0, A^2 g_0, \ldots,$ has only m linearly independent vectors. Thus the conjugate gradient method will terminate in m steps.

We shall later show that the Lanczos process and an associated Krylov sequence also underlies a member of the conjugate gradient family of methods, called the three term occurrence.

Some convergence results very closely related to the above interpretation are given in Luenberger [18], where the c.g. method is viewed as an optimal process over a space of polynomials.

Given an arbitrary starting point x_0 let

$$x_{k+1} = x_0 + P_k(A)g_0$$

where $P_k(A)$ is any polynomial of degree k.

If x^* is the optimum point, then

$$g_0 = A(x_0 - x^*) \tag{2.6}$$

and

$$(x_{k+1} - x^*) = [I + AP_k(A)](x_0 - x^*) \tag{2.7}$$

It can be shown that:

(i) $E(x_{k+1}) \triangleq f(x_{k+1}) - f(x^*) = \frac{1}{2}(x_0-x^*)^T A[I + AP_k(A)]^2 (x_0-x^*)$ (2.8)

(ii) The conjugate gradient method implicitly selects the polynomial $P_k(A)$ of degree k for which E_{k+1} is minimized.

(iii) $E(x_{k+1}) \leq \max_{\lambda_i}[1 + \lambda_i P_k(\lambda_i)]^2 E(x_0)$ (2.9)

where the maximum is taken over all eigenvalues of A. If there are m distinct eigenvalues, then P_m can be chosen so that $E_{m+1} = 0$ and from (1) it follows that the conjugate gradient method converges in as many steps as there are distinct eigenvalues (as was seen above in the discussion on the Lanczos process).

Luenberger [18] also shows that

$$E(x_t) \leq \frac{(\lambda_{n-t} - \lambda_1)^2}{(\lambda_{n-t} + \lambda_1)^2} E(x_0) , \qquad 0 < t < n \qquad (2.10)$$

where $\lambda_1,\ldots,\lambda_n$ are the eigenvalues of A in non-decreasing order.

2.2. Generalizations

Let F be the strictly convex quadratic function

$$F(x) = \frac{1}{2}(x-x^*)^T A(x-x^*) \qquad (2.11)$$

and let H be a symmetric and positive definite matrix $(H > 0)$. H can be factorized in various ways, e.g. as $H = LL^T$, where L is lower triangular and nonsingular.

Let us define the transformation of variables $(x-x^*) = Lz$ and let us represent the function in the z-space by $h(z)$. Then

$$h(z) \triangleq f(x^* + Lz) = f(x) = \frac{1}{2} z^T L^T A L z \qquad (2.12)$$

and

$$\nabla h(z) = (L^T A L) z = L^T \nabla f(x) .$$

Also $\nabla h(0) = 0$, and correspondingly $\nabla f(x^*) = 0$.

Suppose that we apply the conjugate gradient method, say the Fletcher-Reeves to $h(z)$. Let us denote $\nabla h(z_k)$ by $\hat{g}_k$ and search directions in the z-space by $\hat{d}_k$. Thus $\hat{g}_k = L^T g_k$ and $d_k = L\hat{d}_k$. Then:

$$\begin{aligned} \hat{d}_0 &= -\hat{g}_0 \\ \hat{d}_k &= -\hat{g}_k + \frac{\|\hat{g}_k\|^2}{\|\hat{g}_{k-1}\|^2} \hat{d}_{k-1} \end{aligned} \qquad (2.13)$$

Also if α_k is the step from a point x_k along d_k which minimizes $f(x)$, then α_k is also the step from $z = L^{-1}(x_k - x^*)$ along $\hat{d}_k$ which minimizes $h(z_k) \cdot (g(x_k)^T d_k = \hat{g}(z_k)^T \hat{d}_k)$.

In the space of the original variables (2.13) becomes

$$\begin{aligned} d_0 &= -Hg_0 \\ d_k &= -Hg_k + \frac{\|g_k\|_H^2}{\|g_{k-1}\|_H^2} d_{k-1} \end{aligned} \qquad (2.14)$$

where $\|v\|_H = v^T H v$.

We call (2.14) the conjugate gradient method with metric H or preconditioned conjugate gradient method (Axelsson [28]). Some properties of the method, analogous to those discussed in Section 2.1, are:

(i) $\quad g_i^T H g_j = 0, \qquad i \neq j$

(ii) $\quad \hat{E}(z_t) \leq \dfrac{(\sigma_{n-t} - \sigma_1)}{(\sigma_{n-t} + \sigma_1)} \hat{E}(z_0)$ (2.15)

when $\{\sigma_1,\ldots,\sigma_n\}$ are the eigenvalues of L^TAL in increasing order and $\hat{E}(z_t) = \frac{1}{2} z^T L^T A L z = E(x_t)$, and so the conjugate gradient method with metric H satisfies (2.15). If H resembles A^{-1} we can expect that L^TAL "approaches" the identity so that the function values will decrease faster.

Suppose that H was obtained from a quasi-Newton iteration, which for a quadratic satisfies

$$Hy_j = s_j , \qquad j = 1,2,\ldots,t \tag{2.16}$$

when s_j denotes a step and y_j the corresponding change of gradient. Then

$$HAs_j = LL^TA s_j = s_j, \qquad j = 1,2,\ldots,t \tag{2.17}$$

$$(L^TAL)(L^{-1}s_j) = (L^{-1}s_j) , \qquad j = 1,2,\ldots,t \tag{2.18}$$

The vectors $L^{-1}s_j$ are linearly independent so that L^TAL has t unit eigenvalues. The conjugate gradient method with metric H would find the solution in at most $n-t$ steps. Although this result is only true for quadratics, it should motivate the use of the conjugate gradient iteration (2.14) where the metric is obtained by quasi-Newton updates, e.g. Broyden [14], Davidon [19].

2.2.2. Generalization to Arbitrary Starting Direction

So far we have assumed that $d_0 = -g_0$. Beale [20] has shown how d_0 may be taken to be an arbitrary starting direction and the quadratic termination properties of the conjugate gradient method retained by modifying the defining relations as follows:

$$
\begin{aligned}
&d_0 \text{ given} \\
&d_1 = -g_1 + \frac{g_1^T y_0}{d_0^T y_0} d_0 \qquad (2.19) \\
&d_k = -g_k + \frac{g_k^T y_{k-1}}{d_{k-1}^T y_{k-1}} d_{k-1} + \frac{g_k^T y_0}{d_0^T y_0} d_0, \quad k \geq 2 \\
&x_{k+1} = x_k + \alpha_k d_k, \text{ where } \alpha_k \text{ is chosen to minimize the} \\
&\qquad\qquad \text{function along } d_k.
\end{aligned}
$$

Equations (2.19) defines a cycle of n-steps. When the cycle is finished, a new direction d_0 is defined, and a new cycle is stated. Note that when d_0 is the negative gradient, we obtain the usual conjugate gradient method.

It is easily seen that Beale's method applied to a quadratic function develops conjugate directions and find the solution in, at most, n iterations.

Also it is easily seen that

$$d_1 \in [g_0, d_0, Ad_0]$$

$$d_2 \in [g_0, Ag_0, d_0, Ad_0, A^2 d_0]$$

and in general

$$d_k \in [g_0, Ag_0, \ldots, A^{k-1} g_0, d_0, Ad_0, \ldots, A^k d_0].$$

Therefore

$$[d_0,\ldots,d_k] \in [g_0,\ Ag_0,\ldots,A^{k-1}g_0,\ d_0,\ Ad_0,\ \ldots\ ,\ A^k d_0] \qquad (2.20)$$

Let $E(x_k)$ be defined as in (2.8) and suppose that

$$\begin{aligned} 0 < a \le \lambda_1 \le \lambda_2 \le \cdots \le \lambda_{n-k} \le b \\ b < \lambda_{n-k+1} \le \lambda_{n-k+2} \le \cdots \le \lambda_n \end{aligned} \qquad (2.21)$$

where the λ's are the eigenvalues of A.

We now prove the following result, which extends (2.10).

Theorem 2.1. For any $x_0 \in \mathbb{R}^n$, but $x_1, x_2, \ldots, x_n$ be generated by Beale's Method when applied to the quadratic function $\psi(x) = \frac{1}{2}(x-x^*)^T A(x-x^*)$. Assume that d_0 is such that

$$[d_0,\ldots,d_k] = [g_0,\ Ag_0,\ldots,A^{k-1}g_0,\ d_0,\ Ad_0,\ldots,\ A^k d_0] \ ^{(1)} \qquad (2.21a)$$

for $1 \le k \le n$. Then

$$E(x_{k+1}) \le \left(\frac{b-a}{b+a}\right)^2 [E(x_0) + d_0^T A(x_0 - x^* + \tfrac{1}{2} d_0)] .$$

Proof. Beale's method is a conjugate direction method, and therefore minimizes $\psi(x)$ (also the function E) over the space $[d_0,\ldots,d_k]$.

Consider the iteration

$$x_{k+1} = x_0 + P_{k-1}(A)g_0 + S_k(A)d_0 . \qquad (2.22)$$

(1) Conditions which ensure this are given below.

where P_{k-1} and S_k are polynomials in A of degree k-1 and k respectively. Thus the polynomials that minimize $E(x_{k+1})$ are those obtained by Beale's method. Now

$$(x_{k+1} - x^*) = (x_0-x^*) + P_{k-1}(A)\, A(x_0-x^*) + S_k(A)d_0 \qquad (2.23)$$

$$= [I + P_{k-1}(A)A]\, (x_0-x^*) + S_k(A)d_0$$

Choose

$$s_k = (I + P_{k-1}(A)A] \qquad (2.24)$$

We have

$$E(x_{k+1}) \leq \frac{1}{2}\, [(x_0-x^*) + d_0]^T\, [I+P_{k-1}(A)A]\, A[I+P_{k-1}(A)A](x_0-x^*+d_0)]$$

$$= \frac{1}{2}\, (x_0-x^*)^T\, A[I + P_{k-1}(A)A]^2\, (x_0-x^*)$$

$$+ d_0^T A[I + P_{k-1}(A)A]^2\, (x_0-x^*) + \frac{1}{2}\, d_0^T A[I + P_{k-1}(A)A]^2\, d_0$$

(2.25)

Let $\{e_i\}$ be an orthonormal set of eigenvalues of A and let

$$(x_0-x^*) = \sum_{i=1}^{n} \xi_i e_i \quad \text{and} \quad P_{k-1}(A) = \alpha_0 I + \alpha_1 A + \cdots + \alpha_{k-1} A^{k-1} \qquad (2.26)$$

Then

$$P_{k-1}(A)(x_0-x^*) = \alpha_0 + \sum_{i=1}^{n} \xi_i e_i + \cdots + \alpha_{k-1} \sum_{i=1}^{n} \xi_i e_i \lambda_i^{k-1} \qquad (2.27)$$

$$[I + AP_{k-1}(A)](x_0-x^*) = \Sigma\, \xi_i e_i + \alpha_0\, \Sigma\, \xi_i e_i \lambda_i + \cdots + \alpha_{k-1} \Sigma\, \xi_i e_i \lambda_i^k$$

$$= \Sigma\, \xi_i e_i (1 + \alpha_0 \lambda_i + \cdots + \alpha_{k-1} \lambda_i^*) \qquad (2.28)$$

$$P_{k-1}(A)[I + AP_{k-1}(A)](x_0 - x^*)$$

$$= \alpha_0 \Sigma \xi_i e_i (1 + \alpha_0\lambda_i + \cdots + \alpha_{k-1}\lambda_i^k + \cdots + \alpha_{k-1} \Sigma \xi_i e_i \lambda_i^{k-1}(1 + \alpha_0\lambda_i + \cdots + \alpha_{k-1}\lambda_i^k) \quad (2.29)$$

$$[I + AP_{k-1}(A)]^2(x_0 - x^*)$$

$$= \Sigma \xi_i e_i + \alpha_0 \Sigma \lambda_i \xi_i e_i (1 + \cdots + \alpha_{k-1}\lambda_i^k) + \cdots + \alpha_{k-1} \Sigma \xi_i e_i \lambda_i^k (1 + \cdots + \alpha_{k-1}\lambda_i^k) \quad (2.30)$$

$$A[I + AP_{k-1}(A)]^2(x_0 - x^*)$$

$$= \Sigma \xi_i e_i \lambda_i (1 + \alpha_0\lambda_i + \cdots + \alpha_{k-1}\lambda_i^k)(1 + \alpha_0\lambda_i + \cdots + \alpha_{k-1}\lambda_i^k)$$

$$= \Sigma \xi_i e_i \lambda_i [1 + \lambda_i P_{k-1}(\lambda_i)]^2 \quad (2.31)$$

$$(x_0^T - x^*)\, A[I + AP_{k-1}(A)]^2(x_0 - x^*) = \Sigma \xi_i^2 \lambda_i [1 + \lambda_i P_{k-1}(\lambda_i)]^2 .$$

Let $d_0 = \sum_{i=1}^n \beta_i e_i$, then

$$d_0^T A[I + AP_{k-1}(A)]^2(x_0 - x^*) = \Sigma \xi_i \beta_i \lambda_i [1 + \lambda_i P_{k-1}(\lambda_i)]^2 \quad (2.32)$$

$$d_0^T A[I + AP_{k-1}(A)]^2 d_0 = \Sigma \xi_i^2 \lambda_i [1 + \lambda_i P_{k-1}(\lambda_i)]^2 \quad (2.33)$$

Therefore, for any P_{k-1}

$$E(x_{k+1}) \leq \Sigma (\tfrac{1}{2} \xi_i^2 + \xi_i \beta_i + \tfrac{1}{2} \beta_i^2)\, \lambda_i [1 + \lambda_i P_{k-1}(\lambda_i)]^2$$

$$\leq \max_{\lambda_i} [1 + \lambda_i P_{P-1}(\lambda_i)]^2 \, \tfrac{1}{2} \Sigma (\xi_i + \beta_i)^2 \lambda_i \quad (2.34)$$

or alternatively

$$E(x_{k+1}) \leq \max_{\lambda_i} [1 + \lambda_i P_{k-1}(\lambda_i)]^2 [E(x_0) + d_0^T A(x_0 - x^* + \tfrac{1}{2} d_0)] \qquad (2.35)$$

The rest of the proof follows as in Luenberger [18].

Observe that (2.20)

$$[d_0, \ldots, d_k] \in [g_0, Ag_0, \; ; A^{k-1}g_0, \; d_0, Ad_0, \ldots, A^k d_0] \qquad (2.36)$$

only shows that the first space is contained in the other. In order to use Theorem 2.1, we must establish conditions which ensure equality of the two spaces.

(1) Clearly $d_0 = -g_0$ will do, which gives the usual conjugate gradient method.

(2) Another possibility is that d_0 is an eigenvector of A. We do not know these eigenvectors. However this suggests that we consider Beale's method with arbitrary metric H, where the directions are defined by

$$d_k = -Hg_k + \beta_k d_{k-1} + \gamma_k d_0$$

$$\beta_k = g_k^T H y_{k-1} / d_{k-1}^T y_{k-1}$$

$$\gamma_k = \begin{cases} g_k^T H y_0 / d_0^T y_0 & \text{if } k > 1 \\ 0 & \text{if } k = 1 \end{cases} \qquad (2.37)$$

In this case we have that

$$[d_0,\ldots,d_k] \in [Hg_0,(HA)Hg_0,\ldots,(HA)^{k-1}Hg_0,d_0,HAd_0,\ldots,(HA)^k d_0] \ . \quad (2.38)$$

If H was obtained by a quasi-Newton update formula using d_0, then

$$Hy_0 = HAd_0 = d_0 \quad (2.39)$$

so that d_0 is an eigenvalue of HA and (3.38) will hold with equality. Theorem 2.1 will hold (except that the λ now are the eigevalues of a different matrix). Beale's method then takes advantage of the eigenvalue distribution of A, which is a very desirable property.

In short one would implement the method as follows:

(a) Choose any $d_0 \neq 0$.

(b) Find H satisfying $Hy_0 = d_0$, using some quasi-Newton update formula.

(c) Continue with Beale's with metric H, given by (2.37).

Notice that if (2.39) holds then $\beta_1 = 0$ and therefore $d_1 = -Hg_1$. So we obtain the conjugate gradient method with metric H. For inexact line searches or general nonlinear functions $\beta_1 \neq 0$ and a different algorithm will be obtained.

2.3. Strategies

Two strategies which have a great impact on performance are

(1) How often to restart. This is nicely discussed in Powell [7].

(2) Initial scaling of the search direction. For a good discussion of this see Shanno [21].

3. Conjugate Gradient Methods with Variable Metric

An important generalization of the conjugate gradient method (2.1) is based upon the first interpretation, see p. 6 . Two variants that have been suggested are the variable storage generalized conjugate gradient method (VSGCG), Nazareth [15] and the Interleaved quasi-Newton-conjugate gradient method of Buckley [22].

3.1. Variable Storage Generalized Conjugate gradient (VSGCG) method, Nazareth [15].

When line searches are exact, it is shown in [15] that the BFGS method can be stated as follows:

$$d_1^{BFGS} = -H_1 g_1$$

$$d_1^{BFGS} = -H_{j-1}^{\beta} g_j + \left[\frac{y_{j-1}^T H_{j-1}^{\beta} g_j}{y_{j-1}^T d_{j-1}^{BFGS}} \right] d_{j-1}^{BFGS} \qquad (3.1)$$

whose x_1 and $H_1 > 0$ are given, $x_{j+1} = x_j + \lambda_j d_j^{BFGS}$, $\lambda_j = \arg\min_{\lambda} f(x_j + \lambda d_j^{BFGS})$ and H_j^{β} is developed from H_{j-1}^{β} using any member of Broyden's β-class (see Appendix).

By comparing (3.1) and (2.14) it can be seen that the BFGS method can be interpreted as a conjugate gradient method in which the metric is changed at each step. When storage is limited this suggests that some simple H_1 be used, e.g. a diagonal matrix and that the vectors defining the rank 1 or 2 updates be saved. These are then used to define the

metric which can vary or stay the same from one iteration to another, depending on the storage available. The resulting family of algorithms is discussed in Nazareth [15] and is as follows: Let $\{x_1, x_2, \ldots\}$ be the points generated and $\{H_1^1, H_{j_1}^2, H_{j_2}^3, \ldots\}$ the matrices. $H_{j_2}^3$ indicates that it is the third matrix and that it was generated at x_{j_2}. (N.B. In practice these will be defined implicitly by the vectors defined in the update functions.) $d_k^{CG}(H)$ will denote a conjugate gradient at x_k using metric H. Let $T = \{j_1, j_2, \ldots\}$ be the set of indices where updates are performed. The VSGCG iteration is

$$H_k^{r+1} = \begin{cases} U(H_\ell^r,\ s_{k-1},\ y_{k-1}) & \text{if } k \in T \\ \text{undefined for } k \notin T\ . \end{cases}$$

Here U denotes the update function of Broyden's β-class (see Appendix) and $\ell \in T$ is the integer preceding k in T.

$$d_k = d_k^{CG}(H_\ell^r)\ ,$$

$$x_{k+1} = x_k + \alpha_k d_k .$$

Note that matrix used is not the most recent one, but the previous one.

Theorem 3.1. Let H be any symmetric and positive definite matrix. Then the VSGCG method with exact line searches, starting with $H_1^1 = H$ has the quadratic termination property.

Proof. $d_1 = d_1^{CG}(H)$, $d_2 = d_2^{CG}(H)$.

By the orthogonality properties of the CG:

$$g_3^T H g_2 = g_3^T H g_1 = g_2^T H g_1 = 0$$

$$g_3^T d_2 = g_3^T d_1 = g_2^T d_1 = 0 .$$

Assume that $d_k^{CG}(H_{j_m}^m) = d_k^{CG}(H)$ for $2 \leq k$ where $H_{j_m}^m \in \{H_1, H_{j_1}^2, \ldots, H_t^r\}$ and $t \leq k-1$. (That is, we are assuming that it is equivalent to use any of the previous matrices to do the step.) Also assume that

$$\left.\begin{aligned} g_{k+1}^T H g_j &= 0 \\ g_{k+1}^T d_j &= 0 \end{aligned}\right\} \quad j = 1,2,\ldots,k$$

We write Broyden's formula as

$$H_{j+1} = H_j + a_j s_j^T + b_j y_j^T H_j .$$

Then

$$H_{j_m} g_{k+1} = H_{j_{m-1}} g_{k+1} + a_{j_m-1} s_{j_m-1}^T g_{k+1} + b_{j_m-1} y_{j_m-1}^T H_{j_{m-1}} g_{k+1}$$

$$H_{j_{m-1}} g_{k+1} = H_{j_{m-2}} g_{k+1} + a_{j_m-2} s_{j_m-2}^T g_{k+1} + b_{j_m-2} y_{j_m-2}^T H_{j_{m-2}} g_{k+1}$$

$$\vdots$$

$$H_{j_1} g_{k+1} = H g_{k+1} + a_1 s_1^T g_{k+1} + y_1^T H g_{k+1} .$$

We have deleted some superscripts, for simplicity. By the induction hypothesis, the above equations give

$$H_{j_1}^{2} g_{k+1} = Hg_{k+1}, \ldots, H_{j_m}^{m-1} g_{k+1} = Hg_{k+1} ,$$

$$H_{j_m}^{m} g_{k+1} = Hg_{k+1} .$$

Then

$$d_{k+1}^{CG}(H_{j_m}^{m}) = -g_{k+1} + \frac{g_{k+1}^{T} H_{j_m}^{m} y_k}{d_k^{T} y_k} d_k$$

$$= -g_{k+1} + \frac{g_{k+1}^{T} H y_k}{d_k^{T} y_k} d_k = d_{k+1}^{CG}(H) .$$

So the induction holds and shows that each step of the VSGCG method is the same as a CG step with metric H. The result follows from the quadratic termination property of the CG method.

Observe that the above result is independent of what member of Broyden's class one chooses. This is in sharp contrast with the Interleaved Method where BFGS has to be used, as discussed next.

Some specific updating strategies allowed by Theorem 3.1 are the following: (a) updating H_i at every iteration, (b) resetting H_i to H after a certain number of steps, and (c) resetting H_i to any previous matrix H_j.

3.2. Interleaved Quasi-Newton-Conjugate Gradient Method, Buckley [22]

This method performs QN and c.g. steps intermittently. The c.g. iteration is carried out with the metric defined in the previous QN cycle. The metric is not updated during the c.g. iterations. Again the quasi-Newton updates are defined by rank 2 corrections, and they will not be stored in matrix form, but will be kept individually. Again as in the VSGCG method as many corrections are retained as our storage capacity allows us. In what follows, it is only important to keep in mind that during each QN iteration the matrix is updated and during each c.g. iteration it is held fixed.

An interleaved QN-CG has been studied by Buckley. In [22] he states a theorem (see Theorem 3.3 below), which we generalize slightly to show that it does not depend on the use of conjugate gradient iterations. Consider the general iteration

$$\begin{aligned} d_j &= -Hg_j + \sigma_j d_{j-1} \qquad && \sigma_j \text{ is any constant} \\ x_{j+1} &= x_j + \alpha_j d_j \qquad && j = 1,2,\ldots \qquad (3.3a) \\ d_0 &= -Hg_0 \end{aligned}$$

For the case of general nonlinear functions we can ask if the VSGCG method will produce nonsingular matrices, preferably positive definite too. We use the following result of Powell [23] for Broyden's β-class.

Theorem 3.2. Let H_k be symmetric and positive semi-definite, let $s_k \neq 0$ be in the space spanned by the columns of H and let y_k be such that $s_k^T y_k > 0$. Also assume that vector w_k is nonzero. Then if

$$\beta > -\frac{(y_k^T H_k y_k)(s_k^T y_k)^2}{\alpha_k^2(y_k^T H_k y_k)(s_k^T H_k^+ s_k) - (s_k^T y_k)^2} \equiv \beta^* \qquad (3.2)$$

we will have that $\text{rank}(H_{k+1}) = \text{rank}(H_k)$ and H_{k+1} will be positive semidefinite. H^+ is the generalized inverse of H. It can be shown that

$$\beta \equiv t\cdot\beta_{BFGS} + (1-t)\beta_{DFP} > \beta^* \quad \text{for} \quad t \in [0,1] \qquad (3.3)$$

where $\beta_{BFGS} = (y_k^T H y_k/\alpha_k^2)$ gives rise to the BFGS method and $\beta_{DFP} = 0$ to the DFP method.

If H_k is positive definite, any s_k will be in its column space; and all we have to insure is that $s_k^T y_k > 0$. This can always be done by performing a sufficiently accurate line search, see [4]. H_{k-1} will then be positive definite and the VSGCG will be a descent method where H is a symmetric and positive definite matrix and α_j is a steplength. Now consider the interleaved method that uses iteration (3.4) and QN steps from Broyden's β-class (A-1). Let the points generated by this method be

$$x_0 = x_{0,1}, x_{0,2}, \ldots, x_{0,F_0} = x_{1,1}, x_{1,2}, \ldots, x_{1,F_1} = x_{2,1}, \ldots, x_{R,F_R}$$

where the QN steps were performed at $x_{i,1}$, $i = 0,1,\ldots$. H_i is the new matrix obtained at $x_{i,1}$ and $d_{i,j}$ the displacement from x_{ij} to $x_{i,j+1}$.

Now we shall see that in the interleaved method one obtains positive definite matrices for any β satisfying (3.3).

Lemma 3.1. Let H_i be symmetric and positive definite. Consider the interleaved method that uses QN updates and the general iteration (3.1c). If sufficiently accurate line searches are performed (see below) one can choose $\ell \in \{i,1,\ i,2,\ldots,i,F-1\}$ such that the following is true: If $s_{i,\ell}$ and $y_{i,\ell}$ are used in (A.1) to obtain H_{i+1}, and if $w_i \neq 0$, $\beta > \beta^*$ then H_{i+1} will be positive definite.

Proof.

$$d_{i,\ell} = -H_i g_{i,\ell} + \sigma_{i,\ell} d_{i,\ell-1} \tag{3.4}$$

Since H_i is nonsingular $d_{i,\ell}$ is in its column space. Let us drop the first index, i.e., $d_{i\ell} \equiv d_\ell$. Now

$$d_1 = -Hg_1, \qquad d_1^T g_1 < 0$$

$$d_\ell^T g_\ell = -g_\ell^T H g_\ell + \sigma_\ell d_{\ell-1}^T g_\ell \tag{3.5}$$

Let the accuracy of the search be such that

$$|d_j^T g_{j+1}| < \min\left\{\frac{1}{\sigma_j}\, g_{j+1}^T H g_{j+1},\ |d_j^T g_j|\right\} \quad \text{for all } j \tag{3.6}$$

Then from (3.5), $d_\ell^T g_\ell < 0$ and

$$\alpha_\ell d_\ell^T y_\ell = \alpha_\ell [d_\ell^T g_{\ell+1} - d_\ell^T g_\ell] > 0 \ .$$

Therefore $\delta_\ell^T y_\ell > 0$. We assume that $\alpha_j > 0$ for all j. Applying Theorem 3.2 we conclude the proof.

The lemma tells us that we can use any of the general iteration steps to do the next quasi-Newton update and retain positive definiteness. In order to obtain termination for a quadratic we will have to use the last step.

Algorithm 3.1. Consider the interleaved method that uses the general iteration (3.3a) and which satisfies the following:

(a) in the previous iteration to an QN step an exact line search is employed.

(b) for all other iterations we do sufficiently accurate line searches (in the sense of Lemma 3.1).

(c) the QN updates use the last displacement vector.

The following theorem says that the intermediate steps do not undo the progress of the QN steps.

Theorem 3.3. If Algorithm 3.1 is applied to the quadratic function $\psi(x) = \frac{1}{2} (x-x^*)^T A(x-x^*)$, starting from any x_0 then the minimum x^* will be reached after r QN steps, where $0 < r \leq n$.

Proof. Let $S_{ik} = \{v: AH_i v = v,\ v^T H_i g_{i,j} = 0,\ j = 1,2,\ldots,k\}$. First we show that

$$S_{ik} \subseteq S_{i,k+1} \quad \text{for} \quad 1 \leq k < F_i \,. \tag{3.7}$$

Let $v \in S_{i,k}$

$$x_{i,k+1} = x_{i,k} + \sum_{j=1}^{k} \beta_j H_i g_{i,j} \quad \text{for some constants } \beta_j$$

$$g_{i,k+1} = g_{i,k} + \sum_{j=1}^{k} \beta_j A H_i g_{i,j}$$

$$v^T H_i g_{i,k+1} = v^T H_i g_{i,k} + \sum \beta_j g_{i,j}^T H_i A H_i v$$

$$= \sum_{j=1}^{k} \beta_j g_{i,j}^T H_i v = 0 \,.$$

Therefore, $S_{i,k} \subseteq S_{i,k+1}$.

Next we will show that $S_{i,F_i-1} \subseteq S_{i+1,1}$. To simplify the notation we will drop the subindex of F, i.e., $x_{i,F} \equiv x_{i,F_i}$. Let $v \in S_{i,F-1}$ then

$$AH_i v = v,\ v^T H_i g_{i,j} = 0, \qquad j = 1,2,\ldots,F-1 \,.$$

Let us call $\delta = s_{i,F-1}$ and $\gamma = y_{i,F-1}$

$$H_{i+1} = H_i - \frac{H_i \gamma \gamma^T H_i}{\gamma^T H_i \gamma} + \frac{\delta \delta^T}{\delta^T \gamma} + \bar{\beta} w w^T$$

$$w = \alpha \left[\frac{H_i \gamma}{\gamma^T H_i \gamma} - \frac{\delta}{\delta^T \gamma} \right] \tag{3.8}$$

$$AH_{i+1}v = AH_iv - \frac{AH_i\gamma\gamma^TH_iv}{\gamma^TH_i\gamma} + \frac{A\delta\delta^Tv}{\delta^Tv} + \beta Aw\alpha\left[\frac{\gamma^TH_iv}{\gamma^TH_i\gamma} - \frac{\delta^Tv}{\delta^T\gamma}\right]$$

$$= v - \frac{AH_i\gamma\delta^TAH_iv}{\gamma^TH_i\gamma} + \frac{A\delta\delta^Tv}{\delta^T\gamma} + \beta Aw\alpha\left[\frac{\delta^TAH_iv}{\gamma^TH_i\gamma} - \frac{\delta^Tv}{\delta^T\gamma}\right] \qquad (3.9)$$

Now $\delta^TAH_iv = \delta^Tv$

$$\delta = \sum_{j=1}^{F-1} \beta_iH_ig_{i,j} \qquad \text{therefore } \delta^Tv = 0 .$$

Using this in (3.9) we obtain

$$AH_{i+1}v = v . \qquad (3.10)$$

We only need to show that $g_{i+1}^TH_iv = 0$

$$x_{i+1,1} = x_{i,F-1} + \sum_{j=1}^{F-1} \beta_jH_ig_{i,j}$$

$$g_{i+1,1} = g_{i,F-1} + \sum_{j=1}^{F-1} \beta_jAH_ig_{i,j}$$

$$g_{i+1}^T H_{i+1}v = g_{i,F-1}^TH_{i+1}v + \sum_{j=1}^{F-1} \beta_jg_{i,j}^TH_iAH_{i+1}v$$

$$= g_{i,F-1}^TH_{i+1}v + \Sigma\, \beta_jg_{i,j}^TH_iv \quad \text{(from 3.10)}$$

$$= g_{i,F-1}^TH_{i+1}v$$

$$= g_{i,F-1}^TA^{-1}AH_{i+1}v$$

$$= g_{i,F-1}^TA^{-1}AH_iv = 0 \qquad (3.11)$$

Therefore $S_{i,F-1} \subseteq S_{i+1,1}$. Note that we have not used the exact line search hypothesis.

Finally, we will show that if $x_{i,F}$ was obtained by doing an exact line search from $x_{i,F-1}$ then $S_{i,F-1} \subset S_{i+1,1}$. From the quasi-Newton equation, $\delta = H_{i+1}\gamma$, therefore

$$AH_{i+1}\gamma = A\delta = \gamma \tag{3.12}$$

$$\delta^T g_{i+1,1} = 0 \quad \text{(exact search)},$$

then

$$(H_{i+1}^{-1}\delta)^T H_{i+1} g_{i+1,1} = \gamma^T H_{i+1} g_{i+1,1} = 0 . \tag{3.13}$$

Hence $\gamma \in S_{i+1,1}$. Assume that $\gamma \in S_{i,F-1}$:

$$g_{i,F-1}^T H_i \gamma = 0 , \qquad AH_i\gamma = \gamma$$

Therefore

$$g_{i,F-1}^T A^{-1}\gamma = g_{i,F-1}^T \delta = 0 . \tag{3.14}$$

This is not possible; in the proof of Lemma 3.1 it is shown that $g_j^T d_j < 0$ for all j. This shows that $S_{i,F-1} \subset S_{i+1,1}$. So, the linear spaces $S_{i,k}$ are nondecreasing and their dimension increased by at least 1 after the QN-step.

It is clear from the proof that we could do a QN after a step with inexact line searches and this would not destroy the termination property. Theorem 3.3 can be paraphrased as follows: after at most n QN steps that were preceded by exact-line search steps we will reach the minimum x^*. The BFGS update formula is

$$H_{k+1} = H_k + \frac{1}{s_k^T y_k}\left(1 + \frac{y_k^T H_k y_k}{s_k^T y_k} - H_k y_k\right) s_k^T - \frac{s_k y_k^T H_k}{s_k^T y_k} \qquad (3.15)$$

which we will write as

$$H_{k+1} = H_k + a_k s_k^T + b_k y_k^T H_k \qquad (3.16)$$

where the vectors a_k and b_k are found by comparing with (3.15).

Theorem (3.7) is a weak result; we shall now show that these iterations can be chosen so that (n-step) quadratic termination is obtained.

Algorithm 3.2. Consider the Interleaved method that uses BFGS steps and conjugate gradient iterations with respect to the newest H_{BFGS} matrix. An exact line search is performed at each step.

Theorem 3.4. If Algorithm 3.2 is applied to the quadratic function $\psi(x) = \frac{1}{2}(x-x^*)^T A(x-x^*)$ starting from any $x_0 \in R^n$ with any symmetric and positive definite H_0, then the solution x^* will be obtained in at most n steps.

Proof. The Hestenes-Stiefel CG with metric H is

$$d_j^{CG}(H) = -Hg_j + \left[\frac{y_{j-1}^T Hg_j}{y_{j-1}^T s_{j-1}}\right] s_{j-1} . \qquad (3.18)$$

Let $x_{i,j}$ be a point generated by the algorithm. We define

$d_{i,j}$ = displacement generated by Algorithm 3.2 at x_{ij}

$d^{B}_{i,1} = -H_i g_{i1}$, $\quad i = 2,3,\ldots, R$

$d^{CG}_{i,j}$ = (3.18) evaluated at $x_{i,j}$.

We are using here the same notation as in Theorem (3.3) to describe when the updates are done. We will show that $d_{i,j} = d^{CG}_{i,j}(H_0)$ for all (i,j) in the sequence. In other words, the Interleaved method is equivalent to using the CG with metric H_0 throughout.

Assume that at the (j-1) cycle:

$$\left.\begin{aligned} &(1) \qquad d_{s,k} = d^{CG}_{s,k}(H_0)\,, \quad s = 0,\ldots,j-1;\ k = 1,\ldots,F_s \\ &(2) \qquad H_s g_{j-1,t} = H_0 g_{i-1,t}\,, \quad s = 0,\ldots,j-2;\ t = 1,\ldots,F_s \\ &(3) \quad H_{j-1} g_{j-1,t} = H_0 g_{j-1,t}\,, \quad t = 2,3,\ldots, F_{j-1} \end{aligned}\right\} \quad (3.19)$$

The assumption is clearly true for $j = 1$. Now we show that (3.19) holds for the j-th cycle. Recall that $g_{i-1,F_j-1} = g_{j,1}$

$$\begin{aligned} d_{j,1} &= -H_j g_{j,1} = -H_{j-1} g_{j,1} - a_{j-1} s^T_{j-1,F-1} g_{j,1} + b_{j-1} y^T_{j-1,F-1} H_{j-1} g_{j,1} \\ &= -H_0 g_{j,1} - b_{j-1} y^T_{j-1,F-1} H_0 g_{j,1} \\ &= -H_0 g_{j,1} + \frac{y^T_{j-1,F-1} H_0 g_{j,1}}{s^T_{j-1,F-1} y_{j-1,F-1}} s_{j-1,F-1} \quad \text{(see (3.15)-(3.16))} \\ &= d^{CG}_{j,1}(H_0) \end{aligned} \quad (5.20)$$

Using the conjugacy and orthogonality properties of the CG we have

$$H_1 g_{j,2} = H_0 g_{j,2} + a_0 s_{0F}^T g_{j,2} + b_0 y_{0,F}^T H_0 g_{j,2} = H_0 g_{j,2}$$

Assume that $H_k g_{j,2} = H_0 g_{j,2}$ for $1 < k < j$, then

$$H_{k+1} g_{j,2} = H_k g_{j,2} + a_k s_{k,F}^T g_{j,2} + b_k y_{k,F}^T H_k g_{j,2} = H_0 g_{j,2} .$$

Therefore $H_k g_{j,2} = H_0 g_{j,2}$, $k = 1,2,\ldots, j$. Now

$$\begin{aligned} d_{j,2}^{CG}(H_j) &= - H_j g_{j,2} + \frac{y_{j,1}^T H_j g_{j,2}}{y_{j,1}^T d_{j,1}} d_{j,1} \\ &= - H_0 g_{j,2} + \frac{y_{j,1}^T H_0 g_{j,2}}{y_{j,1}^T d_{j,1}} d_{j-1} \\ &= d_{j,2}^{CG}(H_0) . \end{aligned}$$

Reasoning as before we can show that for $k = 1,2,\ldots,j$

$$\left.\begin{aligned} H_k g_{j,i} &= H_0 g_{j,i} \\ d_{j,i}^{CG}(H_j) &= d_{j,i}^{CG}(H_0) \end{aligned}\right\} \quad i = 2,3,\ldots, F_j \qquad (3.21)$$

So that (3.19) holds for the (j-th) cycle. The proof now follows from the quadratic termination of the CG method.

If instead of BFGS one uses some other member of Broyden's β-class (A.1), does one obtain (n-step) quadratic termination?

Lemma 3.2. If in Algorithm 3.2 one uses a member of Broyden's Class (A-1) different from BFGS, then the quadratic termination property is lost.

Proof. We write (A.1) in a slightly different form

$$\bar{H} = H - \frac{Hyy^TH}{y^THy} + \frac{ss^T}{s^Ty} + \beta\left(Hy - \frac{y^THy}{s^Ty}s\right)\left(Hy - \frac{y^THy}{s^Ty}s\right)^T \qquad (3.23)$$

where $\beta_{BFGS} = 1/y^THy$.

Suppose that n-1 CG steps, (n-2) with metric H have been performed and that the solution has not been reached. We now update the matrix, which so far has remained unchanged. From Theorem (3.4) it follows that if the solution is to be obtained in the next step, the new direction should be parallel to the BFGS. Let s be the last displacement and g_+ the current gradient. Recall that we are doing exact line searches:

$$s^Tg_+ = 0$$

$$-d_\beta = \bar{H}g_+ = Hg_+ - \frac{y^THg_+}{y^THy}Hy + \beta\left(Hy - \frac{y^THy}{s^Ty}s\right)y^THg_+$$

$$= Hg_+ + Hy\left(-\frac{y^THg_+}{y^THy} + \beta y^THg_+\right) - s\beta\left(\frac{y^THy}{s^Ty}y^THg_+\right) \qquad (3.24)$$

$$-d_{BFGS} = Hg_+ + Hy\left(-\frac{y^THg_+}{y^THy} + \frac{y^THg_+}{y^THy}\right) - s\left(\frac{y^THg_+}{s^Ty}\right)$$

$$= Hg_+ - \frac{y^THg_+}{s^Ty}\,s \qquad (3.25)$$

Suppose that $k\cdot d_{BFGS} = d_\beta$ for some number k. Then

$$(k-1)Hg_+ + Hy\left(\frac{y^THg_+}{y^THy} - \beta y^THg_+\right) - s\left(\frac{y^THg_+}{s^Ty}\right)(k - \beta y^THy) = 0\ . \qquad (3.26)$$

This equation has the form

$$a_1Hg_+ + a_2Hg + a_3s = 0\ .$$

As $s = \Sigma\,\alpha_iHg_i$, where the summation is over all i such that g_i precedes g_+, and as the gradients are conjugate with respect to H we have $a_1 = a_3 = 0$. But $a_3 = 0$ implies

$$k = \beta y^THy;$$

$$a_1 = (k-1) + \frac{y^THg_+}{y^THy} - \beta y^THg_+ = 0\ ;$$

$$\beta y^THy - 1 = \beta y^THg_+ - \frac{y^THg_+}{y^THy}\ ; \qquad (3.27)$$

$$\beta(y^THy - y^THg_+) = 1 - \frac{y^THg_+}{y^THy} - \frac{y^THy - y^THg_+}{y^THy}$$

Therefore $\beta = (y^THy)^{-1}$ which is BFGS.

The above results show again the special relation between the CG and the BFGS methods discussed in Interpretation I p. 6 . The proof of Theorem 3.4 implies the following: If BFGS and CG are applied to a quadratic function using the same initial matrix, and if exact line searches are used then the displacements generated by the two algorithms are the same in direction and magnitude.

4. Conjugate Gradient Methods with Inexact Line Searches

In this section we discuss variants of the conjugate gradient method which have their basis in the interpretations discussed in Section 2 on p. 6 to 10. The aim of each variation is to drop the requirement that line searches be exact, and still retain the advantages of the basic conjugate gradient method.

We shall give a brief description of each algorithm in Section 4.1.1. We then discuss properties of these algorithms, concentrating on the three term recurrence.

4.1. Basics

4.1.1. Algorithms

a) Dixon's gradient prediction method [24]

The first method along these lines was due to Dixon. His extension of the conjugate gradient method is based upon the following result:

Lemma 4.1. Given an initial point x_0 and a set of conjugate directions $d_0, d_1, \ldots, d_i$ s.t. $d_0 = -g_0$ and $d_j \in [g_0, g_1, \ldots, d_j]$, let a sequence of points $x_1, x_2, \ldots, x_{i+1}$ be developed s.t. $x_{j+1} = x_j + \lambda_j d_j$, where λ_j is an arbitrary step.

Then the gradient g^*_{i+1} at the minimum point x^*_{i+1} in the affine space $\{Z = \{z : z = x_0 + \sum_{j=0}^{i} \alpha_j d_j, \alpha \in \mathbb{R}\}$ can be deduced from $g_j \triangleq \nabla f(x_j)$ and the search directions, and is given by

$$g^*_{i+1} = g_{i+1} - \sum_{j=1}^{i} \left(\frac{g^T_{j+1} d_j}{d^T_j y_j} \right) y_j$$

and

$$x^*_{i+1} = x_{i+1} - \sum_{j=1}^{i} \left(\frac{g^T_{j+1} d_j}{d^T_j y_j} \right) d_j \qquad (4.1)$$

Proof. Implicit in Dixon [24].

g^*_{i+1} can be used to develop a search direction d_{i+1} parallel to that developed by the c.g. method. From (2.1) this is achieved by

$$d_{i+1} = -g^*_{i+1} + \frac{\|g^*_{i+1}\|^2}{\|g^*_i\|^2} d_i \qquad (4.2)$$

From (4.1) it should be clear that only two additional vectors are needed to accumulate the corrections to g_{i+1} and x_{i+1}.

b) Memoryless Quasi-Newton Methods, Shanno [21]

These are based upon the first of the three interpretations in Section 2.1.2, and the subsequent discussion of Section 3.1. It should be clear from (3.1) and (2.1) that the restarted BFGS algorithm ($H^{\beta}_{j-1} = I$) is equivalent to the Hestenes-Stiefel conjugate gradient algorithms (2.1) and (2.3), when line searches are exact. Shanno carries this further by dropping the requirement that line searches be exact, and developing search directions by

$$d_{j+1} = -U_{BFGS}(I, s_j, y_j)g_{j+1}$$

$$= -g_{j+1} - \left(\left(1 + \frac{y_j^T y_j}{d_j^T y_j}\right)\frac{d_j^T g_{j+1}}{d_j^T y_j} - \frac{y_j^T g_{j+1}}{d_j^T y_j}\right) d_j + \frac{d_j^T g_{j+1}}{d_j^T y_j} y_j$$

A number of additions to this basic algorithm contribute to its effectiveness--in particular strategies for scaling and restarting. For details see [21].

c) The multistep method, Nazareth and Nocedal [25]

This is based upon the second of the three interpretations of Section 2.1.2. As noted there the c.g. method develops search directions and gradients which satisfy (2.3a). Let us consider dropping the requirement that line searches be exact and hence the fourth relation $G^TG = \beta$, but let us still insist that the direction gradient relation be satisfied $-G = DR$, and that directions are conjugate, i.e. $D^TAD = \alpha$. In addition the matrix H in the relation $AD\lambda = GH$ must be redefined as

$$H = \begin{bmatrix} -1 & & & & \mu_1 \\ 1 & -1 & & & \vdots \\ & 1 & \ddots & & \vdots \\ & & \ddots & \ddots & \vdots \\ & & & \ddots & \mu_{n-1} \\ & & & 1 & \mu_n \end{bmatrix}, \quad \mu_i \in \mathbb{R} \qquad (4.4)$$

since $g_{n+1} \in [g_1, \ldots, g_n]$ and $g_{n+1} \neq 0$ in general.

The multistep method is based upon the following result, given in [25].

Lemma 4.2. Given matrices G, D, R, H, λ, α as defined above, then R has the form:

$$R = \begin{bmatrix} 1 & \otimes & \alpha & \alpha & \alpha & . & . & . & \alpha \\ & 1 & \otimes & \beta & \beta & & . & . & \beta \\ & & 1 & \otimes & \gamma & & . & . & \gamma \\ & & & . & . & . & & & . \\ & & & & . & . & . & & . \\ & & & & & . & . & . & . \\ & & & & & & . & . & \otimes \\ & & & & & & & & 1 \end{bmatrix}$$

where elements denoted by the same greek letter are equal, and $\otimes$ denotes an element which is, in general, non-zero.

It is clear that for quadratics we have another specialized version of Gram-Schmidt orthogonalization. Mainly for purposes of illustration a particular algorithm is suggested in [25], but a number of alternative formulations come to mind, and it is as yet unclear how to make effective use of Lemma 4.2 in an algorithm for non-linear optimization. The salient point however is this: The usual c.g. method, e.g. Hestenes-Stiefel develops a search direction in $[-g_j, d_{j-1}]$ that is orthogonal to y_{j-1}. Lemma 4.2 suggests that it might be worthwhile to maintain a second vector c_{j-1}, composed of a suitable linear combination of previous directions, and an associated change of gradient f_{j-1}, and to develop $d_j \in [-g_j, d_{j-1}, c_j]$ and orthogonal to y_{j-1} and f_{j-1}.

d) The three term recurrence, Nazareth [17]

As we shall see, in the following section, the method is best thought of as another implicit Lanczos process for symmetric matrices (see p. 8). The defining sections for these three term recurrences are given by

$$d_{j+1} = -y_j + \left(\frac{y_{j-1}^T y_j}{y_{j-1}^T d_{j-1}} \right) d_{j-1} + \left(\frac{y_j^T y_j}{y_j^T d_j} \right) d_j, \qquad j \geq 0 \tag{4.6}$$

$x_{j+2} = x_{j+1} + \lambda_j d_j$ when λ_j is a function reducing step, but not necessarily to the minimum of the function along d_j. Also $d_{-1} \equiv 0$.

Details of the algorithm are given in [17]. Computational experience reported in [27] is encouraging. Shanno [26] however does not obtain good results with the method. A recent hybrid implementation by Gill and Murray [27] combines the TTR with the conjugate gradient method and they also report encouraging computational experience. As we shall see in the next section, the TTR method has certain advantages and disadvantages viz a viz the CG method, and what is clear is that an effective implementation must exploit the positive aspects and circumvent the negative aspects of the TTR.

4.1.2. Properties and Interpretations

a) When line searches are exact then the gradient prediction method is identical to the conjugate gradient method. This holds for arbitrary functions. This property also implies that line search criteria can be found which ensure that the GP method develops descent directions, see Shanno [26]. The GP method has finite termination on quadratics.

b) The memoryless BFGS method does not have finite termination on quadratics. However, by virtue of it being a one step variable metric method it is clear that it develops descent directions, subject to $y_j^T s_j > 0$. This can be assured by the line search.

c) A straightforward implementation of the multistep method, based upon Lemma 4.2, as described in [25], will not assure descent for arbitrary functions. Such a method will retain quadratic termination. As noted earlier, we believe that an algorithm which exploits Lemma 4.2 in a more subtle manner, may be a very useful contribution.

d) We now discuss a number of new properties of the TTR. The first observation of some importance is that the TTR does not require that d_0 be along g_0, in order to develop conjugate directions. This is an advantage since it permits restarts of the algorithm with $d_0 \neq -g_0$. A disadvantage of TTR however is that for arbitrary function d_{j+1} need not be a descent direction, even when line searches are exact.

The TTR is closely related to the Lanczos process for tri-diagonalizing a symmetric matrix. Since $y_j = Ad_j\lambda_j$ we can write (4.6) as

$$Ad_j\lambda_j = -d_{j+1} + \left(\frac{y_{j-1}^T y_j}{y_{j-1}^T d_{j-1}}\right) d_{j-1} + \left(\frac{y_j^T y_j}{y_j^T d_j}\right) d_j \qquad (4.7)$$

Define $D = (d_0, \ldots, d_t)$ $t < n$ where $d_1, \ldots, d_t$ on the set of conjugate directions developed before the algorithm terminates, i.e. $d_{t+1} = 0$. Then (4.7) for $j = 0, 1, \ldots, t$ becomes

$$\left.\begin{aligned} AD &= DT \\ D^T AD &= \alpha \end{aligned}\right\} \qquad (4.8)$$

and by conjugacy

where T is a tridiagonal matrix and α is diagonal, (4.8) can be rewritten as

$$\left.\begin{aligned} \tilde{D}^T A \tilde{D} &= \tilde{T} \\ \tilde{D}^T \tilde{D} &= \alpha \end{aligned}\right\} \qquad (4.9)$$

where $\tilde{D} = A^{1/2} D$ and $\tilde{T} = \alpha T$ is symmetric and tridiagonal. (4.9) defined the Lanczos process.

It also follows directly from the above discussion that

$$d_j \in [d_0, Ad_0, \ldots, A^{j-1} d_0] .$$

Thus the TTR will terminate when the above Krylov sequence $d_0, Ad_0, \ldots$ attains maximum rank. If A has only k distinct eigenvalues, then there can be at most k steps. If $d_0 = -g_0$ then the TTR with exact

or inexact line searches will generate conjugate directions which span the same spaces as would the CG method with exact line searches. When the sequence terminates, the correction step will be to the minimum. If $d_0 \neq -g_0$ then the TTR can terminate (say $d_k = 0$), but the minimum need not lie in the affine space $\{z: z = x_0 + \sum_0^{k-1} \alpha_j d_j, \alpha_j \in \mathbb{R}\}$. This is a disadvantage of the method. We can however show the following.

Lemma 4.1. If the TTR with $d_0 \neq -g_0$ and exact line searches terminates prematurely at x_k, $k < n$, i.e. $g(x_k) \neq 0$ and $d_k = 0$, then $g(x_k)$ is conjugate to $d_1, \ldots, d_{k-1}$.

Proof. g_k is orthogonal to $[d_0, \ldots, d_{k-1}]$ because $d_1, \ldots, d_{k-1}$ are conjugate and line searches are exact. Also by (4.6) $y_j \in [d_0, d_1, \ldots, d_{j+1}]$. Thus $y_0, \ldots, y_{k-2} \in [d_0, \ldots, d_{k-1}]$ and $y_{k-1} \in [d_0, \ldots, d_{k-1}]$ because the process has terminated, i.e. $d_k = 0$. Therefore $[y_0, \ldots, y_{k-1}]$ $= [d_0, \ldots, d_{k-1}]$. Thus g_k is orthogonal to $[y_0, \ldots, y_{k-1}]$, i.e. is conjugate to $d_1, \ldots, d_{k-1}$.

Suppose we drop the requirement that line searches be exact. The next lemma shows that in the quadratic case a vector can be maintained, which permits a restart of the algorithm when premature termination occurs.

Lemma 4.2. Define $n_0 = g_0$

$n_j \in [n_{j-1}, d_{j-1}]$ and n_j orthogonal to y_{j-1}.

Then n_j is orthogoanl to $y_0, \ldots, y_{j-1}$ and n_j is conjugate to $y_0, \ldots, y_{j-2}$.

Proof. By induction, suppose n_k is orthogonal to $y_0, \ldots, y_{k-1}$. Also by conjugacy d_k is orthogonal to $y_0, \ldots, y_{k-1}$.

Since $n_{k+1} \in [n_k, d_k]$ and is chosen to be orthogonal to y_k, it clearly follows that n_{k+1} is orthogonal to $y_0, \ldots, y_k$. Thus

$$n_j^T A[d_0, \ldots, d_{j-1}] = 0$$

$$(An_j)^T [d_0, \ldots, d_{j-1}] = 0$$

Since $[y_0, \ldots, y_{j-2}] \in [d_0, \ldots, d_{j-1}] \Rightarrow An_j$ is orthogonal to $y_0, \ldots, y_{j-2}$.

The above lemmas suggest ways of modifying TTR in order to circumvent its disadvantages discussed above. In particular, Lemma 4.1 justifies the hybrid implementation of Gill and Murray [27], and demonstrates that termination of this implementation will occur in at most n steps from x_0 (N.B. not x_k). We will however defer a more detailed discussion of TTR modified along the lines suggested by Lemma 4.1 and 4.2 so as not to unduly lengthen an already long paper.

It is also clear that methods GP and multistep discussed in the section can be generalized to arbitrary fixed metric and arbitrary starting directions, and that much can be said about strategies of scaling and restarting. Again we do not pursue this here.

5. Inexact Line Search Methods with Variable Metric

In Section 3 we discussed conjugate gradient methods in which the metric is varied. Similar ideas can be applied to the methods of Section 4. Here we discuss only one such method, which seeks to avoid line searches in the conjugate gradient steps and retain quadratic termination by using the TTR method.

Algorithm 5.1. Consider the Interleaved method that uses BFGS and the TTR method in the following way: (a) at the end of a sequence of TTR steps, the correction step, see [17] is done, and (b) every BFGS step is performed with an exact line search.

Theorem 5.1. If Algorithm 5.1 is applied to the quadratic function $\psi(x) = \frac{1}{2}(x-x^*)^T A(x-x^*)$ starting from any $x_0 \in R^n$ and any symmetric and positive definite matrix H_0, then the solution will be obtained in at most n-steps. (As the correction step does not involve function evaluations it is not counted as a step.)

Proof. First we will show that the directions generated by the TTR are parallel to the conjugate gradient directions of $d_0 = -g_0$.

We will denote by $x_1^*, x_2^*, \ldots$ the sequence generated by the CG and $x_1, x_2, \ldots$ that produced by the TTR method.

$$x_1^* = x_0 + \alpha_0 d_0$$

$$x_1 = x_0 + d_0$$

therefore

$$g_1^* = g_1 + (\alpha_0 - 1)y_0 = \alpha_0 y_0 + g_0; \qquad y_0^* = \alpha_0 y_0$$

$$y_0^{*T} g_1 = \alpha_0 y_0^T [g_1 + \alpha_0 y_0 - y_0]$$

$$y_0^{*T} d_0 = \alpha_0 y_0^T d_0 .$$

Using the Hestenes-Stiefel CG we have

$$d_1^* = -\alpha_0 y_0 - g_0 + \alpha_0 \frac{[y_0^T g_1 + y_0^T y_0 \alpha_0 - y_0^0 y_0]}{\alpha_0 y_0^T d_0} d_0$$

$$= -\alpha_0 y_0 + \left[1 + \frac{y_0^T g_1 + \alpha_0 y_0^T y_0 - y_0^T y_0}{y_0^T d_0}\right] d_0$$

$$= -\alpha_0 y_0 + \left[\frac{y_0^T y_0 + \alpha_0 y_0^T y_0 - y_0^T y_0}{y_0^T d_0}\right] d_0$$

$$= -\alpha_0 y_0 + \alpha_0 \frac{y_0^T y_0}{y_0^T d_0} d_0 = \alpha_0 d_1$$

where d_1, d_2, ... are given by (4.6).

Induction: Assume that $d_j^* = \alpha_{j-1} d_j$, i = 1,2,..., k.

From (4.1)

$$g_{k+1}^* = g_{k+1} - \sum_{j=1}^{k} \frac{g_{j+1}^T d_j}{d_j^T y_j} y_j . \qquad (5.1)$$

So

$$y_k^* = y_k - \frac{g_{k+1}^T d_k}{d_k^T y_k} y_k = - \frac{g_k^T d_k}{d_k^T y_k} y_k$$

$$y_k^* = \alpha_k y_k \quad \text{with} \quad \alpha_k = - \frac{g_k^T d_k}{d_k^T y_k} .$$

Now

$$d_{k+1} = - \frac{1}{\alpha_k} y_k^* + \frac{1}{\alpha_k} \frac{y_k^{*T} y_k^*}{y_k^{*T} d_k^*} d_k^* + \frac{1}{\alpha_k} \frac{y_{k-1}^{*T} y_k^*}{y_{k-1}^{*T} d_{k-1}^*} d_{k-1}^*$$

$$= \frac{1}{\alpha_k} \left[-g_{k+1}^* + g_k^* + \frac{y_k^{*T} y_k^*}{y_k^{*T} d_k^*} d_k^* + \frac{y_{k-1}^{*T} y_k^*}{y_{k-1}^{*T} d_{k-1}^*} d_{k-1}^* \right] . \qquad (5.2)$$

$$d_k^* = -g_k^* + \frac{y_{k-1}^{*T} g_k^*}{y_{k-1}^{*T} d_{k-1}^*} d_{k-1}^* . \qquad (5.3)$$

Also

$$-d_k^* + \frac{y_k^{*T} y_k^*}{y_k^{*T} d_k^*} d_k^* = \left[- \frac{y_k^{*T} d_k^* + y_k^{*T} y_k^*}{y_k^{*T} d_k^*} \right] d_k^* .$$

Using (5.3) and the orthogonality of gradients

$$= \frac{y_k^{*T} g_k^* + y_k^{*T} g_{k+1}^* - y_k^* g_k}{y_k^{*T} d_k^*} d_k^* = \frac{y_k^{*T} g_{k-1}^*}{y_k^{*T} d_k^*} d_k^* \qquad (5.4)$$

Substituting (5.3) in (5.2) and using (5.4) and orthogonality

$$d_{k+1} = \frac{1}{\alpha_k}\left[-g^*_{k+1} - d^*_k + \frac{y^{*T}_{k-1} g^*_k}{y^{*T}_{k-1} d^*_{k-1}} d^*_{k-1} + \frac{y^{*T}_k y^*_k}{y^{*T}_k d^*_k} d^*_k + \frac{y^{*T}_{k-1} y^*_k}{y^{*T}_{k-1} d^*_{k-1}} d^*_{k-1}\right]$$

$$= \frac{1}{\alpha_k}\left[-g^*_{k+1} + \frac{y^{*T}_k g^*_{k+1}}{y^{*T}_k d^*_k} d^*_k\right] + \frac{1}{\alpha_k}\left[\frac{y^{*T}_{k-1} g^*_k}{y^{*T}_{k-1} d^*_{k-1}} d^*_{k-1} + \frac{y^{*T}_{k-1} y^*_k}{y^{*T}_{k-1} d^*_{k-1}} d^*_{k-1}\right]$$

$$= \frac{1}{\alpha_k}\left[-g^*_{k+1} + \frac{y^{*T}_k g^*_{k+1}}{y^{*T}_k d^*_k} d^*_k\right] = \frac{1}{\alpha_k} d^*_{k+1} .$$

Induction holds. Therefore CG and the TTR generate parallel directions. After applying the correction step the TTR method produces the same point as the CG method. Now suppose that a cycle of TTR steps plus correction step is completed and that the matrix will be updated. Let s be the last step of the TTR method. Then $s = \lambda s^*$ where s^* is the corresponding CG step and λ is a constant. Then $y = Cs$, $y^* = \lambda Cs$, so $y = \frac{1}{\lambda} y^*$. Looking at the BFGS update formula one readily sees that it is equivalent to use (s,y) or (s^*,y^*). Therefore using the TTR method is equivalent to using the CG method. The result now follows from Theorem 3.3.

Similar results hold for the other methods of Section 4.

APPENDIX

Broyden's β-class

Given x_0 and $n \times n$ matrix H_k, we let $k = 1,2,\ldots$.

$$x_{k+1} = x_k - \alpha_k H_k g_k$$

where α_k is the step length and H_k is defined recursively by

$$H_{k+1} = H_k - \frac{H_k y_k y_k^T H_k}{y_k^T H_k y_k} + \frac{s_k s_k^T}{y_k^T s_k} + \beta\, w_k w_k^T \qquad \text{(A.1)}$$

$$w_k = \frac{\alpha_k H_k y_k}{y_k^T H_k y_k} - \frac{\alpha_k s_k}{s_k^T y_k}$$

$$\beta \geq 0$$

$$s_k \triangleq x_{k+1} - x_k$$

$$y_k \triangleq g_{k+1} - g_k \quad \text{when} \quad g_k \triangleq \nabla f(x_k) .$$

Also

$$d_k^{\beta} \triangleq -H_k g_k .$$

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We prove a number of new properties of algorithms of the Conjugate Gradient type, paying particular attention to methods which utilize variable metric information in determining the conjugate gradient search directions. We attempt a comprehensive discussion of conjugate gradient methods, and present each algorithm within the context of other existing algorithms, an approach which provides fresh insights and some new algorithms.

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