A Step Size Rule for Unconstrained Optimization

J. Rohn[1]

Abstract. We propose an Armijo-type step size rule for solving differentiable unconstrained optimization problems, based on a quadratic approximation. The rule is proved to be finite and to perform the exact line search in one iteration in case of a strictly convex quadratic function. We give convergence results for the steepest descent and for the FR, PR and DFP methods using this rule. Computational evidence shows that the rule performs best when implemented into the DFP or BFGS method.

Key words. Unconstrained optimization, step size rule, convergence

1. Introduction

Gradient methods for solving an unconstrained optimization problem

$$\text{minimize } f(x)$$
$$\text{subject to } x \in R^n ,$$

as e.g. the steepest descent (SD) method or the methods by Fletcher--Reeves (FR), Polak-Ribiére (PR), Davidon-Fletcher-Powell (DFP) or Broyden-Fletcher-Goldfarb-Shanno (BFGS), described in standard textbooks like Luenberger [1], Fletcher [2] or Polak [3], construct a sequence of iterations $\{x_i\}$ according to this general scheme (which we call the ''main algorithm'' to distinguish it from its concrete specifications; we denote $g_i = \nabla f(x_i)$, the gradient of f at x_i):

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[1]Assistant Professor, Faculty of Mathematics and Physics, Charles University, Malostranske nam. 25, 11800 Prague, Czechoslovakia

Main algorithm.

Step 0. Select an $x_0 \in R^n$ and set $i:=0$.

Step 1. If $g_i = 0$, terminate: x_i is a stationary point of f.

Step 2. Otherwise find a search direction d_i such that $d_i^T g_i < 0$.

Step 3. Find a real number α_i satisfying

$$f(x_i + \alpha_i d_i) = \min \{ f(x_i + \alpha d_i) ; \alpha \geq 0 \}.$$

Step 4. Set $x_{i+1} := x_i + \alpha_i d_i$, $i := i + 1$ and go to Step 1.

The methods listed above differ from each other only in the choice of the search direction d_i in Step 2 (to be described later in Section 3). All of them share the common descent property of the main algorithm, namely that $f(x_{i+1}) < f(x_i)$ for each i. The procedure of minimizing the function of one real variable $f(x_i + \alpha d_i)$ over the nonnegative half-ray is called the line search, and the value α_i the step size. In the form stated the main algorithm remains, however, only of conceptual value since generally the exact minimum in Step 3 cannot be found in a finite number of iterations; therefore in practical computations the exact line search in Step 3 must be substituted by some finite procedure (a so-called inexact line search) yielding satisfactory approximate results. Among many options discussed in [1], [2], [3], we shall focus our attention here on the step size rule proposed by Armijo [4], using a preselected parameter $\beta \in (0,1)$:

Step 3A. Set $\alpha_i := \beta^k$, where k is the minimum positive integer satisfying

$$f(x_i + \beta^k d_i) - f(x_i) \leq 0.5 \beta^k d_i^T g_i \ .$$

In view of the choice of d_i made in Step 2, it is easy to see that: (a) such a k exists, and (b) the sequence generated by the main algorithm using this rule satisfies $f(x_{i+1}) < f(x_i)$ for each i, hence the descent property is not violated.

In this paper we shall propose another rule, which is in certain sense similar to that of Armijo's, but based on quadratic considerations. In section 2 we formulate the rule and prove that it is finite and maintains the descent property; moreover, if f is a strictly convex quadratic function, then the line search is exact and the minimizing value is always found in one iteration. In section 3 we state a general convergence result (Theorem 3.1) which is then applied to establish convergence properties of the SD, FR, PR and DFP methods using this rule. Computational experience shows that the rule performs well, especially when implemented into the DFP or BFGS method.

2. The rule

We shall first give an informal description of the basic idea. Assume at the i-th iteration of the main algorithm we have an approximation $\beta_j > 0$ $(j = 0,1,\dots)$ of the exact step size. Assuming f to be at least twice continuously differentiable, let us replace the function $f(x_i + \beta d_i)$ of one real variable β by its truncated Taylor series

$$f(x_i + \beta\, d_i) \doteq f(x_i) + \beta d_i^T g_i + 0.5\, \beta^2 d_i^T H_i d_i \qquad (1)$$

where $H_i = \left(\partial^2 f(x_i)/\partial x_j \partial x_k\right)_{j,k=1}^{n}$ is the Hessian matrix at x_i.
It is obvious that the right-hand side quadratic function achieves its minimum (if it exists) at the point

$$\beta = -(d_i^T g_i)/(d_i^T H_i d_i). \qquad (2)$$

To avoid the necessity of evaluating H_i, let us express the denominator in (2) from the formula (1) applied to the previously computed approximation β_j:

$$d_i^T H_i d_i \doteq (2/\beta_j^2)\left(f(x_i + \beta_j d_i) - f(x_i) - \beta_j d_i^T g_i\right). \qquad (3)$$

Hence, using (2) and (3), we may construct the next approximation by

$$\beta_{j+1} = -0.5\,\beta_j^2 d_i^T g_i/(f(x_i + \beta_j d_i) - f(x_i) - \beta_j d_i^T g_i). \qquad (4)$$

Now observe that this equation implies

$$f(x_i + \beta_j d_i) - f(x_i) = (\beta_j - 0.5\,\beta_j^2/\beta_{j+1})\, d_i^T g_i. \qquad (5)$$

Thus, if

$$\beta_j - 0.5\,\beta_j^2/\beta_{j+1} > 0, \qquad (6)$$

then $f(x_i + \beta_j d_i) - f(x_i) < 0$, so that we may terminate the procedure and set $\alpha_i := \beta_j$, which will enforce the descent property

$$f(x_{i+1}) < f(x_i) \qquad (7)$$

to hold. Since $\beta_j > 0$, we may simplify (6) to

$$\beta_j/\beta_{j+1} < 2.$$

In the opposite case

$$\beta_j/\beta_{j+1} \geq 2$$

we have $\beta_{j+1} > 0$ and setting $j:=j+1$, we may repeat the whole process. Finally, if the denominator in (4) is zero, then we have

$$f(x_i + \beta_j d_i) - f(x_i) = \beta_j d_i^T g_i < 0, \qquad (8)$$

so that we can set $\alpha_i := \beta_j$. Summing up, the line search procedure runs as follows:

<u>Step Size Rule 2.1</u> (to replace Step 3 of the main algorithm).

<u>Step 3.1.</u> Set $\beta_0 := 1$ and $j := 0$.

<u>Step 3.2.</u> Compute $\gamma_j = f(x_i + \beta_j d_i) - f(x_i) - \beta_j d_i^T g_i$.

<u>Step 3.3.</u> If $\gamma_j = 0$, set $\alpha_i := \beta_j$ and go to Step 4.

<u>Step 3.4.</u> Otherwise compute $\beta_{j+1} = -0.5(\beta_j^2/\gamma_j)d_i^T g_i$.

<u>Step 3.5.</u> If $\beta_j/\beta_{j+1} < 2$, set $\alpha_i := \beta_j$ and go to Step 4.

<u>Step 3.6.</u> Otherwise (i.e. if $\beta_j/\beta_{j+1} \geq 2$) set $j := j+1$ and go to Step 3.2.

It follows from Step 3.6 that if the rule does not stop with β_j, then the newly constructed iteration satisfies

$$0 < \beta_{j+1} \leq 0.5\,\beta_j \;. \qquad (9)$$

We shall now prove that α_i is reached after a finite number of iterations:

Proposition 2.1. Let $f \in C^1$. Then the step size rule 2.1 is finite and the main algorithm using this rule generates a sequence of points satisfying

$$f(x_{i+1}) < f(x_i)$$

for each i.

Proof. Assume to the contrary that the rule never terminates for some i, so that it constructs a sequence of numbers $\{\beta_j\}$ tending to zero in view of (9). Hence from (5) we have

$$(f(x_i + \beta_j d_i) - f(x_i))/\beta_j = (1 - 0.5\,\beta_j/\beta_{j+1})\,d_i^T g_i$$

for each j. Since the left-hand side tends to $d_i^T g_i$ as j approaches infinity, we obtain

$$\lim_{j\to\infty} \beta_j/\beta_{j+1} = 0.$$

But this is a contradiction since $\beta_j/\beta_{j+1} \geq 2$ for each j due to Step 3.6. Hence the rule is finite. The fact that the objective strictly decreases has been already established in (7) and (8).

Proposition 2.2. If f is a strictly convex quadratic function, then the line search 3.1-3.6 is exact and $\alpha_i = \beta_1$ for each i.

Proof. Let $f(x) = 0.5x^TCx + b^Tx + a$, where C is a symmetric positive definite matrix. Then for each β we have

$$f(x_i + \beta d_i) = f(x_i) + \beta d_i^T g_i + 0.5\beta^2 d_i^T C d_i,$$

hence $\gamma_j > 0$ since C is positive definite and $d_i \neq 0$ by Step 2, and for each j we have from (4)

$$\beta_{j+1} = -(d_i^T g_i)/(d_i^T C d_i),$$

the right-hand side constant being obviously the exact minimizer of $f(x_i + \beta d_i)$ over the nonnegative half-ray. Hence $\beta_2 = \beta_1$, so that $\alpha_i := \beta_1$ is set in Step 3.5.

3. Convergence properties

In this section we shall first prove in Theorem 3.1 a convergence property for the main algorithm endowed with the step size rule 2.1 and then will use it to establish some convergence results for the SD, FR, PR and DFP methods under the rule 2.1.

For each $i = 0,1,\ldots$, denote by j_i the index j for which $\alpha_i := \beta_j$ is set in Step 3.3 or Step 3.5 of the rule 2.1. If $j_i \geq 1$, denote also $\bar{\alpha}_i = \beta_{j_i - 1}$. Then for each i with $j_i \geq 1$ we have

$$f(x_i + \bar{\alpha}_i d_i) - f(x_i) \geq 0 \tag{10}$$

$$f(x_i + \alpha_i d_i) - f(x_i) < 0 \; . \tag{11}$$

In fact, (11) follows from Proposition 2.1. If $j := j_i \geq 1$, then the rule did not terminate at j-1, which means that it must have been

$$\beta_{j-1}/\beta_j \geq 2$$

in Step 3.6, implying

$$f(x_i + \bar{\alpha}_i d_i) - f(x_i) = \beta_{j-1}(1 - 0.5\,\beta_{j-1}/\beta_j) d_i^T g_i \geq 0$$

due to (5), which proves (10).

Theorem 3.1. Let $f \in C^1$ and let the sequence generated by the main algorithm using the step size rule 2.1 have the property

$$x_{i+1} - x_i \to 0. \tag{12}$$

Then each accumulation point (x_*, d_*) of the sequence $\{(x_i, d_i)\}$ satisfies

$$d_*^T \nabla f(x_*) = 0. \tag{13}$$

Proof. Let $x_i \xrightarrow{K} x_*$, $d_i \xrightarrow{K} d_*$ along some subsequence $K \subset \{0,1,2,\dots\}$ which may be chosen so that $\{\alpha_i\}_{i \in K}$ is convergent (since $0 \leq \alpha_i \leq \max\{0,\beta\}$ for each i). Let $\alpha_i \xrightarrow{K} \alpha$. We shall distinguish two cases:

(a) Let $\alpha > 0$. Then from $\alpha_i d_i = x_{i+1} - x_i \to 0$ we have $d_* = 0$, hence (13) holds.

(b) Let $\alpha = 0$. Since $d_i \xrightarrow{K} d_*$ and $g_i \xrightarrow{K} \nabla f(x_*)$, we have $d_i^T g_i \xrightarrow{K} d_*^T \nabla f(x_*)$. Assume to the contrary that $d_*^T \nabla f(x_*) \neq 0$. Since $\alpha = 0$, it must be $j_i \geq 1$ from some $i \in K$ on and from Step 3.4 we obtain

$$\alpha_i = -(\bar{\alpha}_i^2 / \bar{\gamma}_i) d_i^T g_i,$$

where $\bar{\gamma}_i = \gamma_{j_i - 1}$. Here $\alpha_i \xrightarrow{K} 0$, the sequence $\{\bar{\gamma}_i\}_K$ is bounded and $d_i^T g_i \xrightarrow{K} d_*^T \nabla f(x_*) \neq 0$, which gives $\bar{\alpha}_i \xrightarrow{K} 0$. Now from (10), (11) we have

$$f(x_i + \bar{\alpha}_i d_i) - f(x_i) \geq 0$$
$$f(x_i + \alpha_i d_i) - f(x_i) < 0$$

for sufficiently large $i \in K$, hence by the continuity argument there is an $\alpha_i' \in [\alpha_i, \bar{\alpha}_i]$ such that

$$f(x_i + \alpha_i' d_i) - f(x_i) = 0$$

holds and by the mean-value theorem we have

$$d_i^T \nabla f(x_i + \xi_i d_i) = 0$$

for some $\xi_i \in [0, \alpha_i'] \subset [0, \bar{\alpha}_i]$. Now taking the limit $i \xrightarrow{K} \infty$, from

$\bar{\alpha}_i \xrightarrow{K} 0$ we have $\xi_i \xrightarrow{K} 0$ and hence

$$d_*^T \nabla f(x_*) = 0.$$

This contradicts the assumption $d_*^T \nabla f(x_*) \neq 0$. Hence (13) holds.

Comment. If the line search is exact (as assumed in the original Step 3 of the main algorithm), then taking the derivative of $f(x_i + \alpha d_i)$ at the minimum point, we obtain

$$d_i^T g_{i+1} = 0 \tag{14}$$

for each i (cf. Polak [3]). If $(x_i, d_i) \xrightarrow{K} (x_*, \alpha_*)$ and (12) holds, then $g_{i+1} \xrightarrow{K} \nabla f(x_*)$, hence $g_{i+1} - g_i \xrightarrow{K} 0$ which gives $d_i^T g_i = -d_i^T (g_{i+1} - g_i) \xrightarrow{K} 0 = d_*^T \nabla f(x_*)$. Hence the condition (13) is a generalization of (14).

We shall now apply Theorem 3.1 to establish convergence properties of several known methods under the step size rule 2.1; they arise by specifying the Step 2 of the main algorithm as follows (cf. [1]):

a) The steepest descent method:

$$d_i = -g_i \qquad (i = 0,1,\dots).$$

b) Conjugate gradient methods:

$$d_{i+1} = -g_{i+1} + \delta_i d_i \qquad (i = 0,1,\dots) \tag{15}$$

$$d_o = -g_o$$

where

$$\delta_i = \|g_{i+1}\|_2^2 / \|g_i\|_2^2 \qquad \text{(FR method)} \tag{16}$$

$$\delta_i = g_{i+1}^T (g_{i+1} - g_i) / \|g_i\|_2^2 \qquad \text{(PR method)}. \tag{17}$$

c) The DFP method:

$$d_i = -S_i g_i \qquad (i = 0,1,\dots) \tag{18}$$

where S_o is the unit matrix and updating is done by

$$S_{i+1} = S_i + (p_i p_i^T)/(p_i^T q_i) - (S_i q_i q_i^T S_i)/(q_i^T S_i q_i)$$

where $p_i = x_{i+1} - x_i$, $q_i = g_{i+1} - g_i$, $i = 0,1,\dots$; then all the matrices S_i are symmetric positive definite [1, p. 195].

Notice that the proofs which follow use only the property (13), not the actual construction of the sequence by the rule 2.1. Hence they are valid under any step size rule maintaining the property stated in Theorem 3.1.

Proposition 3.1. Let $f \in C^1$ and let the sequence $\{x_i\}$ constructed by the steepest descent method using the rule 2.1 satisfy (12). Then each accumulation point of $\{x_i\}$ is a stationary point of f.

Proof. If $x_i \xrightarrow{K} x_*$ along some $K \subset \{0,1,\ldots\}$, then $d_i^T g_i = -\|g_i\|_2^2 \xrightarrow{K} -\|\nabla f(x_*)\|_2^2 = 0$ due to Theorem 3.1 and the assertion follows.

Proposition 3.2. Let $f \in C^1$ and let both the sequences $\{x_i\}$, $\{d_i\}$ constructed by the FR (or PR) method using the rule 2.1 be convergent. Then the limit point of $\{x_i\}$ is a stationary point of f.

Proof. Let $x_i \to x_*$, $d_i \to d_*$, so that $g_i \to g_* = \nabla f(x_*)$. Then premultiplying (15) by g_{i+1}, from (16), (17) we have

$$\|g_i\|_2^2(d_{i+1}^T g_{i+1}) = -\|g_i\|_2^2\|g_{i+1}\|_2^2 + \bar{\delta}_i(d_i^T g_i + d_i^T(g_{i+1} - g_i)) \qquad (19)$$

where $\bar{\delta}_i = \|g_{i+1}\|_2^2$ for the FR method and $\bar{\delta}_i = g_{i+1}^T(g_{i+1} - g_i)$ for the PR method. Since $d_i^T g_i \to 0$ according to Theorem 3.1, taking the limit in (19) we obtain $\|g_*\|_2^4 = 0$, hence $g_* = 0$.

Proposition 3.3. Let $f \in C^1$ and let $\{x_i\}$ be constructed by the DFP method using the rule 2.1. Assume that (12) holds and that $S_i \to S$, where S is a positive definite matrix. Then each accumulation point of $\{x_i\}$ is a stationary point of f.

Proof. If $x_i \xrightarrow{K} x_*$, then $g_i \xrightarrow{K} g_* = \nabla f(x_*)$, hence $d_i \xrightarrow{K} -Sg_*$

by (18) and $g_i^T S_i g_i \xrightarrow{K} g_*^T S g_*$, but also $g_i^T S_i g_i = -d_i^T g_i \xrightarrow{K} 0$ by Theorem 3.1, hence $g_*^T S g_* = 0$ and the positive definiteness of S implies $g_* = 0$.

Example. We have tested the rule 2.1 against the Armijo rule (with $\beta = 0.7$) on the example used by Polak in [3], section C.2, for comparing the performances of various methods. The example reads

$$\min \left\{ \exp(x_1^2 + 5x_2^2) + x_1^2 + 80x_2^2;\ x \in R^2 \right\}$$

and clearly has a unique optimal solution $x = (0,0)^T$. We have used throughout Polak's starting point $x_0 = (1.32, -0.07)^T$ and the stopping rule $\|x_k - x_{k-1}\|_\infty < 10^{-3}$. Armijo rule gives the following results (at each method we depict the number of iterations k and the coordinates of the last iteration x_k):

method	k	$(x_k)_1$	$(x_k)_2$
SD	35	2.79333E-02	3.60985E-04
FR	12	1.72954E-03	-1.88560E-05
PR	11	1.11621E-03	1.04664E-04
DFP	10	1.82042E-04	5.48999E-06
BFGS	9	1.97058E-04	-3.23192E-05

Using alternatively the rule 2.1, we obtained these results:

method	k	$(x_k)_1$	$(x_k)_2$
SD	22	3.56810E-02	-6.01563E-03
FR	10	-1.20377E-03	-1.37141E-05
PR	5	1.03677E-02	9.10693E-03
DFP	7	-5.23471E-07	-3.40049E-07
BFGS	6	-9.85223E-07	-5.75616E-07

It can be seen that the rule 2.1 performed approximately equally with SD and FR, a little worse with PR, but essentially better with DFP and BFGS. This particular result corresponds to our overall (although limited) computational experience according to which the rule performs best when incorporated into the DFP or BFGS method.

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