THE CONJUGATE GRADIENT METHOD IN EXTREMAL PROBLEMS*

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THE conjugate gradient method was first described in [1, 2] for solving sets of linear algebraic equations. The method, being iterative in form, has all the merits of iterative methods, and enables a set of linear equations to be solved (or what amounts to the same thing, the minimum of a quadratic functional in finite-dimensional space to be found) after a finite number of steps. The method was later extended to the case of Hilbert space [3-5], and to the case of non-quadratic functionals [6, 7].

The present paper proves the convergence of the method as applied to non-quadratic functionals, describes its extension to constrained problems, considers means for further accelerating the convergence, and describes experience in the practical application of the method for solving a variety of extremal problems.

1. Minimization of Quadratic Functionals

Consider the problem of minimizing the quadratic functional $f(x) = {}^1/_2(Ax, x) - (b, x)$ in Hilbert space H. Here, A is a bounded self-conjugate operator from H into H, and (x, y) is the scalar product. In the conjugate gradient method, an iterative sequence of vectors x^n, $p^n \in H$ is constructed, starting from some $x^0 \in H$, from the expressions

$$x^{n+1} = x^n + \alpha_n p^n, \tag{1}$$

$$p^n = -f'(x^n) + \beta_n p^{n-1}, \tag{2}$$

$$\alpha_n = -\frac{(f'(x^n), p^n)}{(Ap^n, p^n)}, \tag{3}$$

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$$\beta_n = \begin{cases} -\dfrac{(Ap^{n-1}, f'(x^n))}{(Ap^{n-1}, p^{n-1})}, & n \in I_1, \\ 0, & n \in I_2, \end{cases} \tag{4}$$

Here, $f'(x) = Ax - b$ is the gradient of $f(x)$, and I_1 and I_2 are sets of indices such that $I_1 \cup I_2 = \{0, 1, \ldots, n, \ldots\}$, $0 \in I_2$. The n for which $\beta_n = 0$ will be called the instants of renewal of the method. In the general form of the conjugate gradient method, $I_2 = \{0\}$, i.e. renewal is performed only at the first step. In the other extreme case, when $I_2 = \{0, 1, \ldots\}$, i.e., $\beta_n \equiv 0$, we get the method of steepest descent. If $I_2 = \{0, s, 2s, \ldots\}$, the method is identical with the s-step method of steepest descent.

The following propositions hold [1–5, 7].

1. The vectors p^n are A-orthogonal between two renewals, i.e. $(Ap^n, p^k) = 0$ for $n < k$, $\{n+1, n+2, \ldots, k\} \subset I_1$.

2. The vectors $f'(x^n)$ are orthogonal between two renewals, i.e. $(f'(x^n), f'(x^k)) = 0$ for $n < k$, $\{n+1, n+2, \ldots, k-1\} \subset I_1$.

It follows at once from these propositions that α_n and β_n can be evaluated from the following expressions, equivalent to (3) and (4):

$$\alpha_n = \frac{\|f'(x^n)\|^2}{(Ap^n, p^n)}, \tag{3'}$$

$$\beta_n = \begin{cases} \dfrac{\|f'(x^n)\|^2}{\|f'(x^{n-1})\|^2}, & n \in I_1, \\ 0, & n \in I_2. \end{cases} \tag{4'}$$

Many other computational schemes are available for the conjugate gradient method [1–5, 7, 8].

3. If $f(x)$ has a minimum on H, $I_2 = \{0\}$, then x^n is the minimum of $f(x)$ in the subspace passing through x^0 and generated by the vectors $f'(x^0), \ldots, f'(x^{n-1})$.

Hence the minimum of $f(x)$ will be found in N-dimensional space E^N after not more than N steps.

4. If $f(x)$ has a minimum in H, then, whatever I_1 and I_2, the vectors x^n will be convergent to the minimum point x^* (or to the one nearest x^0). Here, if $I_2 = \{0\}$,

$$f(x^n) = \min_{P_n} \int_m^M (1 - tP_n(t))^2 d\mu(t), \tag{5}$$

where m and M are the edges of the spectrum of A (i.e. $0 \leqslant m = \inf_{\|x\|=1}(Ax, x)$, $M = \sup_{\|x\|=1}(Ax, x)$), $P_n(t)$ is an n-th degree polynomial, $d\mu(t) = (dE_t x^0, x^0)$, where E_t is the spectral function of the operator A.

5. If $f(x)$ is strongly convex (i.e. $m > 0$), the rate of convergence for $I_2 = \{0\}$ is estimated from

$$\|x^n - x^*\| \leqslant \frac{(M-m)^n}{(\sqrt{M}+\sqrt{m})^{2n} + (\sqrt{M}-\sqrt{m})^{2n}} C(x^0) \leqslant \left(\frac{\sqrt{M}-\sqrt{m}}{\sqrt{M}+\sqrt{m}}\right)^n C(x^0). \tag{6}$$

Notice, incidentally, that the same estimate (6) is obtained for the two-step of steepest descent. For the ordinary method of steepest descent,

$$\|x^n - x^*\| \leqslant \left(\frac{M-m}{M+m}\right)^n C(x^0), \tag{7}$$

i.e., for $m \ll M$, it is much more slowly convergent than the conjugate gradient method or the two-step method of steepest descent.

Propositions 4 and 5 were first proved in [5], then independently, in [7].

Let us note some further properties of the conjugate gradient method, not all of which seem to have been previously described.

Property 1. If $f(x)$ does not attain a minimum in finite-dimensional space (which is only possible when the matrix A is not positive definite), it turns out that, at one of the steps of the conjugate gradient method, assuming that the process takes place non-degenerately, $(Ap^n, p^n) \leqslant 0$, $f'(x^n) \neq 0$ (i.e. $\alpha_n < 0$ or $\alpha_n = \infty$). The method thus gives a simple means for testing if a matrix is positive definite.

Property 2. If $f(x)$ is not strongly convex (i.e. $m = 0$), the convergence rate given by (5) may be vanishingly small. For example, let

$$f(x) = {}^1/_2 \int_{-1}^{1} t^2 x^2(t)\,dt, \qquad x(t) \in L_2(-1,1), \qquad x^0(t) \equiv 1.$$

Obviously, $x^*(t) \equiv 0$, $f(x^*) = 0$. Since $f'(x) = t^2 x(t)$, the subspace passing through x^0 and generated by $f'(x^0), \ldots, f'(x^{n-1})$, will be a set of even polynomials of degree $2n$, taking the value 1 at 0. These polynomials may be written in the form $\sum_{k=0}^{n} c_k P_{2k+1}(t)/t$, where $P_k(t)$ are Legendre polynomials of degree k, and the c_k have to satisfy

$$\sum_{k=0}^{n} c_k \frac{P_{2k+1}(t)}{t}\Big|_{t=0} = \sum_{k=0}^{n} c_k P'_{2k+1}(0) = 1.$$

Thus, x^n minimizes

$$f(x^n) = {}^1/_2 \int_{-1}^{1} t^2 \left(\frac{\sum_{k=0}^{n} c_k P_{2k+1}(t)}{t} \right)^2 dt = {}^1/_2 \sum_{k=0}^{n} c_k^2 \int_{-1}^{1} P^2_{2k+1}(t)\,dt = \sum_{k=0}^{n} \frac{c_k^2}{4k+3}$$

with the condition $\sum_{k=0}^{n} c_k P'_{2k+1}(0) = 1$. Noting that $P'_{2k+1}(0) = (-1)^k 2^{-2k}$ $(2k+1)C_{2k}^{\,k}$, we can find the c_k by the method of Lagrange multipliers, and and then find

$$f(x^n) = \left(\sum_{k=0}^{n} (2k+1)^2 (4k+3) 2^{-4k-1} (C_{2k}^{\,k})^2 \right)^{-1}.$$

Since $2^{-4k}(C_{2k}^{\,k})^2 \leqslant r_1 / k$, where r_1 is a constant (this follows from Stirling's formula), we have

$$f(x^n) \geqslant \left(\sum_{k=0}^{n} r_2 k^2 \right)^{-1} \geqslant r_3 n^{-3}.$$

Since

$$\|x\|^2 = \int_{-1}^{1} x^2(t)\,dt \geqslant \int_{-1}^{1} t^2 x^2(t)\,dt = 2f(x),$$

we have

$$\|x^n - x^*\| = \|x^n\| \geqslant (2f(x^n))^{1/2} \geqslant r_4 n^{-3/2}.$$

In short, the conjugate gradient method is more slowly convergent than a geometric progression in this example. All in all, given a $\lambda > 0$, an example can be found, in which the convergence is not faster than $n^{-\lambda}$. But notice that the method of steepest descent is always even more slowly convergent.

Property 3. If $f(x) = \|Cx - d\|^2$, where C is a linear operator from H into E^N, and $f(x)$ attains a minimum (which is true in any case if H is finite-dimensional), then the conjugate gradient method (with $I_2 = \{0\}$) converges after not more than N steps, independently of the number of dimensions of H.

Property 4. In the finite-dimensional case the conjugate gradient method may be used, not only to solve a set of linear equations, but also to invert a matrix. In fact, let p^i, $i = 0, \ldots, N-1$, be the vectors obtained by the conjugate gradient method with $I_2 = \{0\}$. We normalize them: $\bar{p}^i = (Ap^i, p^i)^{-1/2} p^i$, and form the matrix P, whose columns are the vectors p^{-i}. We then find, from the property $(Ap^i, p^k) = 0$, $i \neq k$, that $P^*AP = I$, where I is the unit matrix. If A is non-degenerate, and all the p^i non-zero, we have $A^{-1} = PP^*$. Knowing the vectors p^i, therefore, we can easily find A^{-1}. Of course the memory capacity required here is much greater.

Property 5. As already mentioned, the conjugate gradient method is finite in the N-dimensional case. Due to unavoidable computational errors, however, the x^N will not be the exact solution. In reality, therefore, the conjugate gradient method is iterative even in this case. Little attention has been paid to aspects such as the error dependence on the type of computational scheme or on the stipulation of the matrix, and on the best choice of instants of renewal, etc. Some possible means for increasing the accuracy can be indicated. First, the method only requires the multiplication of a matrix by a vector, and the evaluation of scalar products, and the relevant computations can easily be performed to double accuracy. Second, we can utilize the values obtained for the p^i and hence the approximate value PP^* of A^{-1} (see above), to form the new system $PP^*Ax = PP^*b$, which is better posed (this device is discussed in more detail in Section 3 below).

2. Minimization of Non-quadratic Functionals

It was observed in [6] that the conjugate gradient method in the form (1), (2), (3) and (48), can also be used for non-quadratic functionals. Given an N-dimensional function $f(x)$ with the gradient $f'(x)$, the following expressions are used in [6] for computing the coefficients α_n and β_n:

$$\alpha_n : f(x^n + \alpha_n p^n) = \min_{\alpha \geqslant 0} f(x^n + \alpha p^n), \tag{8}$$

$$\beta_n = \begin{cases} \dfrac{\|f'(x^n)\|^2}{\|f'(x^{n-1})\|^2}, & n \neq kN, \\ 0, & n = kN, \quad k = 0, 1, \ldots . \end{cases} \tag{9}$$

Though the results of computations from (1), (2), (8) and (9) are given for a variety of functions in [6], the convergence of the method is not discussed.

An analog of (4) for β_n is given in [7] for a twice differentiable functional $f(x)$ in H, namely,

$$\beta_n = \begin{cases} -\dfrac{(f''(x^n)p^{n-1}, f'(x^n))}{(f''(x^n)p^{n-1}, p^{n-1})}, & n \neq 0, \\ 0, & n = 0, \end{cases} \tag{10}$$

and the convergence of the method (1), (2), (8) and (10) at the rate of a geometric progression is proved under the assumptions of strong convexity and reasonable smoothness of $f(x)$. The method (10) is inconvenient in the sense that the second derivative $f''(x)$ has to be evaluated. The main advantage of the conjugate gradient method over, say, Newton's method is thereby lost (a discussion of the advantages and disadvantages of different minimization methods from the computational point of view may be found in [9]).

We give below an alternative method for finding β_n, which does not involve the evaluation of $f''(x)$ and for which convergence at the rate of a geometric progression can also be proved. In addition, it turns out that, given a reasonably smooth finite-dimensional function, the method is convergent at a squared rate, i.e. much faster than the various versions of the gradient method.

Take the problem of minimizing a differentiable functional $f(x)$ in Hilbert space H. We use the method (1), (2), (8) and (11):

$$\beta_n = \begin{cases} \dfrac{(f'(x^n), f'(x^n) - f'(x^{n-1}))}{\|f'(x^{n-1})\|^2}, & n \in I_1, \\ 0, & n \in I_2. \end{cases} \quad (11)$$

This method is obviously the same as (1)–(4) in the case of a quadratic functional.

Before proving the convergence of the method, we present some obvious relationships.

Lemma 1

We have $(f'(x^n),\ p^{n-1}) = 0$, $(f'(x^n),\ p^n) = -\|f'(x^n)\|^2$, $\|p^n\|^2 = \|f'(x^n)\|^2 + \beta_n^2\|p^{n-1}\|^2 \geqslant \|f'(x^n)\|^2$.

The first of these follows from (8); and then, recalling (2), we obtain the remaining expressions.

We shall first show that, for "poor" functions (not necessarily convex or smooth), the method behaves like the gradient method, i.e. $f'(x^n) \to 0$ in it whatever the initial approximation.

Theorem 1

If $f(x)$ has a lower bound, the set $\{x: f(x) \leqslant f(x^0)\}$ is bounded, $f'(x)$ satisfies a Lipschitz condition, and renewal is carried out after a finite number of steps, then, in method (1), (2), (8) and (11),

$$\varliminf_{n\to 0} \|f'(x^n)\| = 0.$$

Proof. Let $\|f'(x^n)\| \geqslant \varepsilon > 0$ for all n. We first show that $\|p^n\| \leqslant c_n\|f'(x^n)\|$ for all n. In fact, for $n \in I_1$;

$$\beta_n = \frac{(f'(x^n), f'(x^n) - f'(x^{n-1}))}{\|f'(x^{n-1})\|^2} \leqslant \frac{\|f'(x^n)\|\, R\, \|x^n - x^{n-1}\|}{\|f'(x^{n-1})\|^2} \leqslant \frac{Rc\,\|f'(x^n)\|}{\varepsilon\,\|f'(x^{n-1})\|} \leqslant \frac{Rcc_{n-1}}{\varepsilon}\frac{\|f'(x^n)\|}{\|p^{n-1}\|},$$

where $\|x^n - x^{n-1}\| \leqslant c$, since $f(x^n) \leqslant f(x^{n-1}) \leqslant f(x^0)$, while the set $\{x: f(x) \leqslant f(x^0)\}$ is bounded. Hence

$$\|p^n\|^2 = \|f'(x^n)\|^2 + \beta_n^2 \|p^{n-1}\|^2 \leqslant \|f'(x^n)\|^2 + \frac{R^2c^2c_{n-1}^2}{\varepsilon^2}\|f'(x^n)\|^2 = c_n^2\|f'(x^n)\|^2,$$

where $c_n^2 = 1 + R^2c^2c_{n-1}^2 / \varepsilon^2$. Further,

$$\|f'(x^n)\|^2 = -(p^n, f'(x^n)) = -(p^n, f'(x^n) - f'(x^{n+1})) \leqslant \|p^n\|R\|x^n - x^{n+1}\| = R\alpha_n\|p^n\|^2,$$

whence

$$\alpha_n \geqslant \frac{1}{R}\frac{\|f'(x^n)\|^2}{\|p^n\|^2} \geqslant \frac{1}{Rc_n^2} = \delta_n.$$

Since $c_n = 1$ for all instants of renewal ($\|p^n\| = \|f'(x^n)\|$ for $n \in I_2$), while renewal is carried out after a finitė number of steps, then c_n is bounded, so that $\alpha_n \geqslant \delta_n \geqslant \delta > 0$ for all n. Finally,

$$f(x^{n+1}) \leqslant f(x^n + \delta p^n) = f(x^n) + \int_0^1 (f'(x^n + t\delta p^n), \delta p^n)\,dt =$$

$$f(x^n) + \delta(f'(x^n), p^n) + \delta\int_0^1 (f'(x^n + t\delta p^n) -$$

$$f'(x^n), p^n)\,dt \leqslant f(x^n) - \delta\,\|f'(x^n)\|^2 + \delta^2 R\,\|p^n\|^2 \int_0^1 t\,dt \leqslant$$

$$f(x^n) - \delta\,\|f'(x^n)\|^2 + {}^1/_2\,\delta\,\|f'(x^n)\|^2 \leqslant f(x^n) - \frac{\delta\varepsilon^2}{2}.$$

Hence it follows that $f(x^n) \to -\infty$, which contradicts our assumption that $f(x)$ has a lower bound. The theorem is proved.

We shall now show that, in the case of a strongly convex functional, the sequence x^n is convergent to the minimum point x^* at the rate of a geometric progression.

Theorem 2

If $f(x)$ is a strongly convex functional, and $f'(x)$ satisfies a Lipschitz condition, then, whatever the method of selecting the instants of renewal, x^n is convergent in method (1), (2), (8) and (11) to x^* at the rate of a geometric progression.

Proof. Since $f(x)$ is strongly convex, $(f'(x^{n+1}) - f'(x^n), x^{n+1} - x^n) \geqslant m\|x^{n+1} - x^n\|^2$, $m > 0$, whence

$$-\alpha_n(f'(x^n), p^n) \geqslant m\alpha_n^2\|p^n\|^2,$$

$$\alpha_n \leqslant -\frac{1}{m}\frac{(f'(x^n), p^n)}{\|p^n\|^2} = \frac{1}{m}\frac{\|f'(x^n)\|^2}{\|p^n\|^2} \leqslant \frac{1}{m}.$$

Hence, when $n \in I_1$,

$$\beta_n = \frac{(f'(x^n), f'(x^n) - f'(x^{n-1}))}{\|f'(x^{n-1})\|^2} \leqslant \frac{\|f'(x^n)\| R\alpha_{n-1}\|p^{n-1}\|}{\alpha_{n-1} m \|p^{n-1}\|^2} = \frac{R}{m}\frac{\|f'(x^n)\|}{\|p^{n-1}\|}$$

Then,

$$\|p^n\|^2 = \|f'(x^n)\|^2 + \beta_n^2\|p^{n-1}\|^2 \leqslant \|f'(x^n)\|^2 + \frac{R^2}{m^2}\|f'(x^n)\|^2 = \left(1 + \frac{R^2}{m^2}\right)\|f'(x^n)\|^2.$$

Further, as in the proof of Theorem 1,

$$\alpha_n \geqslant \frac{1}{R}\frac{\|f'(x^n)\|^2}{\|p^n\|^2} \geqslant \frac{1}{R(1 + R^2/m^2)} = \delta.$$

Finally, $f(x^{n+1}) \leqslant f(x^n + \delta p^n) \leqslant f(x^n) - (\delta/2)\|f'(x^n)\|^2$. But, in the case of a strongly convex functional, $\|f'(x)\|^2 \geqslant 2m(f(x) - f^*)$, where $f^* = f(x^*) = \min f(x)$. Hence $f(x^{n+1}) - f^* \leqslant f(x^n) - f^* - (\delta/2)\|f'(x^n)\|^2 \leqslant (f(x^n) - f^*)(1 - \delta m)$. This implies the convergence $f(x^n) \to f^*$ at the rate of a geometric progression, while, since $f(x) - f^* \geqslant m\|x - x^*\|^2$, we have $x^n \to x^*$ at the rate of a geometric progression.

With additional assumptions regarding the smoothness of $f(x)$, a more accurate bound might be obtained for the ratio of the progression; but we shall not dwell on this, since Theorem 3 to be proved below, shows that the method is convergent at a squared rate in the case of a finite-dimensional smooth functional.

Theorem 3

Let $x \in E^N$, while $f(x)$ is a twice differentiable strongly convex function, whose second derivative is bounded and satisfies a Lipschitz condition. Then,

$$\|x^{kN} - x^*\| \leqslant cq^{2^k}, \qquad q < 1.$$

in the method (1), (2), (8) and (11) with $I_2 = \{0, N, 2N, \ldots\}$.

Proof. Consider the quadratic functional $\tilde{f}(x) = {}^1/_2(f''(x^*)(x - x^*), x - x^*)$. This has a minimum at the point x^* which is also a minimum point of $f(x)$. Consider the conjugate gradient method, starting from the point $\tilde{x}^0 = x^0$ and applied to the functional $\tilde{f}(x)$:

$$\tilde{x}^{n+1} = \tilde{x}^n + \tilde{\alpha}_n \tilde{p}^n, \qquad \tilde{p}^n = -\tilde{f}'(\tilde{x}^n) + \tilde{\beta}_n \tilde{p}^{n-1},$$

$$\tilde{\alpha}_n = -\frac{(\tilde{f}'(\tilde{x}^n), \tilde{p}^n)}{(f''(x^*)\tilde{p}^n, \tilde{p}^n)}, \qquad \tilde{\beta}_n = \frac{\|\tilde{f}'(\tilde{x}^n)\|^2}{\|\tilde{f}'(\tilde{x}^{n-1})\|^2}, \qquad n \neq 0, \qquad \beta_0 = 0.$$

The basic idea of the proof consists in showing that the points $\tilde{x}^n$ and x^n are close together. We use induction. Let $\|x^n - \tilde{x}^n\| \leqslant c_n\|x^0 - x^*\|^2$, $\|p^{n-1} - \tilde{p}^{n-1}\| \leqslant k_n\|x^0 - x^*\|^2$ (this is certainly true for $n = 0$). It is easy to obtain bounds for the type $\|\tilde{f}''(x) - f''(x)\| \leqslant L\|x - x^*\|$, $\|\tilde{f}'(x) - f'(x)\| \leqslant L\|x - x^*\|^2$, $\|x^n - x^*\| \leqslant (M/m)^{1/2}\| \times \|x^0 - x^*\|$, $m\|p\|^2 \leqslant (f''(x)p, p) \leqslant M\|p\|^2$, $m\|p\|^2 \leqslant (f''(x^*)p, p) \leqslant M\|p\|^2$, $m\|x - x^*\|^2 \leqslant \|f'(x)\|^2 \leqslant M\|x - x^*\|^2$, $m\|x - x^*\|^2 \leqslant \|\tilde{f}'(x)\|^2 \leqslant M\|x - x^*\|^2$, $f'(x) = f''(\xi)(x - x^*)$, $\xi = x + \theta(x - x^*)$, $0 \leqslant \theta \leqslant 1$. Using these, we find after fairly laborious calculations that must be omitted here, that $|\beta_n - \tilde{\beta}_n| \leqslant b_n\|x^0 - x^*\|$, $\|p^n - \tilde{p}^n\| \leqslant k_{n+1}\|x^0 - x^*\|^2$, $|\alpha_n - \tilde{\alpha}_n| \leqslant a_n\|x^0 - x^*\|$ $\|x^n - \tilde{x}^n\| \leqslant c_{n+1}\|x^0 - x^*\|^2$, $b_n, k_{n+1}, a_n, c_{n+1}$ are bounded. Thus, $\|x^n - \tilde{x}^n\| \leqslant c\|x^0 - x^*\|^2$ for all $n \leqslant N$. But $\tilde{x}^N = x^*$ (since the conjugate gradient method is finite for the quadratic functional $f(x)$). Hence $\|x^N - x^*\| \leqslant c\|x^0 - x^*\|^2$. Similarly, we get $\|x^{kN} - x^*\| \leqslant c\|x^{(k-1)N} - x^*\|^2$ for all integral k. Since the convergence of the method was proved in Theorem 2, we have $\|x^{mN} - x^*\| \leqslant p/c$, $p < 1$, for some m. Hence

$$\|x^{(m+k)N} - x^*\| \leqslant \frac{1}{c} p^{2^k} = c' q^{2^{k+m}}, \qquad q^{2^m} = p, \quad c' = \frac{1}{c}.$$

Notice that, under the conditions of the theorem, we can also apply Newton's method locally and obtain for it the bound $\|x^n - x^*\| \leqslant r^{2^n}\|x^0 - x^*\|$, $r < 1$. Thus, N steps of the conjugate gradient method are roughly equivalent to one step of Newton's method (as might naturally be expected). On the other hand, no additional assumptions regarding the closeness of x^0 to the solution are required for the convergence of the conjugate gradient method, as distinct from Newton's method.

In the case of a quadratic functional, Theorem 3 asserts in essence that the method is stable in the presence of errors when computing x^n, $f'(x^n)$, p^n, α_n, and β_n (for x^n, $f'(x^n)$ and p^n the errors may be of the order $\|x^n - x^*\|^2$, and for α_n and β_n of the order $\|x^n - x^*\|$).

3. Further Acceleration of the Convergence

If the memory capacity allows the vectors p^n to be stored, they can be utilized for further accelerating the convergence; in fact, they can be taken as a new basis in the space, in which case the properties of the functional will be considerably improved.

We shall describe the computational procedure in more detail. In N-dimensional space, we perform N iterations in accordance with (1), (2), (8) and (11), without renewal (i.e. $I_2 = \{0\}$). We inspect the $N \times N$ matrix P_1 whose columns are the vectors $\bar{p}^n = (\sqrt{\alpha_n} / \|f'(x^n)\| p^n$. We perform the coordinate transformation $x = P_1 y$, and consider our functional $f(x)$ in the new variables: $\varphi(y) = f(P_1 y) = f(x)$. We use the conjugate gradient method to minimize $\phi(y)$. Since $\varphi'(y) = P_1^* f'(x)$, the method will run thus:

$$y^{n+1} = y^n + \alpha_n s^n, \qquad x^n = P_1 y^n, \qquad s^n = -P_1^* f'(x^n) + \beta_n s^{n-1},$$

$$\alpha_n : \varphi(y^n + \alpha_n s^n) = \min_{\alpha \geqslant 0} \varphi(y^n + \alpha s^n),$$

$$\beta_n = \frac{(P_1 P_1^* f'(x^n), f'(x^n) - f'(x^{n-1}))}{(P_1 P_1^* f'(x^{n-1}), f'(x^{n-1}))}.$$

We write the same method in the initial coordinates, which can be done simply by multiplying the equations for y^{n+1} and s^n by P_1 and writing $p^n = P_1 s^n$:

$$x^{n+1} = x^n + \alpha_n p^n, \qquad n = N, N+1, \ldots, 2N-1,$$

$$p^n = -P_1 P_1^* f'(x^n) + \beta_n p^{n-1},$$

$$\alpha_n : f(x^n + \alpha_n p^n) = \min_{\alpha \geqslant 0} f(x^n + \alpha p^n),$$

$$\beta_n = \frac{(P_1 P_1^* f'(x^n), f'(x^n) - f'(x^{n-1}))}{(P_1 P_1^* f'(x^{n-1}), f'(x^{n-1}))}, \qquad n \neq N, \quad \beta_N = 0.$$

If, after every N iterations, the same process is repeated, we finally obtain the following computational scheme:

$$x^{n+1} = x^n + \alpha_n p^n, \tag{12}$$

$$p^n = -S_k f'(x^n) + \beta_n p^{n-1}, \qquad n = kN + i, \quad 0 \leqslant i \leqslant N-1,$$

$$\alpha_n : f(x^n + \alpha_n p^n) = \min_{\alpha \geqslant 0} f(x^n + \alpha p^n),$$

$$\beta_n = \begin{cases} \dfrac{(S_k f'(x^n), f'(x^n) - f'(x^{n-1}))}{(S_k f'(x^{n-1}), f'(x^{n-1}))}, & n \neq kN, \\ 0, & n = kN, \end{cases}$$

$$S_k = P_k P_k^*, \qquad S_0 = I.$$

Here, P_k is an $N \times N$ matrix, the i-th column of which is $\bar{p}^i = \sqrt{\alpha_n} p^n / (S_k f'(x^n), f'(x^n))^{1/2}$, $n = kN + i$, and I is the unit matrix.

Notice some features of the proposed method. First, if $f(x) = {}^1/_2(Ax, x) - (b, x)$, we obtain in the non-degenerate case (i.e. when $p^n \neq 0$, $n = 0, \ldots, N-1$) $S_1 = P_1 P_1^* = A^{-1} = [f''(x)]^{-1}$ (see the Note in Section 1). In the case of a non-quadratic functional, the matrix S_1 will thus be close to $[f''(x^0)]^{-1}$. Further, while we apply the conjugate gradient method to the function $\phi(y)$, it may easily be verified that $\varphi''(y) = P_1^* f''(x) P_1$. Since P_1^{-1} exists by hypothesis, the matrix $\phi''(y)$ must have the same eigenvalues as $P_1 P_1^* f''(x) = S_1 f''(x)$. But the latter matrix is close to the unit matrix when x is close to x^0. In short, the second cycle of the conjugate gradient method is performed for a functional whose matrix of second derivatives is well-posed. As may be seen from the convergence proofs given in Section 2, the rate of convergence is greater, the closer the numbers m and M (i.e. the better the second derivatives are stipulated). Similarly, in later cycles the matrix S_k becomes a better and better approximation for $[f''(x)]^{-1}$, so that further acceleration of the convergence can be expected.

The method just described has features similar to that given in [10], in which the matrix $[f''(x)]^{-1}$ is likewise obtained by an iterative method. But the computational scheme in [10] is more unwieldy, and what is more important, the convergence is slower, since the method of steepest descent is employed in its coordinate transformations, while in our algorithm the conjugate gradient method is used in the new coordinates.

4. Constrained Problems

Notice first that the conjugate gradient method can be extended immediately to the case of minimizing $f(x)$ on a linear subspace L, provided we replace $f'(x)$ throughout the expressions by the projection $P_L f'(x)$ of the gradient on L. All the convergence theorems remain in force (in particular, if $f(x)$ is quadratic and finite-dimensional, the method is finite).

Now take the problem of minimizing a quadratic finite-dimensional function $f(x)$ under the constraint $x \in Q$, where $Q = \{x: \ a_i \leqslant x_i \leqslant b_i, \ i = 1, \dots, N\}$ (some a_i and b_i may be equal to $\pm\infty$). We shall show that the conjugate gradient method can also be extended to this case, in such a way that it remains finite. We introduce two sets of indices I_n^- and I_n^+, write $I_n = I_n^- \cup I_n^+$ and consider the method

$$x^{n+1} = x^n + \alpha_n p^n, \tag{13}$$

$$p_i^n = \begin{cases} -\dfrac{\partial f(x^n)}{\partial x_i} + \beta_n p_i^{n-1}, & i \notin I_n, \\ 0, & i \in I_n, \end{cases}$$

$$\alpha_n : f(x^n + \alpha_n p^n) = \min_{0 \leqslant \alpha \leqslant \bar{\alpha}_n} f(x^n + \alpha p^n),$$

$$\bar{\alpha}_n = \max\{\alpha: a_i \leqslant x_i^n + \alpha p_i^n \leqslant b_i, \quad i = 1, \dots, N\},$$

$$\beta_n = \begin{cases} \dfrac{\sum_{i \notin I_n} (\partial f(x^n)/\partial x_i)^2}{\sum_{i \notin I_n} (\partial f(x^{n-1})/\partial x_i)^2}, & n \neq 0, \quad I_n = I_{n-1}, \\ 0, & n = 0 \quad I_n \neq I_{n-1}, \end{cases}$$

$$I_n^- = \begin{cases} \{i : x_i^n = a_i, \ \partial f(x^n)/\partial x_i > 0\}, \ n = 0 & \partial f(x^n)/\partial x_i = 0 \\ i \notin I_n, & \\ I_{n-1}^- \cup \{i : x_i^n = a_i\} & \end{cases}$$

$$I_n^+ = \begin{cases} \{i : x_i^n = b_i, \ \partial f(x^n)/\partial x_i < 0\}, \ n = 0 & \partial f(x^n)/\partial x_i = 0 \\ i \notin I_n, & \\ I_{n-1}^+ \cup \{i : x_i^n = b_i\} & \end{cases}$$

Theorem 4

If $f(x)$ is convex and attains its minimum on Q, method (13) is finite: $x^n = x^*$

for some n.

Proof. We shall show that an instant arrives when $\partial f(x^n) / \partial x_i = 0$ for all $i \notin I_n$. In fact, till this happens, the set I_n is merely widened: $I_n \supset I_{n-1}$. But this widening cannot go on indefinitely, so that, as from a certain instant, $I_n = I_{n-1}$. It then follows from the expressions of the method that we shall be applying the conjugate gradient method in a subspace $x_i = a_i$, $i \in I_n^-$, $x_i = b_i$, $i \in I_n^+$. But this method is finite, so that the minimum in this subspace will be found after a finite number of steps. It will then turn out that $\partial f(x^n) / \partial x_i = 0$ for all $i \notin I_n$. Every time, therefore, we arrive after a finite number of steps at the minimum point in some subspace. Further, we transform to a new subspace (the upper line in the definitions of I_n^-, I_n^+). Since the method is monotonic $f(x^{n+1}) \leqslant f(x^n)$, we shall never arrive twice in the same subspace. Since the total number of subspaces is finite, the method must also be finite. It is clear from the expressions for the method that the necessary and sufficient conditions for a minimum of $f(x)$ in Q must be satisfied at a point of the last subspace

This theorem suggests a simple means for solving a set of linear inequalities in finite-dimensional space. For, let the set of inequalities be $Ax = b$, $x \geqslant 0$, so that we have to minimize the quadratic functional $f(x) = \|Ax - b\|^2$ in $Q = \{x \colon x \geqslant 0\}$. We use the method (13). It follows from Theorem 4 that this method, while iterative in form (and possessing all the merits of iterative methods), enables the solution to be found after a finite number of steps.

Since a problem of linear programming may be reduced by various means to the solution of linear inequalities, we have incidentally obtained a method for solving problems of linear programming.

Further, the general problem of quadratic programming min $(Cx, x) - (d, x)$, $Ax \leqslant b$ may be reduced by the duality theorem to minimizing the quadratic function $\varphi(y) = (Gy, y) - (h, y)$, $G = {}^1/_4 AC^{-1}A$, $h = {}^1/_2 AC^{-1}d + b$, under simple constraints $y \geqslant 0$. Our method may be employed for this latter problem (and is much more economic than the Hildreth and d'Esope method for solving the dual problem, see [11], Chapter V).

Finally, the method (13) may also be used for minimizing a non-quadratic function $f(x)$ under constraints $a_i \leqslant x_i \leqslant b_i$, $i = 1, \ldots, N$. Here, β_n have to be evaluated from (11), while the condition $\partial f(x^n) / \partial x_i = 0$, $i \notin I_n$, must be replaced by some condition under which these derivatives are small.

Another way of utilizing the conjugate gradient method in problems of nonlinear programming is given in [12]. In this method, an auxiliary problem of linear programming is solved at each step.

Finally, the conjugate gradient method may be used in conjunction with any algorithm for solving general extremal problems under constraints, in which the problem is reduced to a sequence of unconstrained extremum problems. For instance, there is the method of penalty functions, or the method of selecting Lagrange multipliers with subsequent minimization of the Lagrange function. It only needs to be borne in mind that the conjugate gradient method is only effective for reasonably smooth functions, so that the penalty functions must be reasonably smooth. In particular, the penalty function $Kg_+^2(x)$, $g_+(x) = \max\{0, g(x)\}$, employed for replacing the constraint $g(x) \leq 0$, is of little use, since it is not twice differentiable.

5. Numerical Results

The conjugate gradient method was employed systematically in its standard and modified forms at the Computational Centre of Moscow University to solve a variety of extremal problems. Some results will be briefly described.

1. Unconstrained minimization problems for functions of many variables. In all the examples considered, the conjugate gradient method was much more rapidly convergent than gradient methods (which often stopped in practice a long way from the minimum). In most cases the modified version (11) gave rather better results than (9). To indicate the effectiveness of the method, we shall quote a typical example with 50 variables:

$$f(x) = \sum_{i=1}^{51} \left(\frac{0.0016 + (x_i - x_{i-1})^2}{0.04i}\right)^{1/2}, \qquad x_0 = 0, \qquad x_{51} = 1.19254566.$$

This is the discrete version of the familiar brachistochrone problem. For the initial approximation, $f(x^0) - f(x^*) = 0.21$, $\|x^0 - x^*\| = 4.0$. After 370 iterations the conjugate gradient method gave an approximation in which all 9 places were correct for $f(x)$ and 8 places for x_i. Here, 1508 gradient computations were required. The results with the same number of iterations in the method of steepest descent are, for comparison: $f(x^n) - f(x^*) = 0.13$, $\|x^n - x^*\| = 3.5$ and for the simple gradient method: $f(x^n) - f(x^*) = 0.09$, $\|x^n - x^*\| = 3.0$.

In the majority of problems, the conjugate gradient method is quite rapidly convergent and acceleration of the convergence rate is unnecessary. An example of a function of quite a small number of variables, where the method (12) was required, is

$$f(x) = A^{-2} \sum_{j=1}^{10} (Ae^{-0.2j} + 2Ae^{-0.4j} - x_1 e^{-0.2jx_2} - x_3 e^{-0.2jx_4})^2.$$

When $A = 1$, 640 iterations were needed, in order to obtain

$$f(x^n) - f(x^*) = 0.5 \cdot 10^{-13}, \qquad \|x^n - x^*\| = 0.2 \cdot 10^{-4}$$

(when $f(x^0) - f(x^*) = 0.5$, $\|x^0 - x^*\| = 1.7$). At the same time, after only 50 iterations of method (12), we had $f(x^n) - f(x^*) < 10^{-19}$, $\|x^n - x^*\| = 10^{-8}$. When $A = 1000$, the conjugate gradient method is not practicable. The fact is that the orders of the derivatives with respect to the different variables are sharply different in this problem. In view of this, the size of a_n varies widely from step to step and its selection from condition (8) becomes a difficult problem. In the method (12), a_n can be shown to be always of the order of unity (for reasonably smooth functions). Hence method (12) is applicable even when $A = 1000$, and after 240 iterations, gives $f(x^n) - f(x^*) < 10^{-19}$, $\|x^n - x^*\| = 0.5 \cdot 10^{-5}$. It must be mentioned that, when $N > 10$, it is often more slowly convergent than the conjugate gradient method.

Two standard programs for the M-20 computer were devised by V. V. Skokov. The first realized the method (1), (2), (8) and (11), when $N \leqslant 620$; the second realized method (12), when $N \leqslant 50$. To use these programs, it is only necessary to specify a subprogram for computing $f'(x)$.

2. Problems of linear and quadratic programming. The problem

$$\min (c, x) + (Ax, x), \quad Bx = d, \quad x \geqslant 0,$$

reduces by means of penalty functions to

$$\min (c, x) + (Ax, x) + K\|Bx - d\|^2, \quad x \geqslant 0,$$

after which the method described in Section 4 can be employed [13]. Since this method requires no transformations of the initial matrices, and the latter are sparsely filled, it can be applied to problems with a large number of dimensions. The standard program for the BESM-4 computer devised by E. N. Belov enables problems of linear programming to be solved with $m + 2n \leqslant 1504$, $P \leqslant 4000$ (m is the number of equations, n the number of variables, and P the number of non-zero elements in the matrix). From 2 to 4 hours per problem were required when solving a variety of problems with $m = 314$, $n = 505$, $P = 1000$

3. Optimal control problems. In the problem

$$\min f(u) = \int_0^T F(x, u, t)\,dt + \Phi(x(T)),$$

$$\frac{dx}{dt} = \varphi(x, u, t), \qquad x(0) = c, \qquad a(t) \leqslant u(t) \leqslant b(t)$$

the gradient can be written down without difficulty and the conjugate gradient method applied. A detailed description of the algorithm and computational results for several examples may be found in [14]. If the phase coordinates are constrained in the problem (in particular, if there is a condition on $x(T)$), the method of penalty functions can be used. If time T is not fixed, we can perform the transformation $t \to \tau$ in accordance with $dt = v(\tau)d\tau$, $v(\tau) \geqslant 0$, $0 \leqslant \tau \leqslant 1$ and take $v(\tau)$ as the new control.

4. Integral equations of the 1st kind. Solution of the equation

$$\int_0^1 K(s, t)\,x(s)\,ds = a(t)$$

is replaced by minimization of the quadratic functional

$$f(x) = \int_0^1 \left(\int_0^1 K(s, t)\,x(s)\,ds - a(t) \right)^2 dt.$$

The resulting problem is incorrectly posed: not every minimizing sequence is convergent. A detailed numerical check on the conjugate gradient method for such problems was given in [15]. It was found that, in spite of rounding errors, the method is stable and yields a convergent sequence. The choice of the metric of the space in which the minimization is performed has an important influence. For instance, if a fairly smooth solution exists, the method is much more rapidly convergent in space W_2^1 than in L_2.

5. Partial differential variational problems. Many problems of mathematical physics may be stated in terms of variational principles. We can usually write down the gradient of the resulting functional, and then employ the conjugate

gradient method. Computational experience in one such problem is described in [16], namely, choice of the boundary condition for the equation of heat conduction, such that the least deviation from a given temperature state is obtained.

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