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GRADIENT METHODS IN MATHEMATICAL PROGRAMMING
PART 1 - REVIEW OF PREVIOUS TECHNIQUES

by

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Gradient Methods in Mathematical Programming

Part 1 - Review of Previous Techniques[1]

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Abstract. This report is the first of a series on gradient methods in mathematical programming. It considers the problem of minimizing a function f(x), where f is a scalar function and x is an n-vector whose components are unconstrained. For this problem, three previous methods are reviewed, namely, the ordinary gradient method, the conjugate-gradient method, and the variable-metric method. A new intuitive derivation of the last two algorithms is presented.

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1. Definitions

The following definitions are used throughout the paper:

(a) The symbol x denotes the position vector

$$x = \begin{bmatrix} x^1 \\ x^2 \\ . \\ . \\ . \\ . \\ x^n \end{bmatrix} \tag{1}$$

whose scalar components are $x^1, x^2, \ldots, x^n$.

(b) The symbol f denotes a scalar function of the vector x, that is

$$f = f(x) \tag{2}$$

(c) The symbol g denotes the column vector

$$g(x) = \begin{bmatrix} \partial f/\partial x^1 \\ \partial f/\partial x^2 \\ . \\ . \\ . \\ . \\ \partial f/\partial x^n \end{bmatrix} \tag{3}$$

whose components are the first partial derivatives of f with respect to the scalar variables $x^1, x^2, \ldots, x^n$. This is the gradient of the function f.

(d) The symbol H denotes the square matrix

$$H(x) = \begin{bmatrix} \partial^2 f/\partial x^1 \partial x^1 & \partial^2 f/\partial x^1 \partial x^2 & \cdots\cdots & \partial^2 f/\partial x^1 \partial x^n \\ \partial^2 f/\partial x^2 \partial x^1 & \partial^2 f/\partial x^2 \partial x^2 & \cdots\cdots & \partial^2 f/\partial x^2 \partial x^n \\ \cdots\cdots & \cdots\cdots & \cdots\cdots & \cdots\cdots \\ \partial^2 f/\partial x^n \partial x^1 & \partial^2 f/\partial x^n \partial x^2 & \cdots\cdots & \partial^2 f/\partial x^n \partial x^n \end{bmatrix} \tag{4}$$

whose components are the second partial derivatives of the function f with respect to the scalar variables $x^1, x^2, \ldots, x^n$.

(e) The symbol x denotes the nominal point. The symbol $\tilde{x}$ denotes the point following x. The symbol $\hat{x}$ denotes the point preceding x.

(f) The symbol $\delta(\ldots)$ denotes the displacement leading from a point to the next point. Therefore, the following relations hold:

$$\begin{aligned} \tilde{x} &= x + \delta x \\ x &= \hat{x} + \delta\hat{x} \end{aligned} \tag{5}$$

(g) The superscript T denotes the transpose of a matrix.

2. Introduction

A basic problem of mathematical programming is that of finding the minimum of a function

$$f = f(x) \tag{6}$$

where f is a scalar function and x is an n-vector. If the n components of the vector x are unconstrained, the extremum of (6) occurs when the following necessary condition is satisfied:

$$g(x) = 0 \tag{7}$$

where g is the gradient of the function f with respect to the vector x. For a minimum, the matrix of the second derivatives (4) must be positive definite at the point x defined by (7).

If the function (6) is quadratic, the gradient g(x) is linear with respect to x. Hence, Eq. (7) can be solved analytically. On the other hand, if (6) is nonquadratic, the gradient g(x) is nonlinear. This being the case, approximate methods must be employed to solve Eq. (7). One possible method consists of quasilinearizing (7) about a nominal point. Another method, the descent method, consists of constructing corrections δx leading from a nominal point x to a varied point $\tilde{x}$ such that

$$f(\tilde{x}) < f(x) \tag{8}$$

Thus, by an iterative procedure (that is, through successive decreases in the value of the function f), it is hoped that the minimum of f is approached to any desired degree of accuracy.

This report is the first of a series on gradient methods in mathematical programming. It reviews three of the existing techniques, namely, the ordinary gradient method, the conjugate-gradient method (Refs. 1-3), and the variable-metric method (Refs. 4-5). For the last two methods, a new intuitive derivation is presented.

3. Ordinary Gradient Method

To first-order terms, the values of the function (6) at the varied point and the nominal point are related by

$$f(\tilde{x}) \cong f(x) + \delta f(x) \tag{9}$$

where the first variation $\delta f(x)$ is given by

$$\delta f(x) = g^T(x)\delta x \tag{10}$$

with

$$\delta x = \tilde{x} - x \tag{11}$$

Also to first-order terms, the greatest decrease in the value of the function is achieved if the first variation (10) is minimized. Here, we limit our analysis to those variations δx which satisfy the constraint

$$K = \delta x^T \delta x \tag{12}$$

where K is a prescribed quantity.

3.1. Derivation of the Algorithm. Standard methods of the theory of maxima and minima show that the fundamental function of this problem is the scalar function

$$F = g^T(x)\delta x + (1/2\alpha)\delta x^T \delta x \tag{13}$$

where $1/2\alpha$ is a constant Lagrange multiplier. The optimum system of variations must be such that

$$G(\delta x) = 0 \tag{14}$$

where G is the gradient of the function F with respect to the scalar variables $\delta x^1, \delta x^2, \ldots, \delta x^n$. In the light of (13), the explicit form of (14) is the following:

$$\delta x = -\alpha g(x) \tag{15}$$

and shows that the optimum correction δx has the gradient direction. This is why the method is called the ordinary gradient method. Upon substituting (15) into (12), we see that

$$K = \alpha^2 g^T(x) g(x) \tag{16}$$

Therefore, a one-to-one correspondence exists between the value of the constant K and the value of α. This being the case, one can bypass prescribing K and reason directly on α, as in the considerations which follow.

3.2. Descent Property. Upon combining Eqs. (10) and (15), we see that the first variation becomes

$$\delta f(x) = -\alpha g^T(x) g(x) \tag{17}$$

and is negative for $\alpha > 0$. Therefore, if α is sufficiently small, the function f decreases. This guaranteed decrease of f at every step is the most important property of the gradient method.

3.3 Optimum Stepsize. The next step is to assign a value to the parameter α, the stepsize of the gradient method. There are two situations to be avoided: (a) if the stepsize α is exceeedingly small, the decrease of the function is guaranteed but very small; therefore, the number of iterations necessary for convergence is large; and (b) if the stepsize α is too large, the first variation may be only a small part of the total variation; therefore, the function f may actually increase. In order to prevent the occurrence of (a) and (b), the stepsize α must be in the proper range.

If Eqs. (11) and (15) are combined, the position vector at the end of any iteration becomes

$$\tilde{x} = x - \alpha g(x) \tag{18}$$

For each point x, Eq. (18) defines a one-parameter family of points $\tilde{x}$ for which the function f takes the form

$$f(\tilde{x}) = f(x - \alpha g(x)) = F(\alpha) \tag{19}$$

The greatest decrease in the function $F(\alpha)$ occurs if the parameter α satisfies the following necessary condition:

$$F_\alpha = 0 \tag{20}$$

On account of (19), the following relation holds:[5]

$$F_\alpha = -g^T(\tilde{x})g(x) \tag{21}$$

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[5] At $\alpha = 0$, the derivative (21) is given by $F_\alpha = -g^T(x)g(x)$ and is negative, since $g^T(x)g(x) > 0$.

Therefore, Eq. (20) becomes

$$g^T(\tilde{x})g(x) = 0 \tag{22}$$

and shows that the gradient $g(\tilde{x})$ is orthogonal to the gradient $g(x)$.

3.4. Summary of the Algorithm. Equations (15), (17), and (22) summarize the general properties of the ordinary gradient algorithm. They are valid regardless of the function $f(x)$, as long as it is continuous and has continuous first derivatives.

For any given iteration, the algorithm can be summarized as follows: (a) for a given nominal point x, the gradient $g(x)$ is known from Eq. (3); (b) the optimum value of the stepsize α must be determined by solving Eq. (20) with a one-dimensional search, as in Section 7; (c) the correction δx to the position vector x is determined using Eq. (15); and (d) the new position vector $\tilde{x}$ is computed through Eq. (11). Next, the position vector $\tilde{x}$ becomes the nominal point x for the subsequent iteration, and the procedure is repeated until a predetermined stopping condition is satisfied (see Section 8).

4. Modifications of the Ordinary Gradient Method

The ordinary gradient method is conceptually simple and stable in that the function $f(x)$ is reduced at every iteration; however, it has the drawback of slow convergence. For this reason, methods have been developed to reduce the number of iterations required for convergence. In this connection, let the displacement vector δx be written in the form

$$\delta x = -\alpha p \tag{23}$$

where p is the search direction. The following are particular forms of the vector p:

$$p = g(x) + q \tag{24}$$

and

$$p = Ag(x) \tag{25}$$

where q is an n-vector and A is an n x n symmetric matrix. In Section 5, the conjugate-gradient algorithm is derived by reasoning on (24); in Section 6, the variable-metric algorithm is derived by reasoning on (25).

5. Conjugate-Gradient Method

In this section, we consider the algorithm

$$\tilde{x} = x + \delta x, \qquad \delta x = -\alpha p, \qquad p = g(x) + q \tag{26}$$

where q is an n-vector to be specified. The first variation of the function (6) is given by Eq. (10) which, in the light of (26), becomes

$$\delta f(x) = -\alpha[g^T(x)g(x) + g^T(x)q] \tag{27}$$

We note that $g^T(x)g(x) > 0$. Therefore, for $\alpha > 0$, the descent property of this algorithm is ensured if one chooses q so that

$$g^T(x)q = 0 \tag{28}$$

If Eqs. (26-1) and (26-2) are combined, the position vector at the end of any iteration becomes

$$\tilde{x} = x - \alpha p \tag{29}$$

For a given point x and a given vector p, Eq. (29) defines a one-parameter family of points $\tilde{x}$ for which the function f takes the form

$$f(\tilde{x}) = f(x - \alpha p) = F(\alpha) \tag{30}$$

The greatest decrease in the function $F(\alpha)$ occurs if the parameter α satisfies the following necessary condition:

$$F_\alpha = 0 \tag{31}$$

On account of (30), the following relation holds:

$$F_\alpha = -g^T(\tilde{x})p \tag{32}$$

Therefore, Eq. (31) becomes

$$g^T(\tilde{x})p = 0 \tag{33}$$

and shows that the gradient $g(\tilde{x})$ is orthogonal to the search direction p.

Next, we apply Eq. (33) to the previous iteration and obtain

$$g^T(x)\hat{p} = 0 \tag{34}$$

By comparing (28) and (34), we conclude that one possible choice of the vector q is the following:

$$q = \gamma\hat{p} \tag{35}$$

where γ is a constant. As a consequence, the algorithm (26) can be rewritten as

$$\tilde{x} = x + \delta x\,, \quad \delta x = -\alpha p\,, \quad p = g(x) + \gamma\hat{p} \tag{36}$$

The next step is to determine the constant γ. If Eqs. (36) are combined, the position vector at the end of any iteration becomes

$$\tilde{x} = x - \alpha g(x) - \alpha\gamma\hat{p} \tag{37}$$

For a given point x and a given vector $\hat{p}$, Eq. (37) defines a two-parameter family of points $\tilde{x}$ for which the function f takes the form

$$f(\tilde{x}) = f(x - \alpha g(x) - \alpha\gamma\hat{p}) = F(\alpha, \gamma) \tag{38}$$

The greatest decrease in the function $F(\alpha, \gamma)$ occurs if the parameters α, γ satisfy the following necessary conditions:

$$F_\alpha = 0 , \quad F_\gamma = 0 \tag{39}$$

On account of (36-3) and (38), the following relations hold:

$$F_\alpha = - g^T(\tilde{x})p \quad , \quad F_\gamma = -\alpha g^T(\tilde{x})\hat{p} \tag{40}$$

Therefore, Eqs. (39) become

$$g^T(\tilde{x})p = 0 \quad , \quad g^T(\tilde{x})\hat{p} = 0 \tag{41}$$

and show that the gradient $g(\tilde{x})$ is orthogonal to the search directions p and $\hat{p}$. A mathematical consequence of Eqs. (36-3) and (41) is that

$$g^T(\tilde{x})g(x) = 0 \tag{42}$$

showing that the gradients $g(\tilde{x})$ and $g(x)$ are orthogonal.

5.1. Quadratic Function. Now, consider the particular case of a quadratic function, that is, a function of the form

$$f(x) = a + b^T x + \frac{1}{2} x^T H x \tag{43}$$

where a is a constant scalar, b is a constant n-vector. and H is a constant, symmetric n x n matrix. For this function, the gradient is a linear function of x, that is,

$$g(x) = b + Hx \tag{44}$$

Since

$$g(\tilde{x}) = b + H\tilde{x} \tag{45}$$

relations (44) and (45) imply that

$$g(\tilde{x}) = g(x) + H\delta x = g(x) - \alpha Hp \tag{46}$$

Next, we introduce Eqs. (46) into (41) and, after laborious manipulations, obtain the solutions (Ref. 1)

$$\alpha = \frac{g^T(x)g(x)}{p^T Hp} \quad , \quad \gamma = \frac{g^T(x)g(x)}{g^T(\hat{x})g(\hat{x})} \tag{47}$$

where p is given by (36-3).

For a quadratic function, Hestenes and Stiefel (Ref. 1) proved that, if the first step of the descent process is a gradient step, the following relations hold:

$$g^T(x)g(x_*) = 0 \quad , \quad g^T(x)p_* = 0 \quad , \quad p^T Hp_* = 0 \tag{48}$$

where x_* denotes any state preceeding x. Equation (48-1) states that the gradient at each iteration is orthogonal to the gradient at every previous iteration. Equation (48-2) states that the gradient at each iteration is orthogonal to the search direction at every previous iteration. Finally, Eq. (48-3) states that the search direction at each iteration and the search direction at every previous iteration are conjugate with respect to the constant matrix H; this is why the algorithm is called the conjugate-gradient method. The algorithm (36) with α and γ defined by (47) reduces the gradient to zero in no more than n steps; therefore, the minimum of f(x) is reached in no more than n steps.

5.2. Nonquadratic Function. For a nonquadratic function, solving Eqs. (41) for α and γ requires a two-dimensional search (Ref. 6). The difficulty of this process can be avoided if one optimizes α exactly and uses an approximate value for γ, namely, that given by Eq. (47-2). This leads to the algorithm (Ref. 3)

$$\tilde{x} = x + \delta x, \quad \delta x = -\alpha p \quad , \quad p = g(x) + \frac{g^T(x)g(x)}{g^T(\hat{x})g(\hat{x})}\hat{p} \tag{49}$$

in which α is optimized by searching for the minimum of f along the direction defined by (49). Theoretically, therefore, the optimization of α requires that the relation (41-1) be satisfied.

For any iteration except the first, the complete algorithm can be stated as follows: (a) for a given nominal point x, the gradient g(x) is known; since the gradient $g(\hat{x})$ and the search direction $\hat{p}$ are known from the previous iteration, the search direction p can be determined with Eq. (49-3); (b) the optimum stepsize α must be determined by minimizing the function f along the search direction p, as in Section 7; (c) the correction δx to the position vector x is determined using Eq. (49-2); and (d) the new position vector $\tilde{x}$ is computed through Eq. (49-1). Next, the position vector $\tilde{x}$ becomes the nominal point for the subsequent iteration, and the procedure is repeated until a predetermined stopping condition is satisfied (see Section 8). To start the algorithm, one bypasses (49-3) and sets p = g(x), equivalent to stating that the first step is a gradient step.

In closing, the following comments are pertinent: (a) in the conjugate-gradient method, it is important that the stepsize α be determined accurately, while this is not the case with the ordinary gradient method; (b) theoretical considerations and numerical experience show the desirability of restarting the process every n or n + 1 iterations, that is, resetting p = g(x) every n or n + 1 iterations (Ref. 3).

6. Variable-Metric Algorithm

In this section, we consider the algorithm

$$\tilde{x} = x + \delta x , \qquad \delta x = -\alpha p , \qquad p = Ag(x) \tag{50}$$

where A is a symmetric n x n matrix to be specified. The first variation of the function (6) is given by Eq. (10) which, in the light of (50), becomes

$$\delta f(x) = -\alpha g^T(x) A g(x) \tag{51}$$

We note that, if the matrix A is positive definite, $g^T(x)Ag(x) > 0$. Therefore, for $\alpha > 0$, the descent property of this algorithm is ensured.

Now, consider the points $\hat{x}$ and x. At point $\hat{x}$, the gradient $g(\hat{x})$ and the matrix $\hat{A}$ are known; at point x, the gradient g(x) is known. Therefore, the differences

$$\delta\hat{x} = x - \hat{x}, \qquad \Delta\hat{g} = g(x) - g(\hat{x}) \tag{52}$$

are available. We wish to determine the matrix A so that the relation

$$A\Delta\hat{g} = \delta\hat{x} \tag{53}$$

is satisfied. After defining the matrix difference

$$\Delta\hat{A} = A - \hat{A} \tag{54}$$

we combine (53)-(54) to obtain

$$\Delta\hat{A}\Delta\hat{g} = \delta\hat{x} - \hat{A}\Delta\hat{g} \tag{55}$$

in which the only unknown is $\Delta\hat{A}$. Equation (55) admits the solution

$$\Delta\hat{A} = \frac{\delta\hat{x}\, y^T}{y^T \Delta\hat{g}} - \frac{\hat{A}\Delta\hat{g}\, z^T}{z^T \Delta\hat{g}} \tag{56}$$

where y and z denote arbitrary n-vectors. Therefore, the matrix A must be updated according to the relation

$$A = \hat{A} + \frac{\delta\hat{x}\, y^T}{y^T \Delta\hat{g}} - \frac{\hat{A}\Delta\hat{g}\, z^T}{z^T \Delta\hat{g}} \tag{57}$$

In particular, if one chooses

$$y = \delta\hat{x}\,, \quad z = \hat{A}\Delta\hat{g} \tag{58}$$

Eq. (57) becomes

$$A = \hat{A} + \frac{\delta\hat{x}\,\delta\hat{x}^T}{\delta\hat{x}^T \Delta\hat{g}} - \frac{\hat{A}\Delta\hat{g}\Delta\hat{g}^T\hat{A}}{\Delta\hat{g}^T\hat{A}\Delta\hat{g}} \tag{59}$$

Note that the second and third matrices on the right-hand side of (59) are symmetric; therefore, if $\hat{A}$ is symmetric, A is also symmetric.

6.1. Quadratic Function. Now, consider the particular case of a function having the form (43). For this quadratic function, the following properties can be shown to hold (Refs. 4-5 and 7-8):

(a) If the initial matrix A is chosen to be the inverse of the second derivative matrix H, that is, if

$$A = H^{-1} \tag{60}$$

at the initial point, the variable-metric algorithm exhibits one-step convergence. This is due to the fact that the variable-metric algorithm becomes identical with quasilinearization.

(b) If the initial matrix A is chosen to be positive definite, any subsequent matrix A is also positive definite. With this understanding, the following relations hold:

$$g^T(x)p_* = 0, \quad p^T H p_* = 0 \tag{61}$$

Equation (61-1) states that the gradient at each iteration is orthogonal to the search direction at every previous iteration. Equation (61-2) states that the search direction at each iteration and the search direction at every previous iteration are conjugate with respect to the constant matrix H. As the algorithm progresses, the matrix A tends to the inverse of the second derivative matrix H, and relation (60) becomes satisfied exactly when convergence is achieved. The algorithm (50), with A updated according to (59), reduces the gradient to zero in no more than n steps; therefore, the minimum of f(x) is reached in no more than n steps.

(c) As a particular case of (b), the initial matrix can be chosen to be

$$A = I \tag{62}$$

where I is the n x n identity matrix. Under these conditions, the variable-metric algorithm becomes identical with the conjugate-gradient algorithm of Section 5.

6.2. Nonquadratic Function. For a nonquadratic function, the variable-metric algorithm is represented by

$$\tilde{x} = x + \delta x, \quad \delta x = -\alpha p, \quad p = Ag(x) \tag{63}$$

with

$$A = \hat{A} + \frac{\delta\hat{x}\,\delta\hat{x}^T}{\delta\hat{x}^T\Delta\hat{g}} - \frac{\hat{A}\Delta\hat{g}\Delta\hat{g}^T\hat{A}}{\Delta\hat{g}^T\hat{A}\Delta\hat{g}} \tag{64}$$

The stepsize α is to be optimized by searching for the minimum of f along the direction defined by (63).

For any iteration except the first, the complete algorithm can be stated as follows: (a) for a given nominal point x, the gradient g(x) is known; since $g(\hat{x})$, $\delta\hat{x}$, $\hat{A}$ are known from the previous iteration, the matrix A can be computed with (64) and the search direction p with (63-3); (b) the optimum stepsize α must be determined by minimizing the function f along the search direction p, as in Section 7; (c) the correction δx to the position vector x is determined using Eq. (63-2); and (d) the new position vector $\tilde{x}$ is computed through Eq. (63-1). Next, the new position vector $\tilde{x}$ becomes the nominal point for the subsequent iteration and the procedure is repeated until a predetermined stopping condition is satisfied (see Section 8). To start the algorithm, one bypasses (64) and sets A equal to any symmetric, positive-definite matrix (for instance, the identity matrix).

In closing, the following comments are pertinent: (a) in the variable-metric method, it is important that the stepsize α be determined accurately; (b) restarting the algorithm every n or n + 1 iterations is not necessary; however, restarting is indispensable whenever the positive-definiteness of the matrix A is violated, for example, if the stepsize α becomes negative.

7. Search Technique

In each of the previous methods, the stepsize α must be optimized. In this section, we present techniques to solve the equation

$$F_\alpha(\alpha) = 0 \tag{65}$$

that is, to find the minimum of the function $F(\alpha)$ given by Eq. (19) for the ordinary gradient algorithm or Eq. (30) for the conjugate-gradient and variable-metric algorithms. Since the techniques in question involve the consideration of the first derivative F_α and perhaps the second derivative $F_{\alpha\alpha}$, we summarize these derivatives below.

For all of the previous methods, we have

$$F_\alpha(\alpha) = -g^T(\tilde{x})p \ , \quad F_{\alpha\alpha}(\alpha) = p^T H(\tilde{x})p \tag{66}$$

where

$$\tilde{x} = x - \alpha p \tag{67}$$

The search direction is given by $p = g(x)$ for the ordinary gradient method, Eq. (49-3) for the conjugate-gradient method, and Eq. (63-3) for the variable-metric method. Of course, Eq. (66-2) requires that the second-derivative matrix $H(x)$ be explicitly available. If this is not the case, one can use the difference scheme

$$\begin{aligned} F_{\alpha\alpha}(\alpha) &= (1/2\theta)[F_\alpha(\alpha + \theta) - F_\alpha(\alpha - \theta)] \\ &= (1/2\theta)[g(\tilde{x} + \theta p) - g(\tilde{x} - \theta p)]^T p \end{aligned} \tag{68}$$

In practice, one may choose

$$\theta = \epsilon_1 / |p| \tag{69}$$

where ϵ_1 is a small number.

7.1. Cubic Interpolation. Let the values of the function $F(\alpha)$ and its derivative $F_\alpha(\alpha)$ be computed for two different values of α, namely, α_1 and α_2, with $\alpha_2 > \alpha_1 \geq 0$. If α_1 and α_2 are such that

$$F_\alpha(\alpha_1) < 0 \quad , \quad F_\alpha(\alpha_2) > 0 \tag{70}$$

then the minimum of the function $F(\alpha)$ occurs for some value α in the range

$$\alpha_1 < \alpha < \alpha_2 \tag{71}$$

In this range, we represent the function $F(\alpha)$ with the cubic

$$F(\alpha) = A + B(\alpha - \alpha_1) + C(\alpha - \alpha_1)^2 + D(\alpha - \alpha_1)^3 \tag{72}$$

whose first and second derivatives are given by

$$F_\alpha(\alpha) = B + 2C(\alpha - \alpha_1) + 3D(\alpha - \alpha_1)^2 \quad , \quad F_{\alpha\alpha}(\alpha) = 2C + 6D(\alpha - \alpha_1) \tag{73}$$

The scalar coefficients A, B, C, D are determined by requiring (72) to match the ordinate and the slope of the curve $F(\alpha)$ at α_1 and α_2. Therefore, one has to solve the linear equations

$$\begin{aligned} F(\alpha_1) &= A \ , \qquad F(\alpha_2) = A + B(\alpha_2 - \alpha_1) + C(\alpha_2 - \alpha_1)^2 + D(\alpha_2 - \alpha_1)^3 \\ F_\alpha(\alpha_1) &= B, \qquad F_\alpha(\alpha_2) = B + 2C(\alpha_2 - \alpha_1) + 3D(\alpha_2 - \alpha_1)^2 \end{aligned} \tag{74}$$

Once the coefficients of the cubic (72) are known, the optimum value of α is determined by the condition (65). Therefore, in the light of (73), one arrives at the solution

$$\alpha = \alpha_1 + (1/3D)[-C + \sqrt{(C^2 - 3BD)}] \tag{75}$$

At this point, one recomputes the function $F(\alpha)$ and the derivative $F_\alpha(\alpha)$. Then, the process is iterated until a predetermined stopping condition is satisfied. For instance, one may require that

$$|F_\alpha(\alpha)| \leq \epsilon_2 \tag{76}$$

or that

$$|F_\alpha(\alpha)| \leq \epsilon_3 |F_\alpha(0)| \tag{77}$$

where ϵ_2 and ϵ_3 are prescribed small numbers.

7.2. Quasilinearization. An alternate technique for computing the optimum stepsize, that of quasilinearization with built-in safeguards to ensure that the function decreases at every step of the iterative search, is now presented. Let

$$\delta\alpha = \alpha - \alpha_o \tag{78}$$

denote the correction to α starting from an arbitrary nominal value α_o. If quasilinearization is applied to Eq. (65), one obtains the linear algebraic equation

$$F_{\alpha\alpha}(\alpha_o)\delta\alpha + F_\alpha(\alpha_o) = 0 \tag{79}$$

Next, we imbed Eq. (79) in the more general equation

$$F_{\alpha\alpha}(\alpha_o)\delta\alpha + \mu\rho F_\alpha(\alpha_o) = 0 \tag{80}$$

where μ denotes a scaling factor and ρ a direction factor such that

$$0 < \mu \leq 1 \quad , \quad \rho = \pm 1 \tag{81}$$

Equation (80) admits the solution

$$\delta\alpha = -\mu\rho F_\alpha(\alpha_o)/F_{\alpha\alpha}(\alpha_o) \tag{82}$$

The direction factor ρ is determined in such a way that the first variation

$$\delta F(\alpha_o) = F_\alpha(\alpha_o)\delta\alpha \tag{83}$$

is negative. From (82)-(83), we obtain

$$\delta F(\alpha_o) = -\mu\rho F_\alpha^2(\alpha_o)/F_{\alpha\alpha}(\alpha_o) \tag{84}$$

Therefore, $\delta F(\alpha_o)$ is negative if the direction factor ρ is chosen as follows:

$$\rho = \text{sign } F_{\alpha\alpha}(\alpha_o) \tag{85}$$

Because of this choice, the correction (82) becomes

$$\delta\alpha = -\mu F_\alpha(\alpha_o)/|F_{\alpha\alpha}(\alpha_o)| \tag{86}$$

To perform the search, a nominal value must be given to α_o. Then, one sets $\mu = 1$, computes $\delta\alpha$ from Eq. (86) and α from Eq. (78). If $F(\alpha) < F(\alpha_o)$, the scaling factor $\mu = 1$ is acceptable. If $F(\alpha) > F(\alpha_o)$, the previous value of μ must be replaced by some smaller value in the range $0 \leq \mu \leq 1$ until the condition $F(\alpha) < F(\alpha_o)$ is met; this can be obtained through bisection, that is, by successively dividing the value of μ by 2. At this point, the search step is completed. The value obtained for α becomes the nominal value α_o for the next search step, and the procedure is repeated until a desired degree of accuracy is obtained, that is, until Ineq. (76) or (77) is satisfied. In the absence of better information, the first step of the search procedure can be made with $\alpha_o = 0$.

8. Termination of the Algorithm

One way to terminate the gradient algorithm is to impose a condition on the modulus of the gradient, for example,

$$g^T(x)g(x) \leq \epsilon_4 \tag{87}$$

where ϵ_4 is a prescribed small number. If the function f(x) is rather flat in the neighborhood of the minimum, then Eq. (87) may not yield precise coordinates. In this case, the following additional condition is suggested:

$$\delta x^T \delta x \leq \epsilon_5 \tag{88}$$

where ϵ_5 is a prescribed small number.

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