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N-Step Conjugate Gradient Minimization Scheme for Nonquadratic Functions

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Introduction

In a recent report,[1] Jacobson and Oksman describe a new algorithm for function minimization. The novel and most prominent feature of this algorithm is its ability to minimize in $N + 2$ steps not only quadratics but also a larger class of homogeneous functions. In this regard this algorithm may prove superior (as shown experimentally in Ref. 1) to the widely used conjugate direction techniques as adapted to the minimization of nonquadratic functions by Davidon,[2] Fletcher and Powell,[3] and Fletcher and Reeves.[4] Both the variable metric technique of Davidon and that of Jacobson and Oksman require the storage and updating of an $N \times N$ full or half matrix.

One of the important uses of the minimization scheme is for solving the large algebraic systems generated by the finite element (or any other discretization) method applied to nonliner problems via a direct search[5,6] for the minimum. The number of variables may be so large in such cases that the $N \times N$ matrix will no longer fit into the core, and both the variable metric method as well as the method of Jacobson and Oksman may prove to be disadvantageous from the point of view of the programing and execution time. The marked advantage of the conjugate gradient method lies precisely in the avoidance of this matrix.

It is the purpose of this Note to present a new conjugate gradient algorithm which, like that of Jacobson and Oksman, minimizes a larger class of nonquadratic functions in no more than N steps. The algorithm presented here, however, does not require the storage and handling of large full matrices.

Minimization Scheme

Consider the function

$$f = (1/2r)[(x - \xi)^T K(x - \xi)]^r + c \tag{1}$$

where K is an $N \times N$ positive definite matrix. The function f has its minimal value, $f = c$, at $x = \xi$. In the present discussion it is assumed that c is known and for the sake of simplicity set equal to zero. For $r = 1$ the method of conjugate gradients will minimize f in no more than N steps. As will now be shown, the conjugate gradient algorithm can be modified to insure the convergence of f in N steps not only for $r = 1$ but for any r.

The gradient $g = \nabla f$ of f is written concisely as

$$g = FK(x - \xi) \tag{2}$$

where $F = [(x - \xi)^T K(x - \xi)]^{r-1}$. Starting with x_0, the gradient $g_0 = \nabla f(x_0)$ is calculated. Then the next x, x_1 is sought along the search vector $p_0 = g_0$ such that $x_1 = x_0 + \alpha_0 p_0$. Also α_0 is fixed by the condition that f assumes a local minimum with respect to α_0. The next gradient, g_1, can be calculated (assuming for the moment that K is given) by $g_1 = F_1(g_0/F_0 + \alpha_0 K p_0)$. As in the quadratic case, the next search direction p_1 is obtained from $p_1 = g_1 + \beta_0 p_0$. The third gradient, g_2, is given by

$$g_2 = F_2(g_1/F_1 + \alpha_1 K g_1 + \alpha_1\beta_0 K p_0) \tag{3}$$

and β_0 is obtained from the condition that g_2 is orthogonal to g_0 (and g_1). Hence

$$\beta_0 = -g_0{}^T K g_1/g_0{}^T K g_0 \tag{4}$$

Multiplying

$$g_1 = F_1(g_0/F_0 + \alpha_0 K p_0) \tag{5}$$

by g_1 and g_0 yields $g_1{}^T K g_0 = g_1{}^T g_1/F_1\alpha_0$ and $g_0{}^T K g_0 = -g_0{}^T g_0/P_0\alpha_0$, and with these β becomes

$$\beta_0 = g_1{}^T g_1 F_0/g_0{}^T g_0 F_1 \tag{6}$$

The gradient g_2 is now normal to both g_1 and g_0. Continuing this scheme will generate, as in the quadratic case, a complete set of N orthogonal gradients. Since there can be only N nonzero orthogonal vectors in the N-dimensional space, the $(N + 1)$th gradient must vanish.

For a general function neither r nor K is known, and the F needed for calculating β in Eq. (6) should be obtained from f and g. Equation (1) readily leads to

$$F_0/F_1 = (f_0/f_1)^{(r-1)/r} \tag{7}$$

Also

$$F_0/F_1 = g_0{}^T(x_1 - \xi)/g_1{}^T(x_0 - \xi) \tag{8}$$

and

$$g_0{}^T\xi = g_0{}^T x_0 - 2rf_0, \quad g_1{}^T\xi = g_1{}^T x_1 - 2rf_1 \tag{9}$$

Then, since $g_1{}^T(x_0 - x_1) = -g_1 p_0 \alpha_0 = 0$, introduction of Eq. (9) into Eq. (8) results in

$$F_0/F_1 = (\alpha_0 g_0{}^T p_0 + 2rf_0)/2rf_1 \tag{10}$$

The exponent r is obtained from the equation

$$(f_1/f_0)^t = 1 + \alpha_0 p_0{}^T g_0 t/2f_0 \qquad t = 1/r \tag{11}$$

resulting from equating Eqs. (10) and (7). Equation (11) is written concisely as

$$a^t = 1 + bt \tag{12}$$

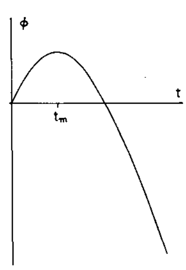

Fig. 1 The function $\varphi = -a^t + 1 + bt$. It attains its maximal value at $t = t_m$.

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where $t = 1/r$. This equation is then solved by iteratively searching for the zero value of the function φ

$$\varphi = -a^t + 1 + bt \tag{13}$$

The form of φ is shown in Fig. 1, and it can be seen that φ has a maximum at the point $t_m = \ln(b/\ln a)/\ln a$ and that $2t_m$ is a reasonable first approximation for t. For any $t_0 > t_m$ the Newton-Raphson scheme

$$t_{j+1} = t_j - \varphi_j'/\varphi_j, \quad \varphi' = -a^t \ln a + b \tag{14}$$

converges to the correct solution, computer experiments showing that about four steps (for $a = 0.98$) are required for full convergence.

The general minimization algorithm is then as follows. Start:

$$x_0, \quad f_0 = f(x_0), \quad g_i = \nabla f_0, \quad p_0 = g_0$$

Iterate: Obtain α_i from: $\partial f(x_i + \alpha_i p_i)/\partial \alpha_i = 0$

$$x_{i+1} = x_i + \alpha_i p_i, \quad f_{i+1} = f(x_{i+1}), \quad g_{i+1} = \nabla f_{i+1}$$

Obtain t_i from: $(f_{i+1}/f_i)^{t_i} = 1 + \alpha_i p_i{}^T g_i t_i / 2f_i$

$$\begin{aligned} \gamma_i &= (f_i/f_{i+1})^{1-t_i}, \quad \beta_i = g^T{}_{i+1} g_{i+1}/g_i{}^T g_i \\ p_{i+1} &= g_{i+1} + \beta_i \gamma_i p_i \end{aligned} \tag{15}$$

In algorithm (15) it was assumed that $f = 0$ at the minimum. If at the minimum $f = c$, f should be replaced by $f - c$ in algorithm (15). If only an estimate of c is used, the algorithm will assume that f is quadratic near (depending on the closeness of $f_{\min}$ to c) the minimum. If $f_{\min} > 0$, but $c = 0$, algorithm (15) will minimize $f = 1/2r[(x - \xi)^T K(x - \xi) + f_{\min}]^r$.

Numerical Example

The present algorithm was used for minimizing

$$f = (\tfrac{1}{2}x^T K x + x^T b + \tfrac{1}{4})^r$$

$$K = \begin{pmatrix} 4.5 & 7 & 3.5 & 3 \\ 7 & 14 & 9 & 8 \\ 3.5 & 9 & 8.5 & 5 \\ 3 & 8 & 5 & 7 \end{pmatrix} \qquad b = \begin{vmatrix} -0.5 \\ -1.0 \\ -1.5 \\ 0 \end{vmatrix}$$

for $r = \frac{1}{2}$ and $r = 2$. The case $r = 2$ was also tested in Ref. 1. In both cases the starting point was (4, 4, 4, 4), f attaining its minimal value, $f = 0$, at (0.5, −0.5, 0.5, 0). Calculation was carried out in double precision (14 decimal places). With the present algorithm, f was minimized ($f = 10^{-14}$) in no more than five steps, the fifth step resulting from round-off errors. For $r = 2$ the conjugate gradient scheme of Fletcher and Reeves required 69 iterations to reach $f = 10^{-14}$. For $r = \frac{1}{2}$, 300 iterations were needed to reduce f to 10^{-14}. In both cases iteration was not restarted. Generally, restarting the iterations in the Fletcher and Reeves scheme may reduce the total number of steps required for convergence.

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Approximate Analytic Solution for the Position and Strength of Shock Waves about Cones in Supersonic Flow

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SIMPLE analytic equations are derived for the position and strength of the shock wave emitted by an axisymmetric cone in a steady supersonic flow. These equations are valid for higher Mach numbers and/or larger cone semiangles than the equations derived previously by Lighthill[1] and Whitham.[2] Even though the complete solution of the conical flow problem is well documented in various tables and computer programs, an analytic expression is useful for preliminary design estimates and for ascertaining the relative effects of the various parameters on the shock wave. In addition, these equations may have an important effect on shock wave calculations when applied to sonic boom problems. Recent experiments[3] have shown that theoretical sonic boom signatures emitted by bodies at higher Mach numbers and/or lower fineness ratios are generally longer than the corresponding experimentally determined signatures, that is, the shock wave stands out too far ahead of the freestream Mach cone emitted by the vertex of the body. The results of this Note tend to alleviate this lengthening effect by placing the shock wave closer to the undisturbed Mach cone from the vertex.

The equation derived in this Note is obtained by applying both the Whitham procedure for calculating a uniformly valid first-order solution, and the simplification afforded by the conical symmetry of the flow. In this derivation, only the details of the second order characteristics† are used in order to obtain a solution. Any further increase in accuracy or increases to higher Mach numbers (and/or larger cone semiangles) would necessarily have to include complicated third-order effects on the characteristics.

The Whitham theory is a powerful tool for the determination of the strength and location of weak shock waves in a supersonic flowfield. The theory is based on the premise that a uniformly valid first-order expression for the perturbation quantities can be obtained by fitting the first order perturbations to the second-order characteristics (or a suitable approximation to them). Consider, for example, the disturbance field created by a symmetric cone, of semiangle δ, placed in a steady, supersonic stream flowing with a velocity V. Let the speed of propagation of small disturbances in the free stream be denoted by a_∞, and define the Mach number M and the quantity β by V/a_∞ and $[(V/a_\infty)^2 - 1]^{1/2}$, respectively. A cylindrical coordinate system (x,r,θ) is introduced with its origin at the vertex of the cone, and the x axis along the cone's axis of symmetry. With respect to this

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† The second-order characteristic represents an expansion of the exact Mach angle up to terms linear in the perturbation velocities.