A Family of Variable-Metric Methods Derived by Variational Means

By Donald Goldfarb

Abstract. A new rank-two variable-metric method is derived using Greenstadt's variational approach [*Math. Comp.*, this issue]. Like the Davidon-Fletcher-Powell (DFP) variable-metric method, the new method preserves the positive-definiteness of the approximating matrix. Together with Greenstadt's method, the new method gives rise to a one-parameter family of variable-metric methods that includes the DFP and rank-one methods as special cases. It is equivalent to Broyden's one-parameter family [*Math. Comp.*, v. 21, 1967, pp. 368–381]. Choices for the inverse of the weighting matrix in the variational approach are given that lead to the derivation of the DFP and rank-one methods directly.

In the preceding paper [6], Greenstadt derives two variable-metric methods, using a classical variational approach. Specifically, two iterative formulas are developed for updating the matrix H_k, (i.e., the inverse of the variable metric), where H_k is an approximation to the inverse Hessian $G^{-1}(x_k)$ of the function being minimized.*

Using the iteration formula

$$H_{k+1} = H_k + E_k$$

to provide revised estimates to the inverse Hessian at each step, Greenstadt solves for the correction term E_k that minimizes the norm

$$N(E_k) = \mathrm{Tr}\,(WE_kWE_k^T)$$

subject to the conditions

$$E_k^T = E_k \tag{1}$$

and

$$E_ky_k = \sigma_k - H_ky_k\,. \tag{2}$$

W is a positive-definite symmetric matrix and Tr denotes the trace.

The first condition is a symmetry condition which ensures that all iterates H_k will be symmetric as long as the initial estimate H_0 is chosen to be symmetric. The second condition ensures that the updated matrix H_{k+1} satisfies the equation

$$H_{k+1}y_k = \sigma_k$$

and hence, that the method is of the "quasi-Newton" type [1].

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* The reader is referred to Greenstadt's paper [6] for a more detailed discussion of variable-metric methods and for definitions of some of the terms used here.

If the function being minimized were quadratic, H_{k+1} would operate on the vector y_k as would the matrix G^{-1}. The norm chosen by Greenstadt is essentially a weighted Euclidean norm.

Solving this constrained minimization problem using Lagrange multipliers, Greenstadt obtained the following formula for E_k:

$$E_k = \frac{1}{(y^TMy)} \Big\{ \sigma y^T M + My\sigma^T - Hyy^TM - Myy^TH - \frac{1}{(y^TMy)} [(y^T\sigma) - (y^THy)]Myy^TM \Big\}, \tag{3}$$

where $M = W^{-1}$.

If the current approximation H to G^{-1} is substituted for M, Greenstadt's first formula is obtained:

$$E_H = \frac{1}{(y^THy)} \left\{ \sigma y^T H + Hy\sigma^T - \left[1 + \left(\frac{y^T\sigma}{y^THy}\right)\right] Hyy^TH \right\}.$$

(Throughout the remainder of the note no superscript will indicate the kth iterate and a (*) superscript will denote the $(k + 1)$st iterate.)

If, instead, H^* is substituted for M in Eq. (3),

$$E_{H^*} = \frac{1}{(y^T\sigma)} \left\{ -\sigma y^T H - Hy\sigma^T + \left[1 + \frac{(y^THy)}{(y^T\sigma)}\right] \sigma\sigma^T \right\}$$

is obtained. The above two correction terms appear to be similar, at least in part, to both the Davidon-Fletcher-Powell (or DFP) rank-2 correction term

$$E_{R2} = \frac{\sigma\sigma^T}{\sigma^Ty} - \frac{Hyy^TH}{y^THy}$$

and the rank-1 correction term [1], [3], and [7]

$$E_{R1} = \frac{(\sigma - Hy)(\sigma - Hy)^T}{(\sigma - Hy)^Ty}.$$

In fact, all four corrections terms E_H, E_{H^*}, E_{R1}, and E_{R2} give rise to algorithms that locate the exact minimum of a strictly convex quadratic objective function of N variables in N steps. They also result in a matrix H which after those N steps is exactly equal to G^{-1}. Proofs of this property, which we shall refer to as "exactness" following Broyden [1], were given for E_{R2}, E_{R1}, and E_H by Fletcher and Powell [4], Broyden [1], and Bard [6, Appendix], respectively.

It is easy to show that this property also holds for variable-metric algorithms with correction term E_{H^*}. For example, Bard's proof may be followed almost entirely, except for some obvious and trivial changes.

E_{R2} and E_{H^*}, moreover, share the additional property of preserving the positive-definiteness of the approximating matrix H. This ensures the stability of the corresponding variable-metric algorithms that search for a minimum along the direction $-Hg$ at each step. Fletcher and Powell proved this for E_{R2}. The proof for E_{H^*} follows from the observation that

$$x^T(E_{H^*} - E_{R2})x = x^T E_{H^*} x - x^T E_{R2} x = \frac{[(y^T Hy)(x^T\sigma) - (y^T\sigma)(x^T Hy)]^2}{(y^T\sigma)^2(y^T Hy)} \geqq 0 .$$

It may seem then that the iteration scheme $H^* = H + E_{H^*}$ would be less likely to generate a sequence of matrices $\{H_i\}$ that tends toward singularity than would the DFP iteration scheme $H^* = H + E_{R2}$. One should not count this apparent improvement too heavily, for the behavior of a variable-metric algorithm and its convergence to a stationary point depend upon the sequence $\{H_i\}$ being bounded above as well as being bounded away from singularity [5].

The resemblances between the correction terms E_{R2}, E_{R1}, E_H and E_{H^*} suggest that each can be written as a linear combination of the others. This is indeed the case: E_{R2} and E_{R1} can be expressed directly as weighted sums of E_H and E_{H^*}, and vice versa.

$$\text{(4)} \quad \begin{aligned} E_{R2} &= \frac{(y^T Hy)E_H + (y^T\sigma)E_{H^*}}{y^T Hy + y^T\sigma} = \frac{(y^T Hy)E_H + (y^T H^* y)E_{H^*}}{y^T Hy + y^T H^* y} , \\ E_{R1} &= \frac{(y^T Hy)^2 E_H - (y^T\sigma)^2 E_{H^*}}{(y^T Hy)^2 - (y^T\sigma)^2} = \frac{(y^T Hy)^2 E_H - (y^T H^* y)^2 E_{H^*}}{(y^T Hy)^2 - (y^T H^* y)^2} , \end{aligned}$$

$$\text{(5)} \quad \begin{aligned} E_H &= \gamma E_{R2} + (1 - \gamma)E_{R1} , \\ E_{H^*} &= 1/\gamma E_{R2} + (1 - 1/\gamma)E_{R1} , \end{aligned}$$

where

$$\gamma = \left(\frac{y^{T\sigma}}{y^T Hy}\right) .$$

It is especially interesting that the two variationally derived correction terms E_H and E_{H^*} give rise to a one-parameter family of correction terms $E = \alpha E_H + (1 - \alpha) E_{H^*}$ whose corresponding variable-metric methods are "exact." The DFP-rank-2 and rank-1 correction terms are members of this one-parameter family that correspond to particularly interesting choices for the parameter α. This family includes all symmetric variable-metric correction terms that have been published [1], [2], [3], [4], [6], [7].**

In fact, it is equivalent to the one-parameter family given by Broyden's algorithm 2 [1]. The equivalence can be obtained by setting

$$\text{(6)} \qquad \alpha = \frac{(1 - \beta y^T\sigma)y^T Hy}{y^T Hy + y^T\sigma} ,$$

where β is Broyden's parameter.

Broyden's algorithm 1 (i.e., the rank-1 algorithm) is just a special case of his algorithm 2 [1], with $\beta = 1/(y^T Hy - y^T\sigma)$; a point that seems to have been overlooked by Broyden himself.

It is also possible to obtain E_{R1} and E_{R2} directly from Eq. (3) by choice of a suitable M. For the rank-1 case a choice that works is

$$M_{R1} = H^* - H = E .$$

However, using $M_{R1} = M$ in Eq. (3) yields $E = E_{R1}$ which has rank 1 and, hence, M_{R1} has no inverse.

** Davidon's variance algorithm [3] multiplies the rank-1 correction term E_{R1} by a scalar function of $(g^T Hg^*/g^{*T} Hg^*)$ so as to ensure the stability of the method.

Before going further, we note that:

(i) Formula (3) is homogeneous in M; therefore, replacing M by μM, where μ is a scalar, has no affect on the resultant E.

(ii) M always appears in conjunction with y in formula (3) either as My or as y^TM; therefore, the replacement of $(y^THy)H$ by Hyy^TH and $(y^T\sigma)H^* = (y^TH^*y)H^*$ by $H^*yy^TH^*$ as terms of M has no affect on the resultant E.

Hence the substitution of either

$$M_{R1} = H^* - \frac{Hyy^TH}{y^THy} \tag{7}$$

or

$$M_{R1} = H - \frac{\sigma\sigma^T}{\sigma^Ty} \tag{8}$$

for M in Eq. (3) also yields E_{R1}.

Substitution of any of the forms of M_{R2} given below in Eq. (3) is sufficient to show that all give rise to the DFP correction term E_{R2}.

$$\begin{aligned} M_{R2} &= (y^THy)^{1/2}H^* - (y^T\sigma)^{1/2}H\,, \\ M_{R2} &= (y^TH^*y)^{-1/2}H^* - (y^THy)^{-1/2}H\,, \\ M_{R2} &= H^* - \left(\frac{y^T\sigma}{y^THy}\right)^{1/2}\frac{Hyy^TH}{y^THy}\,, \\ M_{R2} &= H - \left(\frac{y^THy}{y^T\sigma}\right)^{1/2}\frac{\sigma\sigma^T}{y^T\sigma}\,. \end{aligned} \tag{9}$$

Although the matrices M_{R1} and M_{R2} given by expressions (7) through (9) are, in general, nonsingular, these choices for M and hence, the corresponding W's are not necessarily positive-definite. Thus, their substitution in Eq. (3) is somewhat contrived. Just what role they play in the variational derivation of the rank-1 and DFP rank-2 methods remains confusing.

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