Minimizing a function without calculating derivatives

By Willard I. Zangwill*

In an important contribution Powell has suggested an approach for determining the unconstrained minimum of a function of several variables, and determining it without calculating derivatives. This paper studies his approach in some detail. It is first shown by counter-example that his basic method for minimizing a quadratic function in a finite number of iterations contains an error. His modification of his basic method is then simplified, and the simplification proven to converge for strictly convex functions. Finally, we pose a new method not only which converges in a finite number of iterations for a quadratic, but also for which theoretical convergence is established in the strictly convex case.

1. Introduction

In a recent and important paper, Powell (1964) has suggested a new procedure for calculating the minimum of a function of several variables. The key advantage of his approach is that it does not require explicit evaluation of derivatives. In his paper he purports to have shown that his method will converge in a finite number of iterations to the minimum of a quadratic function. Regrettably, there is a minor flaw in his theory and in Section 2 of this paper a counter-example is posed. The counter-example reveals that Powell's method not only does not converge to the minimum of a quadratic in a finite number of iterations, but it will not converge in any number of iterations. It seems that Powell himself perceived some problems with his method as he reports encountering difficulties when applying the method to a function of five or more variables. The counter-example in this paper requires only three variables. The precise place at which the slip occurs in his proof is also pin-pointed.

Because of the difficulties he perceived, he developed a second method which, he suggests, might not converge to the minimum of a quadratic in a finite number of steps, but appears useful for more general functions. In the third section of this paper his second method is simplified, and the simplification proven to converge to the minimum of a strictly convex function.

The fourth portion of this paper develops a new method which has both the property that it will converge to the minimum of a quadratic in a finite number of steps, and the property that it will converge at least theoretically, to the minimum of a strictly convex function.

The notation of Powell's paper will be used as much as possible.

2. Non-convergence of Powell's Method

Let f be a real-valued function on E^n, Euclidean n-space. Powell first suggested the following procedure for determining a point p^*, called optimal, which minimizes f over E^n.

The First Powell Procedure

Initially choose $\xi_1, \ldots, \xi_n$ to be the n coordinate directions, and let p_0 be the starting point.

Step (i): For $r = 1, 2, \ldots, n$ calculate λ_r to minimize $f(p_{r-1} + \lambda_r \xi_r)$ and set $p_r = p_{r-1} + \lambda_r \xi_r$.

Step (ii): For $r = 1, 2, \ldots, n-1$ replace ξ_r by ξ_{r+1}, and replace ξ_n by $(p_n - p_0)$.

Step (iii): Choose λ to minimize $f(p_n + \lambda\{p_n - p_0\})$, replace p_0 by $p_0 + \lambda(p_n - p_0)$, and start the next iteration from step (i).

Roughly speaking, calculate $p_1, \ldots, p_n$ by successively minimizing in the directions $\xi_1, \ldots, \xi_n$. Then define a new set of directions by first deleting the old ξ_1, letting the new ξ_r be the old ξ_{r+1} $r = 1, \ldots, n-1$, and finally defining the new ξ_n by $\xi_n = p_n - p_0$. The new p_0 is found by minimizing from the old p_0 using the new ξ_n direction. The entire cycle from one p_0 to the next p_0 comprises one iteration.

A counter-example will now be posed.

Let

$$f(x, y, z) = (x - y + z)^2 + (-x + y + z)^2 + (x + y - z)^2.$$

It is easy to show that f is a strictly convex quadratic function with a unique minimum at $(x, y, z) = (0, 0, 0)$.

Choose as the initial point $(\frac{1}{2}, 1, \frac{1}{2})$.

DIRECTION ALONG WHICH TO MINIMIZE	POINT OBTAINED AFTER MINIMIZATION IN THE GIVEN DIRECTION
Initial point	$(\frac{1}{2}, 1, \frac{1}{2}) = p_0$
x	$(\frac{1}{2}, 1, \frac{1}{2}) = p_1$
y	$(\frac{1}{2}, \frac{1}{3}, \frac{1}{2}) = p_2$
z	$(\frac{1}{2}, \frac{1}{3}, \frac{5}{18}) = p_3$

The new direction would be

$$\xi_3 = p_3 - p_0 = (\tfrac{1}{2}, \tfrac{1}{3}, \tfrac{5}{18}) - (\tfrac{1}{2}, 1, \tfrac{1}{2}) = \left(0, \frac{-2}{3}, \frac{-2}{9}\right).$$

* *Center for Research in Management Science, University of California, Berkeley, California, U.S.A.*

The new set of directions becomes

$$\xi_1 = (0, 1, 0) = y$$
$$\xi_2 = (0, 0, 1) = z$$
$$\xi_3 = \left(0, \frac{-2}{3}, \frac{-2}{9}\right).$$

Observe that the x component of all three directions is zero, so that the x component can never again change. However, the x component of $p_3 = (\frac{1}{2}, \frac{1}{3}, \frac{-5}{18})$ is not zero. The optimal point $(0, 0, 0)$ can thus be never achieved, even in the limit.

Although the above is a counter-example to the original Powell procedure, he in an example (page 159 of his paper) modified his original procedure. The modification appears first to optimize along each coordinate direction before starting the usual procedure. Thus a new set of directions is not formed until the coordinate directions have been used twice: the first time in a special initialization iteration, the second as required by the method. The above function can also be used as a counter-example to the modified procedure. Start at the point $(100, -1, \frac{5}{2})$. After minimization first along the x direction and then along the y and z directions the point $(\frac{1}{2}, 1, \frac{1}{2})$ is reached. We then continue as in the previous counter-example.

To point out the place at which the error occurs in Powell's proof let f be quadratic so that

$$f(x) = xAx + bx + c, \tag{1}$$

where now $x \epsilon E^n$. Two directions p and q in E^n are said to be conjugate if

$$pAq = 0. \tag{2}$$

Powell states the following two theorems assuming the requisite minima are achieved.

Theorem 1: If $q_1, \ldots, q_m, m \leqslant n$, are mutually conjugate directions, then the minimum of the quadratic $f(x)$ in the m-dimensional space containing x_0, and the directions $q_1, \ldots, q_m$ may be found by searching along each of the directions once only.

Theorem 2: If x_0 is a minimum of the quadratic $f(x)$ in a space containing q, and x_1 is also a minimum in such a space, then the direction $(x_1 - x_0)$ is conjugate to q.

Finally, Powell employs the above two theorems to prove that at the end of n iterations, the directions $\xi_1, \ldots, \xi_n$ are mutually conjugate, and hence by Theorem 1 the minimum will have been found.

The difficulty with the above proof is in Theorem 1 because the $q_1, \ldots, q_m$ may not span an m-dimensional space. For example, the zero vector is trivially conjugate to any other vector. Regrettably, the Powell procedure may generate directions which are linearly dependent, and when it does, convergence may not occur.

We revise Theorem 1 to be:

Theorem 1-*A*: Theorem 1 with the additional hypothesis that the $q_i, i = 1, \ldots, m$ span the m-dimensional space.

3. A simplification of Powell's Second Procedure

Observing that his first method might encounter difficulties, Powell suggested a second procedure. The key notion behind his second procedure was that it might be unwise to replace a previous direction by a new direction if in doing so the new set of directions became linearly dependent. We pose a simplification of this procedure and then give a convergence proof. In the following $||.||$ denotes Euclidean norm.

Powell's Second Procedure (*simplified*)

Let the coordinate directions $\xi_1^1, \xi_2^1, \ldots, \xi_n^1$, an initial point p_0^1, and a scalar ϵ, $1 \geqslant \epsilon > 0$ be given. Also assume the directions are normalized to unit length so that $||\xi_r^1|| = 1, r = 1, \ldots, n$. Set $\delta^1 = 1$. Go to iteration k with $k = 1$.

Iteration k

(i) For $r = 1, 2, \ldots, n$ calculate λ_r^k to minimize $f(p_{r-1}^k + \lambda_r^k \xi_r^k)$, and define $p_r^k = p_{r-1}^k + \lambda_r^k \xi_r^k$.

(ii) Define $\alpha^k = ||p_n^k - p_0^k||$ and $\xi_{n+1}^k = (p_n^k - p_0^k)/\alpha^k$. Calculate λ_{n+1}^k to minimize $f(p_n^k + \lambda_{n+1}^k \xi_{n+1}^k)$ and set $p_0^{k+1} = p_{n+1}^k = p_n^k + \lambda_{n+1}^k \xi_{n+1}^k$.

(iii) Let $\lambda_s^k = \max\{\lambda_r^k | r = 1, \ldots, n\}$.
Case (*a*). If $\lambda_s^k \delta^k / \alpha^k \geqslant \epsilon$, let $\xi_r^{k+1} = \xi_r^k$ for $r \neq s$, $\xi_s^{k+1} = \xi_{n+1}^{k+1}$, and set $\delta^{k+1} = \lambda_s^k \delta^k / \alpha^k$.
Case (*b*). If $\lambda_s^k \delta^k / \alpha^k < \epsilon$,
let $\xi_r^{k+1} = \xi_r^k$, $r = 1, \ldots, n$ and set $\delta^{k+1} = \delta^k$.

Go to iteration k with $k + 1$ replacing k.

It is assumed that all minima are achieved.

Theorem 3: $\delta^k = \det|\xi_1^k, \ldots, \xi_n^k|$, the determinant of the matrix whose columns are $\xi_1^k, \ldots, \xi_n^k$.

PROOF: For $k = 1$ as ξ_r^1 are the unit coordinate vectors the result holds.

Assume the theorem for k. Since

$$p_n^k - p_0^k = \sum_{r=1}^{n} \lambda_r^k \xi_r^k = \alpha^k \xi_{n+1}^k$$

$$\begin{aligned}\det|\xi_1^k, \ldots, \xi_{s-1}^k, \xi_{n+1}^k, \xi_{s+1}^k, \ldots, \xi_n^k| &= (\lambda_s^k/\alpha^k)\det|\xi_1^k, \ldots, \xi_n^k| \\ &= (\lambda_s^k/\alpha^k)\delta^k.\end{aligned}$$

In step (ii) if Case (*a*) occurs, the new set of directions is the old set but with ξ_{n+1}^k replacing ξ_s^k. In this case $\delta^{k+1} = \lambda_s^k \delta^k / \alpha^k$. If Case (*b*) holds then the new set of directions is the same as the old set, so $\delta^{k+1} = \delta^k$.

Q.E.D.

Corollary 3.1: $\text{Det}|\xi_1^k, \ldots, \xi_n^k| \geqslant \epsilon$ for all k.

PROOF: Step (iii) ensures $\delta^k \geqslant \epsilon$ for all k. Q.E.D.

Step (iii) is thus seen to preserve the linear independence of the directions at each iteration.

In the remainder of the paper the letter K, perhaps with a superscript, will denote an infinite subsequence of the integers. The notation $K^1 \subset K$ means the infinite subsequence K^1 is a subsequence of K. Writing $\{p_1^k\}_{k \epsilon K}$ means the subsequence formed by the p_1^k for $k \epsilon K$. The subsequence $\{p_1^{k+1}\}_{k \epsilon K}$ is the subsequence formed by adding 1 to each $k \epsilon K$. If a subsequence $\{p_r^k\}_{k \epsilon K}$ converges to p_r^∞, we write $p_r^k \to p_r^\infty k \epsilon K$ or $\lim_{k \epsilon K} p_r^k = p_r^\infty$.

The next three theorems establish that Powell's Second Procedure (simplified) is well behaved in that any convergent subsequence must converge to a point at which the gradient of f, denoted ∇f, is zero for f a strictly convex function. Such a point will be the optimal point.

Theorem 4: Given any infinite subsequence of the integers K, there exists a $K^1 \subset K$ such that

$$\xi_r^k \to \xi_r^\infty \; k \epsilon K^1, \qquad r = 1, \ldots, n$$

where $||\xi_r^\infty|| = 1$, $r = 1, \ldots, n$. Furthermore, the ξ_r^∞, $r = 1, \ldots, n$ are linearly independent.

PROOF: As the ξ_r^k are normalized to unit length and are thus contained in a compact set, there must be a $K^1 \subset K$ such that

$$\xi_r^k \to \xi_r^\infty \; k\epsilon K' \text{ where } ||\xi_r^\infty|| = 1, \; r = 1, 2, \ldots, n. \quad (3)$$

By Corollary 3.1 $\det|\xi_1^k, \ldots, \xi_n^k| \geqslant \epsilon$ for all k. But $\det|\xi_1^k, \ldots, \xi_n^k| \to \det|\xi_1^\infty, \ldots, \xi_n^\infty| \; k\epsilon K^1$ from equation (3). Thus

$$\det|\xi_1^\infty, \ldots, \xi_n^\infty| \geqslant \epsilon,$$

and the ξ_r^∞, $r = 1, \ldots, n$ are linearly independent. Q.E.D.

The next theorem is stated in a more general framework as it will also be useful in Section 4 of this paper.

Theorem 5: Let f be a continuously differentiable strictly convex function, x^k for all k and x^∞ be points in E^n, η^k for all k and η^∞ be directions in E^n, and let β^k for all k and β^∞ be scalars. Assume there is a procedure which generates

$$f(x^{k+1}) \leqslant f(x^k) \qquad k = 1, 2, \ldots \quad (4)$$

Given K, an infinite subsequence of the integers, assume $x^k \to x^\infty$, $\eta^k \to \eta^\infty \neq 0$, and $x^{k+1} \to x^{\infty+1}$, $k\epsilon K$. Also for $k\epsilon K$ let

$$x^{k+1} = x^k + \beta^k \eta^k$$

where β^k is chosen to minimize $f(x^k + \beta\eta^k)$.

Then

$$x^{\infty+1} = x^\infty.$$

PROOF: By (4) the sequence $\{f(x^k)\}_{k=1}^\infty$ is monotonic so that

$$\lim_{k\to\infty} f(x^k) = \lim_{k\epsilon K} f(x^k) = \lim_{k\epsilon K} f(x^{k+1}).$$

By continuity of f

$$\lim_{k\epsilon K} f(x^k) = f(x^\infty) \quad \text{and} \quad \lim_{k\epsilon K} f(x^{k+1}) = f(x^{\infty+1})$$

hence

$$f(x^{\infty+1}) = f(x^\infty). \quad (5)$$

Also observe as $x^k \to x^\infty$, $x^{k+1} \to x^{\infty+1}$ and $\eta^k \to \eta^\infty \neq 0$, it must be that $\beta^k \to \beta^\infty k\epsilon K$ where β^∞ is the limit.

By hypothesis $f(x^{k+1}) = f(x^k + \beta^k\eta^k) \leqslant f(x^k + \beta\eta^k)$ for any β fixed. Continuity of f ensures that

$$f(x^{\infty+1}) = f(x^\infty + \beta^\infty\eta^\infty) \leqslant f(x^\infty + \beta\eta^\infty)$$

for any β. But strict convexity requires that $\beta^\infty = 0$. Hence as $x^{\infty+1} = x^\infty + \beta^\infty\eta^\infty$

$$x^{\infty+1} = x^\infty. \qquad \text{Q.E.D.}$$

The convergence can now be established.

Theorem 6: Let f be a strictly convex continuously differentiable function. Assume for $k\epsilon K$ that

$$p_r^k \to p_r^\infty, \qquad r = 0, \ldots, n.$$

Then $p_0^\infty = p_1^\infty = \ldots = p_n^\infty$, and p_0^∞ is such that

$$\nabla f(p_0^\infty) = 0.$$

That is, p_0^∞ is optimal.

PROOF: Via Theorem 4 there is a $K^1 \subset K$ such that

$$\xi_r^k \to \xi_r^\infty \; k\epsilon K', \quad ||\xi_r^\infty|| = 1, \quad r = 1, \ldots, n.$$

The hypotheses of Theorem 5 hold so that

$$p_0^\infty = p_1^\infty = \ldots = p_n^\infty. \quad (6)$$

Now for $r = 1, \ldots, n$

$$f(p_r^k) \leqslant f(p_{r-1}^k + \lambda\xi_r^k) \quad \text{for all } \lambda.$$

By continuity of f and equation (6)

$$f(p_0^\infty) \leqslant f(p_0^\infty + \lambda\xi_r^\infty), \quad r = 1, \ldots, n \quad \text{and all } \lambda. \quad (7)$$

But Theorem 4 guarantees that the ξ_r^∞, $r = 1, \ldots, n$ are linearly independent and thus span the entire space. Hence equation (7) could only hold if $\nabla f(p_0^\infty) = 0$, for otherwise there would be some s such that $\nabla f(p_0^\infty)\xi_0^\infty \neq 0$. Q.E.D.

The procedure is seen to converge for a strictly convex continuously differentiable function.

4. A new procedure

A new procedure based upon Powell's theorems will now be developed. The procedure will, whenever it encounters a quadratic with positive definite Hessian matrix of second partial derivatives, converge in a finite number of iterations. Theoretical convergence is also established for a strictly convex continuously differentiable function. No results are available, however, to enable an assessment to be made of the rate of convergence of this procedure relative to Powell's Second Procedure (or its simplification above) on general practical problems.

The new procedure requires a slight departure from Powell's notation, although as much notational consistency as possible will be maintained.

The procedure

Let c_r, $r = 1, \ldots, n$ be the coordinate directions and assume they are normalized to unit length.

Initialization step: Let an initial point p_n^0, and n normalized directions ξ_r^1, $r = 1, \ldots, n$ be given. Calculate λ_n^0 to minimize $f(p_n^0 + \lambda_n^0\xi_n^1)$ and let $p_{n+1}^0 = p_n^0 + \lambda_n^0\xi_n^1$. Set $t = 1$ and go to iteration k with $k = 1$.

Iteration k: p_{n+1}^{k-1}, ξ_r^k, $r = 1, \ldots, n$ and t are given.

Step (i): Find α to minimize $f(p_{n+1}^{k-1} + \alpha c_t)$. Update

t by

$$t \leftarrow \begin{cases} t+1 & \text{if} \quad 1 \leqslant t < n \\ 1 & \text{if} \quad t = n. \end{cases}$$

If $\alpha \neq 0$, let $p_0^k = p_{n+1}^{k-1} + \alpha c_t$. If $\alpha = 0$, repeat step (i). Should step (i) be repeated n times in succession, stop; the point p_{n+1}^{k-1} is optimal.

Step (ii): For $r = 1, \ldots, n$ calculate λ_r^k to minimize

$$f(p_{r-1}^k + \lambda_r^k \xi_r^k)$$

and define $\quad p_r^k = p_{r-1}^k + \lambda_r^k \xi_r^k.$

Let $\quad \xi_{n+1}^k = (p_n^k - p_{n+1}^{k-1})/||p_n^k - p_{n+1}^{k-1}||.$

Determine λ_{n+1}^k to minimize $f(p_n^k + \lambda_{n+1}^k \xi_{n+1}^k)$

and set $\quad p_{n+1}^k = p_n^k + \lambda_{n+1}^k \xi_{n+1}^k.$

Define $\quad \xi_r^{k+1} = \xi_{r+1}^k \; r = 1, \ldots, n.$

Go to iteration k with $k + 1$ replacing k.

All minima are assumed to exist.

Some discussion of the procedure may be in order. Step (i) proceeds cyclically through the coordinate directions. That is, each time we return to step (i) we use the next coordinate direction, repeating c_1 after using c_n. Every $n + 1$ times step (i) is employed the same coordinate direction is employed. The t indexes the coordinate direction to be used. If step (i) is repeated n times in succession, then all n coordinate directions have been attempted and no change in the point has occurred. Such a situation can only occur if at that point the gradient of the function f is zero. As we assume f strictly convex and continuously differentiable, that point is optimal.

In general step (i) is repeated until a new point is generated. In step (ii) the procedure continues as in the earlier procedures. It is important to observe that after at most n iterations, all coordinate directions have been used.

The quadratic case follows Powell's argument but ensures that Theorem 1-A holds instead of Theorem 1.

Theorem 7 (Quadratic Convergence): Let f be quadratic with a positive definite Hessian A. Then the procedure stops at an optimal point in step (i) of iteration k where $k \leqslant n$.

PROOF: Assume at the beginning of iteration k, $k \leqslant n - 1$, that the direction $\xi_{n-k+1}^k, \xi_{n-k+2}^k, \ldots, \xi_n^k$, are mutually conjugate and linearly independent. If the procedure does not stop in step (i) of iteration k then $p_{n+1}^{k-1} \neq p_0^k$ and as A is positive definite $f(p_o^k) < f(p_{n+1}^{k-1})$. By monotonicity of the procedure $f(p_n^k) \leqslant f(p_0^k) < f(p_{n+1}^{k-1})$ so that

$$p_{n+1}^{k-1} \neq p_n^k \quad \text{and} \quad \xi_{n+1}^k \neq 0.$$

At iteration $k - 1$, because $\xi_{r+1}^{k-1} = \xi_r^k$, the last k directions to be employed were $\xi_{n-k+1}^k, \ldots, \xi_n^k$. Since these directions are linearly independent the point p_{n+1}^{k-1} is a minimum in the k-dimensional space containing $\xi_{n-k+1}^k, \ldots, \xi_n^k$ via Theorem 1-A. Similarly the point p_n^k is such a point. Thus from Theorem 2 ξ_{n+1}^k is mutually conjugate to $\xi_{n-k+1}^k, \ldots, \xi_n^k$. Furthermore, $\xi_{n-k+1}^k, \ldots, \xi_n^k, \xi_{n+1}^k$ are all non-zero hence, as A is positive definite, they are linearly independent. Thus $\xi_{n-(k+1)+1}^{k+1}, \ldots, \xi_n^{k+1}$ are linearly independent and mutually conjugate.

Clearly the same argument holds for $k = 1$ establishing the induction.

Thus if the procedure has not stopped by the beginning of iteration n, we have generated n mutually conjugate and linearly independent directions. In step (ii) of iteration $n - 1$ we have optimized over these n directions, so that the point p_{n+1}^{n-1} must be optimal. The procedure will then stop in step (i) of iteration n. Q.E.D.

The convergence of the procedure for f strictly convex will now be established. Since finite convergence has been discussed in reference to step (i) only the situation in which the procedure generates an infinite sequence of points will be considered. The proof will be brief as it follows the proof of Theorem 6 closely.

Theorem 8: Let f be strictly convex and continuously differentiable. Assume all points p_r^k, $r = 0, \ldots, n + 1$ for all k are contained in a compact set. Let $p_s^k \rightarrow p_s^\infty$ $k \epsilon K$ for some K and fixed s. Then p_s^∞ is optimal.

PROOF: Since all points are in a compact set there must be a $K^1 \subset K$ such that for $k \epsilon K^1$

$$_{s+i}^{k+j} \rightarrow p_{s+i}^{\infty+j}, k \epsilon K^1, \quad i = -s, -s+1, \ldots, -1, 0, +1, \ldots, n+1-s \quad \text{and} \quad j = 0, \ldots, n-1.$$

Here we are considering all points generated on iterations $k, k + 1, \ldots, k + n - 1$ for $k \epsilon K$.

As the directions are normalized, by extracting subsequences if necessary, Theorem 5 ensures that

$$p_s^\infty = p_{s+i}^{\infty+j}, \quad i = -s, \ldots, n+1-s, \quad j = 0, \ldots, n-1.$$

But during any successive n iterations all n coordinate directions must have been used. Again using subsequences if necessary, and calling upon the ideas leading to equation (7) in Theorem 6, we obtain

$$f(p_s^\infty) \leqslant f(p_s^\infty + \beta c_r) \text{ for all } \beta \text{ and } r = 1, \ldots, n.$$

But as the c_r are the coordinate directions, p_s^∞ must be optimal. Q.E.D.

Acknowledgement

This research was supported by a grant from the Ford Foundation to the Graduate School of Business Administration, and administered through the Center for Research in Management Science.

Reference

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