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AN EFFECTIVE ALGORITHM FOR MINIMIZATION

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Abstract

An algorithm is proposed for minimizing certain nice C^2 functions f on E_n assuming only a computational knowledge of f and ∇f. It is shown that the algorithm provides global convergence at a rate which is eventually superlinear and possibly quadratic. The algorithm is purely algebraic and does not require the minimization of any functions of one variable.

Numerical computation on specific problems with as many as six independent variables has shown that the method compares very favorably with the best of the other known methods. The method is compared with the Fletcher and Powell method for a simple two dimensional test problem and for a six dimensional problem arising in control theory.

This note proposes an algorithm for minimizing certain nice C^2 functions f on E_n assuming only a computational knowledge of f and ∇f. It is shown that the algorithm provides global convergence at a rate which is eventually superlinear and possibly quadratic. The algorithm is purely algebraic and does not require the minimization of any functions of one variable.

In the following, let δ and r be positive numbers with $\delta < \frac{1}{2}$. Let f be a real-valued function defined on E_n, x^o be an arbitrary point of E_n, and I_i be the i^{th} column of the $n \times n$ identity matrix, I. Let S denote the level set of f at x^o, viz.: $S = \{x \in E_n: f(x) \leq f(x^o)\}$. Assume that for some open convex set $\hat{S}$ containing S, $f \in C^2(\hat{S})$. Let $H(x)$ denote the Hessian of f at x. Assume that for all $u \in E_n$ and for all $x \in S$, there exists a constant $\omega > 0$ such that $[u,H(x)u] \geq \omega||u||^2$.

An algorithm for minimizing $f(x)$ consists of performing the following computations for $k = 0,1,2,...$:

1. Compute the $n \times n$ matrix $Q(x^k)$ whose j^{th} column is

$$\frac{\nabla f(x^k+\theta_k I_j)-\nabla f(x^k)}{\theta_k}$$

where $\theta_0 = r$ and

$$\theta_k = r||\phi(x^{k-1})|| \text{ for } k = 1,2,3,...,$$

in which ϕ is defined as follows:

(a) If $k = 0$, or if $Q(x^k)$ is singular, or if

$$[\nabla f(x^k), Q^{-1}(x^k)\nabla f(x^k)] \leq 0,$$

set $\phi(x^k) = \nabla f(x^k)$.

(b) Otherwise, set $\phi(x^k) = Q^{-1}(x^k)\nabla f(x^k)$.

2. Consider the function

$$\gamma \to g(x^k,\gamma) = \frac{f(x^k)-f(x^k-\gamma\phi(x^k))}{\gamma[\nabla f(x^k),\phi(x^k)]},$$

If $g(x^k,1) < \delta$, choose γ_k so that $\delta \leq g(x^k,\gamma_k) \leq 1-\delta$; otherwise set $\gamma_k = 1$.

3. Set $x^{k+1} = x^k - \gamma_k\phi(x^k)$.

<u>Theorem</u>: *Under the assumptions stated above,*

1) the sequence $\{x^k\}$ converges to a point z minimizing f,

2) there exists a number N such that if $k > N$ then $\gamma_k = 1$, and

3) the rate of convergence of $\{x^k\}$ is superlinear.

Before proving this theorem we shall first establish 2 lemmas.

<u>Lemma 1</u>. If the sequence $\{\theta_k\}$ of the above theorem converges to 0, then $\{\|Q(x^k)-H(x^k)\|\} \to 0$ and for some K, there exists a positive number ω' such that for all $k \geq K$ and any $h \in E_n$, $[h,Q(x^k)h] \geq \omega'\|h\|^2$.

<u>Proof</u>. The existence of $H(x)$ implies that given $\varepsilon > 0$ there exists $\delta > 0$ such that for all $h \in E_n$, $\|h\| < \delta$, we have the validity of the inequality $\|\nabla f(x+h)-\nabla f(x)-H(x)h\| < \varepsilon\|h\|$. For large k we have that $\|\theta_k I_j\| < \delta$, $1 \leq j \leq n$, and therefore

$\left\| \frac{\nabla f(x^k+\theta_k I_j)-\nabla f(x^k)}{\theta_k} - H_j(x^k) \right\| < \varepsilon$, $(1 \le j \le n)$, where $H_j(x^k)$ denotes the j^{th} column of $H(x^k)$. Thus $\{\| Q(x^k)-H(x^k) \|\} \to 0$.

To complete the proof observe that because $\frac{[h,H(x^k)h]}{\|h\|^2}$ is bounded below and $Q(x^k)$ is eventually close to $H(x^k)$, it follows that $\frac{[h,Q(x^k)h]}{\|h\|^2}$ is also eventually bounded below.

Lemma 2. Assume A and B are square matrices satisfying $\| (A-B)A^{-1} \| < 1$. Then B^{-1} exists and

$$\| A^{-1}-B^{-1} \| \le \|A-B\| \cdot \|A^{-1}\|^2 \cdot (1-\| A-B \| \, \|A^{-1}\|)^{-1}.$$

Proof. Set $C = B-A$, and compute that

$$\| A^{-1}-B^{-1} \| = \| A^{-1}-(A+C)^{-1} \| = \| A^{-1}(I-[(A+C)A^{-1}]^{-1}) \|$$

$$= \| A^{-1}(I-[I+CA^{-1}]^{-1}) \| .$$

By hypotheses $\|CA^{-1}\| < 1$, whence:

$$[I+CA^{-1}]^{-1} = I - CA^{-1} + (CA^{-1})^2 - \dots = AB^{-1}.$$

Thus $\|A^{-1}-B^{-1}\| \le \| A^{-1} \| \, \|(CA^{-1}(I-CA^{-1}+\dots))\|$

$$\le \|C\| \, \|A^{-1}\|^2(1-\|CA^{-1}\|)^{-1}.$$

We now turn to the proof of the theorem.

Proof of Theorem.

We show first that the set S is bounded. If not, there is an unbounded sequence say $\{z^k\}$ in S. Take $u \varepsilon S$. Then by Taylor's theorem and the fact that $H(x)$ is bounded below by ω on S we get $f(z^k) \geq f(u) + \|z^k-u\|[(\|z^k-u\|)\frac{\omega}{2} - \|\nabla f(u)\|]$, showing that $f(z^k) \geq f(x^\circ)$ for large k; thus S must be bounded.

Clearly, by definition of $\phi(x^k)$, $\nabla f(x^k) \neq 0$ implies $[\nabla f(x^k),\phi(x^k)] > 0$. Arguing as in [1] p. 148, after we observe that ϕ is bounded on S, we conclude that $\{[\nabla f(x^k),\phi(x^k)]\} \to 0$.

Let $\{x^n\}$ be a subsequence of $\{x^k\}$ with the property that $\{x^{n+1}-x^n\} \to 0$. By Lemma 1, $[\nabla f(x^n),Q(x^n)\nabla f(x^n)] \geq \|\nabla f(x^n)\|^2\omega'$ for all n sufficiently large. Take M so that $\|Q(x^n)\| \leq M$, $n = 1,2,\ldots$. Then $[\nabla f(x^n),Q^{-1}(x^n)\nabla f(x^n)] = [\nabla f(x^n),\phi(x^n)] \geq M^{-2}\omega'\|\nabla f(x^n)\|^2$, showing that $\{\nabla f(x^n)\} \to 0$. If z is any cluster point of $\{x^n\}$, clearly $\nabla f(z) = 0$. Because $f(x) - f(z) \geq \frac{1}{2}\|x-z\|^2\omega$, it follows that z is the unique minimizer of f; moreover, since $\{f(x^k)\}$ is strictly decreasing, both $\{f(x^k)\}$ and $\{f(x^n)\}$ converge downward to $f(z)$. Thus if z' is any cluster point of $\{x^k\}$, $f(z') = f(z)$, which implies that $z' = z$. Consequently, $\{x^k\} \to z$. This implies that $\phi(x^k) \to 0$.

We now turn to the proof of 2). In what follows the superscripts k on x^k will often be omitted. By Taylor's theorem we may write:

$$g(x,\gamma) = 1 - \frac{[H(\xi)h,h]}{2[\nabla f(x),h]}$$

where $h = \gamma Q^{-1}(x)\nabla f(x)$, and ξ lies "between" x and $x+h$.
Set $H(\xi) = Q(x) + H(\xi) - Q(x)$, then we calculate that:

$$g(x,\gamma) = 1 - \frac{\gamma}{2} - \frac{\gamma[(H(\xi)-Q(x))Q^{-1}(x)\nabla f(x), Q^{-1}(x)\nabla f(x)]}{2[\nabla f(x), Q^{-1}(x)\nabla f(x)]}.$$

As above we have that

$$[u, Q^{-1}(x)u] \geq \omega' M^{-2} \| u \|^2$$

whence:

$$\left|1 - \frac{\gamma}{2} - g(x,\gamma)\right| \leq \frac{\gamma \| H(\xi)-Q(x) \| M^2}{2\omega'^3}.$$

Since $\{\| \xi^k - x^k \|\} \to 0$, we have by uniform continuity on S that $\{\| H(\xi^k) - Q(x^k) \|\} \to 0$. Thus eventually γ_k can be taken always to be unity.

To conclude the proof we write:

$$\begin{aligned} x^{k+1} - z &= x^k - z - \gamma_k Q^{-1}(x^k)\nabla f(x^k) \\ &= x^k - z - \gamma_k Q^{-1}(x^k)Q(x^k)(x^k - z) + \gamma_k Q^{-1}(x^k)[H(x^k)(x^k-z) - \nabla f(x^k)] \\ &\quad + \gamma_k Q^{-1}(x^k)[Q(x^k) - H(x^k)](x^k - z). \end{aligned}$$

Since $|H(x^k)(x^k-z) - \nabla f(x^k)| < \varepsilon \| x^k - z \|$, whenever $\| x^k - z \|$ is sufficiently small, we get that

$$\begin{aligned} \| x^{k+1} - z \| &\leq |1-\gamma_k| \, \| x^k - z \| + \varepsilon \gamma_k \| Q^{-1}(x^k) \| \, \| x^k - z \| \\ &\quad + \gamma_k \| Q^{-1}(x^k) \| \, \| Q(x^k) - H(x^k) \| \, \| x^k - z \|. \end{aligned}$$

Choose k sufficiently large so that $\gamma_k = 1$ and $||Q(x^k) - H(x^k)|| < \varepsilon$. Then $||x^{k+1}-z|| \leq \frac{2\varepsilon}{\omega'} ||x^k-z||$, showing the superlinear convergence.

Remarks.

1. $Q(x^k)$ can be any sequence of $n \times n$ matrices with the property that $||Q(x^k)-H(x^k)|| \to 0$. The hypothesis that $H(x)$ is bounded below by ω on S can be replaced by the hypothesis that S is bounded and f has a unique point z where the gradient vanishes and $H(x)$ is bounded below by ω on some neighborhood of z. Indeed it is sufficient that $H(x^k)$ be bounded below on any infinite subsequence of $\{x^k\}$.
2. If $f \in C^3$ on S then by the application of Kantorovich's [2] theorem, the ultimate rate of convergence is actually quadratic.

<u>Numerical Results</u>

The method of this paper has been used on some dozen test problems. For comparison, the method of Fletcher and Powell [3] and in some cases the method of steepest descent have also been tried on the same problems. In all cases the method of steepest descent converged very much more slowly than the other two methods.

Table 1 shows the results when the faster two methods were tried on a simple test problem of Fletcher and Powell [3] (originally given by Rosenbruck)

$$f(x_1,x_2) = (x_2-x_1^2)^2 + .01(1-x_1)^2.$$

The number of steps required by the Fletcher and Powell method was about the same as for the method of this paper. It is hard to compare the time required by the two methods, particularly because of the fact that in the Fletcher and Powell method, it is easy to waste a lot of time obtaining a more accurate minimum than is really essential in the direction the method specifies. However, the method of Fletcher and Powell *does* specify that the function be minimized in this direction, and one needs to have some reasonable criteria satisfied for the approximate minimum. The "number of function and gradient evaluations" column in Table 1 is not absolutely accurate because the number of function evaluations required is not exactly the same as the number of gradient evaluations required. However, the numbers in the columns are approximately correct. In the case of the Fletcher and Powell method, if a less stringent minimization requirement were used, it is possible that the number of functional evaluations could be cut somewhat.

Figure 1 shows the results when all three methods were tried on a six dimensional problem in control theory. The problem consists of minimizing the function $w(\lambda)$ where λ is a 6-dimensional vector. The vector $x(\lambda)$ is defined as

$$x(\lambda) = \int_0^T B(\tau)G(\lambda,\tau)d\tau$$

where

$$B(\tau) = \begin{pmatrix} (-4 \sin \tau + 3\tau) & 2(1-\cos \tau) & 0 \\ (4 \cos \tau - 3) & -2 \sin \tau & 0 \\ 2(\cos \tau - 1) & -\sin \tau & 0 \\ 2 \sin \tau & \cos \tau & 0 \\ 0 & 0 & -\sin \tau \\ 0 & 0 & \cos \tau \end{pmatrix}$$

T is constant, and the 3-component vector

$$G(\lambda,\tau) = \begin{cases} \dfrac{\lambda \cdot B(\tau)}{\| \lambda \cdot B(\tau) \|} & \text{if } \| \lambda \cdot B(\tau) \| > 1 \\ 0 & \text{if } \| \lambda \cdot B(\tau) \| \leq 1. \end{cases}$$

x^o is a fixed 6-dimensional vector, and the scalar $y = \int_0^T \| G(\lambda,\tau) \| d\tau$.

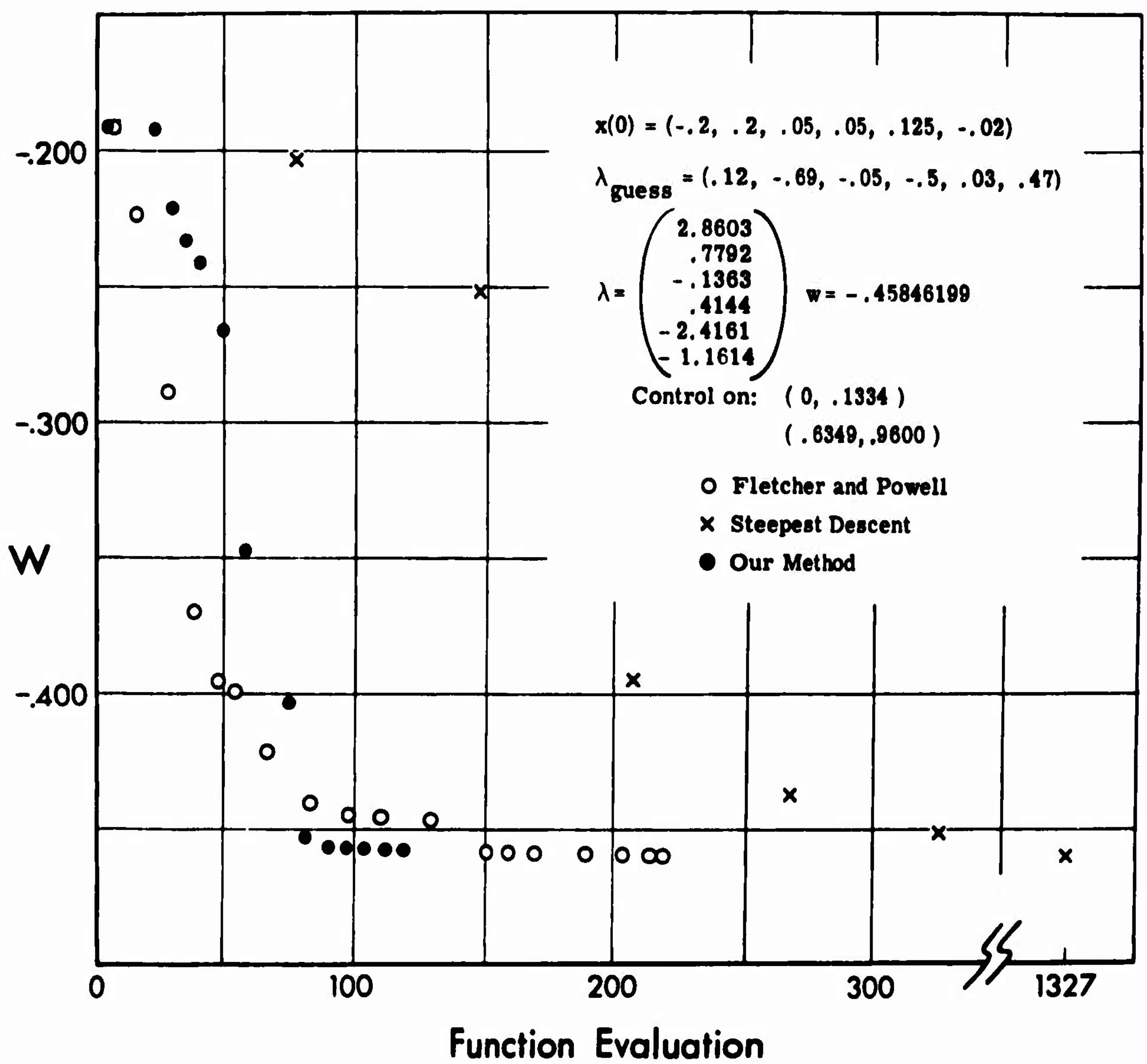
Then

$$w(\lambda) = [\lambda, x(\lambda) - x^o] - y.$$

In Figure 1 each dot represents a single step in the iterative process. The crosses each represent *ten* steps in the method of steepest descent. In all cases the same final results were obtained. Notice that the Fletcher and Powell method starts out faster than the present method but that the ultimate convergence is more rapid for this new method. Such behavior seems to occur quite often.

Table 1 $f(x_1,x_2) = (x_2-x_1^2)^2 + .01(1-x_1)^2$

Iteration Number k	Fletcher and Powell Method: Number of function and gradient evaluations carred out	Fletcher and Powell Method: $f(x_1,x_2)$	Our Method: Number of function and gradient evaluations carried out	Our Method: $f(x_1,x_2)$
0		.242		.242
1	4	$.413\times10^{-1}$	5	$.490\times10^{-1}$
2	11	$.385\times10^{-1}$	3	$.380\times10^{-1}$
3	12	$.353\times10^{-1}$	4	$.334\times10^{-1}$
4	17	$.187\times10^{-1}$	3	$.252\times10^{-1}$
5	9	$.179\times10^{-1}$	4	$.214\times10^{-1}$
6	12	$.144\times10^{-1}$	3	$.158\times10^{-1}$
7	13	$.111\times10^{-1}$	4	$.129\times10^{-1}$
8	12	$.886\times10^{-2}$	3	$.939\times10^{-2}$
9	11	$.686\times10^{-2}$	3	$.688\times10^{-2}$
10	10	$.596\times10^{-2}$	3	$.450\times10^{-2}$
11	14	$.357\times10^{-2}$	5	$.329\times10^{-2}$
12	11	$.222\times10^{-2}$	3	$.186\times10^{-2}$
13	8	$.202\times10^{-2}$	4	$.125\times10^{-2}$
14	13	$.690\times10^{-3}$	3	$.642\times10^{-3}$
15	8	$.523\times10^{-3}$	3	$.281\times10^{-3}$
16	9	$.245\times10^{-3}$	3	$.959\times10^{-4}$
17	10	$.312\times10^{-5}$	3	$.215\times10^{-4}$
18	4	$.167\times10^{-5}$	3	$.221\times10^{-5}$
19	8	$.759\times10^{-8}$	3	$.435\times10^{-7}$
20	4	$.107\times10^{-9}$	3	$.241\times10^{-10}$
21	5	$.156\times10^{-15}$	3	$.171\times10^{-16}$



-.200
-.300
-.400
W
0
100
200
300
1327
Function Evaluation
x(0) = (-.2, .2, .05, .05, .125, -.02)
λguess = (.12, -.69, -.05, -.5, .03, .47)
λ = (2.8603, .7792, -.1363, .4144, -2.4161, -1.1614)
w = -.45846199
Control on: (0, .1334)
(.6349, .9600)
Fletcher and Powell
Steepest Descent
Our Method

Figure 1

References

1. Goldstein, A. A.: On Steepest Descent. *SIAM J. on Control, A*, V. 3, 1(1965) pp 147-151.

2. Kantorovich, L. V. and Akilov, G. P.: Functional Analysis in Normed Spaces. Macmillan (1964).

3. Fletcher, R. and Powell, M. J. D.: A rapidly convergent descent method for minimization. *Computer J.* (July 1963) p 163-168.