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PROPERTIES OF THE CONJUGATE GRADIENT AND DAVIDON METHODS

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PROPERTIES OF THE CONJUGATE GRADIENT AND DAVIDON METHODS*

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ABSTRACT

Two quadratically convergent gradient methods for minimizing an unconstrained function of several variables are examined. The heart of the Fletcher and Powell reformulation of Davidon's method is a variable H matrix. The eigenvalues and eigenvectors of this matrix for a quadratic function are explored, leading to a proof that the gradient vectors at each step are mutually orthogonal. From this is derived a geometric interpretation of the H matrix in terms of the projection of the gradient into a solution subspace.

These properties are used to arrive at the main result, which states that, for a quadratic function, the direction vectors generated by the Davidon algorithm and the conjugate gradient algorithm of Hestenes and Stiefel are scalar multiples of each other, provided the initial step each takes is in the direction of steepest descent. Assuming no round-off and a perfect one-dimensional search, the methods will generate identical steps leading to the minimum.

It is also shown that, for a quadratic function, the Davidon algorithm has a simplified version which searches in the same directions. However, the unique advantage of the original scheme, that it yields the curvature of the function at the minimum, is sacrificed for simplicity.

Although these results all apply to the case of a quadratic function, a comparative study of the same algorithms for a general function can be found in a companion paper.

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INTRODUCTION

Consider the problem of finding the minimum of an unconstrained function, f, where f has continuous partial derivatives of at least second order. Then f can be expanded about the minimum point $x = h$ in the Taylor series:

$$f(x) = f(h) + \frac{1}{2}(x-h)^T A(x-h) + R$$

where n-vector of variables and A is the positive definite Hessian matrix. remainder R estimates the error between f and its quadratic approximation. Since R becomes negligible when x is sufficiently close to h, the general function is approximated by a quadratic in a neighborhood of the minimum; hence, algorithms converging rapidly for quadratics are of interest.

Two methods for locating the minimum of a general function are examined in this paper for their terminal phase properties, that is, R is assumed to be zero and f is quadratic. A more complete picture can be found in a companion paper (Ref. 1) where a comparison of the analytic and numeric properties of the same methods is presented for the non-quadratic case. Since f is assumed quadratic, its gradient vector $g(x)$ equals $A(x-h)$ and is represented at any point x_i by g_i.

Both minimizing procedures rely upon the method of successive linear searches. This means h is located as the limit of a sequence $x_o, x_1, x_2, \ldots$ where x_o is an initial approximation of h, and x_{i+1} is the minimum of the function along the line passing through x_i in some specified direction p_i. The step Δx_i from x_i to x_{i+1} equals $-k_i p_i$ where k_i is a scalar step parameter satisfying $\frac{d f(x_i - k p_i)}{dk} = 0$ or equivalently

$$(p_i, g_{i+1}) = p_i^T g_{i+1} = 0 \qquad \text{for all } i \tag{1}$$

It remains to examine algorithms for generating p_i.

A frequent choice for p_i is g_i, referred to as the method of steepest descent. Although this method is stable, that is, a decrease in f is assured after each step, the minimum is approached asymptotically, resulting in very slow convergence.

It is shown in Reference 2 that if the direction vectors have the property of A-conjugacy, that is, for a quadratic function:

$$p_i^T A \; p_j = 0 \qquad i \neq j \tag{2}$$

then

$$p_i^T g_j = 0 \qquad i < j \tag{3}$$

which implies convergence in n steps (or fewer should any $k_i = 0$, $i < n$).

Two methods generating a sequence of A-conjugate directions for a quadratic function are the Davidon variable metric algorithm (Ref. 3) as reformulated by Fletcher and Powell (Ref. 4) and the conjugate gradient algorithm of Hestenes and Stiefel (Ref. 5). The attractive property of rapid convergence, combined with stability and simplicity (only first order partial derivatives are required), make these two of the most powerful and practical methods known.

THE ALGORITHMS REVIEWED

The direction vectors of the Davidon scheme are given by

$$p_i = H_i g_i \qquad 0 \leq i \leq n \tag{4}$$

where H_0 is any positive definite, symmetric matrix and H_{i+1} is defined by the recursion formula:

$$H_{i+1} = H_i + Y_i - Z_i \tag{5}$$

where

$$Y_i = \frac{\Delta x_i \, \Delta x_i^T}{\Delta x_i^T \, \Delta g_i} \tag{6}$$

and

$$Z_i = \frac{H_i \, \Delta g_i \, \Delta g_i^T \, H_i}{\Delta g_i^T \, H_i \, \Delta g_i} \tag{7}$$

For a quadratic function, the change in the gradient $\Delta g_i = g_{i+1} - g_i = A \, \Delta x_i$. It is shown in Reference 4 that H_i is a positive definite symmetric matrix, from which the stability property is derived. A-conjugacy of the direction vectors is established together with the property that

$$A^{-1} = H_n = \sum_{i=0}^{n-1} Y_i \tag{8}$$

By combining (1) with the symmetry of H_i, equation (7) reduces to

$$Z_i = \frac{H_i \, \Delta g_i \, \Delta g_i^T \, H_i}{g_{i+1}^T \, H_i \, g_{i+1} + g_i^T \, H_i \, g_i} \tag{9}$$

and the following relationships hold

$$Y_{i-1} \, g_i = 0$$

and

$$Z_{i-1} \, g_i = \frac{H_{i-1} \, \Delta g_{i-1} (g_i^T \, H_{i-1} \, g_i)}{g_i^T \, H_{i-1} \, g_i + g_{i-1}^T \, H_{i-1} \, g_{i-1}}$$

implying

$$p_i = H_{i-1} \, g_i - \frac{H_{i-1} \, \Delta g_{i-1} (g_i^T \, H_{i-1} \, g_i)}{g_i^T \, H_{i-1} \, g_i + g_{i-1}^T \, H_{i-1} \, g_{i-1}} \tag{10}$$

H_o is chosen as the identity matrix, causing the first step to be in the direction of steepest descent.

The direction vectors of the conjugate gradient algorithm, represented by r_i to distinguish them from those of the Davidon method, are specified by:

$$r_o = g_o$$

and

$$r_i = r_{i-1} \frac{|g_i|^2}{|g_{i-1}|^2} + g_i \qquad 1 \leq i \leq n \tag{11}$$

where $|g_i|^2 = g_i^T \, g_i$.

The property of A-conjugacy of the vectors r_i is inherent in their derivation via the Gram-Schmidt orthogonalization procedure, from which the following are immediate for a quadratic function

$$g_i^T g_j = 0 \qquad i \neq j \quad i, j \leq n$$

and

$$g_j^T r_i = |g_i|^2 \qquad i \geq j \tag{12}$$

Stability is proved in Reference 6.

EIGENVALUES OF THE DAVIDON H MATRIX

Since each H_i matrix of the Davidon algorithm is positive definite and symmetric, its eigenvalues are positive real numbers. In particular, it shall be shown that at least $(n-i-1)$ of these are unity when the function is quadratic.

Lemma 1: $g_j^T H_{i-1} g_i = 0 \quad$ for $i < j \leq n$

From A-conjugacy, we have that

$$g_j^T p_i = 0 \qquad i < j \leq n$$

so

$$g_j^T H_{i-1} g_i - \frac{g_j^T H_{i-1} \Delta g_{i-1}(g_i^T H_{i-1} g_i)}{g_i^T H_{i-1} g_i + g_{i-1}^T H_{i-1} g_{i-1}} = 0 \qquad \text{by (10)}$$

But

$$g_j^T H_{i-1} \Delta g_{i-1} = g_j^T H_{i-1} g_i \qquad \text{by (3)}$$

implying

$$g_j^T H_{i-1} g_i \left[1 - \frac{g_i^T H_{i-1} g_i}{g_i^T H_{i-1} g_i + g_{i-1}^T H_{i-1} g_{i-1}} \right] = 0$$

For the factor on the right to be zero, $g_{i-1}^T H_{i-1} g_{i-1}$ must be zero, which is impossible since g_{i-1} is assumed non-zero and H_{i-1} is positive definite.

So $g_j^T H_{i-1} g_i = 0$ and the lemma is proved.

Theorem 1: $\underline{H_i g_j = g_j \qquad i < j \leq n}$

$$H_i g_j = H_{i-1} g_j + Y_{i-1} g_j - Z_{i-1} g_j \qquad \text{by (5)}$$

where

$$Y_{i-1} g_j = 0 \qquad \text{by (3) and (6)}$$

and

$$Z_{i-1} g_j = \frac{H_{i-1} \Delta g_{i-1}}{\Delta g_{i-1}^T H_{i-1} \Delta g_{i-1}} (g_i^T H_{i-1} g_j - g_{i-1}^T H_{i-1} g_j) \qquad \text{by (7)}$$

But

$$g_i^T H_{i-1} g_j = 0 \qquad \text{by Lemma 1}$$

and

$$g_{i-1}^T H_{i-1} g_j = 0 \qquad \text{by (3)}$$

implying

$$H_i g_j = H_{i-1} g_j$$

By repeated application

$$H_i g_j = H_{i-1} g_j = \cdots = H_o g_j = g_j$$

This demonstrates that the gradients g_j are eigenvectors with unit eigenvalue of the matrix H_i, $i < j \leq n$.

An immediate consequence is the mutual orthogonality of the gradient vectors, for if

$$g_i^T g_j = g_i^T H_i g_j \qquad i < j \leq n$$

then

$$g_i^T g_j = p_i^T g_j = 0 \qquad \text{by (3)}$$

and, by symmetry,

$$g_i^T g_j = 0 \qquad i \neq j \tag{13}$$

Since mutual orthogonality of non-zero vectors implies linear independence, it is confirmed that unity is an eigenvalue of H_i of multiplicity n-i-1.

A further consequence of the theorem is that the algorithm for the direction vectors (10) for a quadratic function is reduced to the recursion formula:

$$p_i = \frac{(g_i\, g_{i-1}^T + |g_i|^2\, I)\, p_{i-1}}{|g_i|^2 + g_{i-1}^T\, p_{i-1}} \qquad 0 < i \le n \qquad (14)$$

EQUIVALENCE OF THE CONJUGATE GRADIENT AND DAVIDON METHODS FOR QUADRATIC FUNCTIONS

By an inductive argument, it shall be shown that p_i as given by (14) and r_i as given by (11) are scalar multiples of each other. This implies that, at each step, the Davidon and conjugate gradient schemes search along the same straight line. Assuming the one-dimensional search for the minimum of f along this line is free from numerical error, both methods will generate identical sequences leading to the minimum of the quadratic function f.

Theorem 2: $p_i = \alpha_i\, r_i \qquad 0 \le i < n$

where α_i is a positive, non-zero scalar

Since

$$r_o = g_o = p_o \qquad \text{and} \qquad \alpha_o = 1$$

both methods have identical values for x_1 and g_1.

$$p_1 = \frac{(g_1\, g_o^T + |g_1|^2\, I)\, p_o}{|g_1|^2 + g_o^T\, p_o} = \frac{g_1 |g_o|^2 + |g_1|^2 g_o}{|g_1|^2 + |g_o|^2} \qquad (15)$$

and

$$r_1 = r_o \frac{|g_1|^2}{|g_o|^2} + g_1 = \frac{g_o |g_1|^2 + g_1 |g_o|^2}{|g_o|^2}$$

implying

$$p_1 = \alpha_1 r_1$$

with

$$\alpha_1 = \frac{|g_o|^2}{|g_1|^2 + |g_o|^2} > 0$$

Assume $p_j = \alpha_j r_j$ with $\alpha_j > 0$ for all $j \leq i < n$ and therefore both algorithms generate identical values for x_k, g_k $k = 0, 1, ---, i, i+1$

$$p_{i+1} = \frac{g_{i+1} g_i^T p_i + |g_{i+1}|^2 p_i}{|g_{i+1}|^2 + g_i^T p_i} \qquad \text{by (14)}$$

$$= \frac{g_{i+1} g_i^T \alpha_i r_i + |g_{i+1}|^2 \alpha_i r_i}{|g_{i+1}|^2 + g_i^T \alpha_i r_i} \qquad \text{by inductive hypothesis}$$

$$= \frac{\alpha_i}{|g_{i+1}|^2 + \alpha_i |g_i|^2} \left[g_{i+1} |g_i|^2 + |g_{i+1}|^2 r_i \right] \qquad \text{by (12)}$$

$$= \frac{\alpha_i |g_i|^2}{|g_{i+1}|^2 + \alpha_i |g_i|^2} \left[g_{i+1} + \frac{|g_{i+1}|^2}{|g_i|^2} r_i \right]$$

$$= \alpha_{i+1} r_{i+1} \qquad \text{with} \qquad \alpha_{i+1} > 0$$

and the theorem is proved.

GEOMETRIC INTERPRETATION OF THE DAVIDON H MATRIX FOR QUADRATIC FUNCTIONS

Because of the relationship between p_i and r_i, the space W spanned by p_i, - - -, p_{n-} is also spanned by r_i, - - -, r_{n-1}. It is shown in Reference 6 that

$$r_i = c_i g_i + \sum_{j=0}^{i-1} c_j A r_j \qquad i < n$$

where c_j $j = 0, - - -, i$ are scalars. Since the vectors $A r_j$ $(j = 0, - - -, i-1)$ span $W^{\perp}$, the orthogonal complement of W, r_i is a scalar multiple of the projection of g_i on W.

By noting that

$$A p_j = -\frac{1}{k_j} A \Delta x_j = -\frac{1}{k_j} \Delta g_j$$

the inductive proof of Theorem 3 demonstrates that p_i is the projection of g_i in W.

Theorem 3: $\underline{p_i = g_i - \sum_{j=0}^{i-1} s_j \Delta g_j \qquad i < n}$

$\underline{\text{where } s_j \text{ are scalars}}$

Since $p_o = g_o$, the induction is valid for $i = 0$. Assume

$$p_{i-1} = g_{i-1} - \sum_{j=0}^{i-2} c_j \Delta g_j \qquad i < n$$

where c_j are scalars $j = 0, ---, i-2$.

Combining the inductive hypothesis with (13) gives

$$g_{i-1}^T p_{i-1} = (1 + c_{i-2}) |g_{i-1}|^2 \tag{16}$$

Substituting (16) and the inductive hypothesis into (14) gives that

$$p_i = \frac{g_i(1 + c_{i-2}) |g_{i-1}|^2 + |g_i|^2 g_{i-1} - |g_i|^2 \sum_{j=0}^{i-2} c_j \Delta g_j}{|g_i|^2 + (1 + c_{i-2}) |g_{i-1}|^2}$$

Defining

$$s_{i-1} = \frac{|g_i|^2}{|g_i|^2 + (1 + c_{i-2}) |g_{i-1}|^2}$$

and

$$s_j = s_{i-1} c_j \qquad j = 0, ---, i-2$$

gives

$$p_i = g_i - s_{i-1} \Delta g_{i-1} - \sum_{j=0}^{i-2} s_j \Delta g_j$$

and the theorem is proved.

Since $p_i = H_i g_i$, it follows that the transformation represented by the H_i matrix projects the gradient g_i into W. This projected gradient becomes the next direction of search for the minimum of the quadratic function in the subspace W.

A MODIFIED VERSION OF THE DAVIDON METHOD

Noting the disappearance of the matrix Y_i in equation (10), it is tempting to redefine the Davidon direction vector p_i as

$$p_i' = Q_i g_i \qquad i = 0, ---, n \tag{17}$$

where $Q_o = H_o$ and

$$Q_{i+1} = Q_i - Z_i' \tag{18}$$

$$Z_i' = \frac{Q_i \Delta g_i \Delta g_i^T Q_i}{\Delta g_i^T Q_i \Delta g_i} \tag{19}$$

and investigate the relationship between p_i and p_i'. It is quickly seen that Q_i is symmetric and positive semi-definite, but it cannot be immediately assumed that the direction vectors p_i' are A-conjugate.

With $H_o = Q_o = I$, formula (5) can be written

$$H_{i+1} = I + \sum_{j=0}^{i} Y_j - \sum_{j=0}^{i} Z_j \qquad i < n \tag{20}$$

and (18) can be written

$$Q_{i+1} = I - \sum_{j=0}^{i} Z_j' \qquad i < n \tag{21}$$

Showing that $Z_j = Z_j'$ $(j = 0, ---, n-1)$ is then equivalent to proving that $p_i = p_i'$ $(i = 0, ---, n)$.

Theorem 4: <u>The Davidon method and its modified version generate identical direction vectors for a quadratic function</u>

By definition

$$Z_o = Z_o' = \frac{\Delta g_o \Delta g_o^T}{\Delta g_o^T \Delta g_o}$$

Assuming $Z_j = Z_j'$ $(j = 0, ---, i-1)$ implies that

$$H_k g_k = Q_k g_k \qquad k = 0, ---, i \tag{22}$$

and

$$H_i = Q_i + \sum_{j=0}^{i-1} Y_j \tag{23}$$

The inductive hypothesis (22) implies that $g_{i+1}^T p_{i-1}' = 0$ and $g_{i-1}^T p_{i-1}' \neq 0$ by properties of p_{i-1}. Starting with $g_{i+1}^T p_i' = 0$ by (1) and substituting these properties in the argument of Lemma 1, it is seen that $g_{i+1}^T Q_{i-1} g_i = 0$. The symmetry of Q_{i-1}, together with the above relationships and the logic of Theorem 1, will give the desired result that

$$Q_i g_{i+1} = g_{i+1} \tag{24}$$

Substituting (24) into (19) gives

$$Z_i' = \frac{(g_{i+1} - Q_i g_i)\Delta g_i^T Q_i}{\Delta g_i^T (g_{i+1} - Q_i g_i)}$$

By (7) and Theorem 1

$$Z_i = \frac{(g_{i+1} - H_i g_i)\Delta g_i^T H_i}{\Delta g_i^T (g_{i+1} - H_i g_i)}$$

By (23)

$$\Delta g_i^T H_i = \Delta g_i^T Q_i + \sum_{j=0}^{i-1} \frac{(\Delta g_i^T \Delta x_j)\Delta x_j^T}{\Delta x_j^T \Delta g_j}$$

which by (3) reduces to

$$\Delta g_i^T H_i = \Delta g_i^T Q_i \qquad (25)$$

Using (25) and (22) it is shown that

$$Z_i' = Z_i$$

and therefore

$$p_i = p_i'$$

and

$$H_i = Q_i + \sum_{j=0}^{i-1} Y_j \qquad (26)$$

for all values of $i \leq n$.

Although both algorithms generate the same steps to the minimum of the quadratic function, only the original Davidon H matrix yields the curvature of the function at that minimum. In particular, by comparing (26) and (8), it is seen that $H_n = A^{-1}$ while $Q_n = 0$. The implication for a non-quadratic function is that Q_n should be replaced by the estimate of A^{-1} given by $\sum_{i=0}^{n-1} Y_i$ and the same process repeated every n iterations.

CONCLUDING REMARKS

For a quadratic function, it has been shown that the Davidon method, its modified version, and the conjugate gradient method theoretically generate identical steps leading to the minimum. Reference 1 contains a comparison of the numerical efficiencies of the schemes when programmed for the IBM 7094 computer, using identical routines for the one-dimensional search (Ref. 8) and the closed form evaluation of a quadratic function and its gradient. By using the Davidon method and its modified version, almost identical solutions were obtained which were more accurate than those obtained using three theoretically equivalent representations of the conjugate gradient scheme.

Also contained in Reference 1 is a comparative study of the same five algorithms applied to a non-quadratic function. The Davidon method, closely followed by its modified version, clearly exhibited the best convergence in examples with small numerical error, that is, with all computations done in double precision arithmetic (sixteen decimal digits) and with closed form evaluation of the function and its gradient. To simulate the effects of numerical error, the computations were repeated in single precision (eight decimal digits). The deterioration exhibited by all the algorithms was especially severe for the Davidon scheme on account of the appearance of gradient differences in the metric. Less seriously affected was the modified Davidon algorithm, probably because of the systematic discarding of this error accumulation every n cycles. However, both schemes were ultimately susceptible to loss of the descent property. The simplest version of the conjugate gradient algorithm proved the least susceptible to error propagation influences.

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