On the Rate of Convergence of the Conjugate Gradient Reset Method with Inaccurate Linear Minimizations

KAZUHIKO KAWAMURA AND RICHARD A. VOLZ

Dear Dick,

As your first Ph.D. student, it is my great honor to dedicate our paper to you. I still remember the day Mary and you came with your first baby to our wedding in a snowy day in Ann Arbor. Time has indeed passed.

Ethel and I send you and Mary our best wishes!

Yours sincerely,

Kaz Kawamura
School of Engineering
Vanderbilt University

On the Rate of Convergence of the Conjugate Gradient Reset Method with Inaccurate Linear Minimizations

KAZUHIKO KAWAMURA AND RICHARD A. VOLZ

Abstract—Recently Klessig and Polak have shown that a variation of the Polak–Ribière conjugate gradient reset algorithm converges n-step quadratically even if the one-dimensional search is not performed exactly. It is shown here that n-step quadratic convergence is also obtained for a modification of the Fletcher–Reeves conjugate gradient reset algorithm with inaccurate one-dimensional search.

Manuscript received November 1, 1972; revised March 19, 1973. Paper recommended by E. R. Barnes, Chairman of the IEEE S-CS Computational Methods, Discrete Systems Committee.
K. Kawamura is with the Electrical Engineering Section, University of Michigan, Dearborn, Mich. 48128.
R. A. Volz is with the Department of Electrical and Computer Engineering, University of Michigan, Ann Arbor, Mich. 48104.

I. Introduction

In recent years the problem of minimizing functions of n variables by conjugate gradient methods has been receiving much attention, and the convergence and rate of convergence of these methods have been extensively studied (e.g., see [1], [2], [5], [7], and [8]). Recently Klessig and Polak have further shown [6] that the Polak–Ribière conjugate gradient reset algorithm converges n-step quadratically even if the one-dimensional search is not performed exactly. It is the purpose of this paper to illustrate that n-step quadratic convergence is also obtained for the Fletcher–Reeves conjugate gradient reset algorithm with inaccurate one-dimensional search.

Let $f: E_n \to E_1$ be twice continuously differentiable and let there exist $\mu, \lambda > 0$ such that $\mu\|y\|^2 \le \langle y, Q(x)y\rangle \le \lambda \|y\|^2$ for all $x, y \in E_n$ where $Q(x) = \partial^2 f(x)/\partial x^2$ is the Hessian matrix. The problem is to find the element $z \in E_n$ that minimizes $f(x)$ on E_n. The Fletcher–Reeves conjugate gradient algorithm with reset for finding z proceeds as follows. Choose an arbitrary point $x_0 \in E_n$, and set $p_o = -g(x_o)$, where $g(x)$ is the gradient of f at x. Then for $i = 0,1,2,\cdots$, set

$$x_{i+1} = x_i + \alpha_i p_i \tag{1.1}$$

$$p_{i+1} = -g_{i+1} + \beta_i p_i, \qquad g_{i+1} = g(x_{i+1}) \tag{1.2}$$

where α_i is the least positive root of $\langle g(x_i + \alpha p_i), p_i\rangle = 0$, and

$$\beta_i = \begin{cases} 0 & \text{if } i+1 = 0 \ (\text{modulo } q), \quad q \ge n \\ \|g_{i+1}\|^2/\|g_i\|^2 & \text{otherwise.} \end{cases} \tag{1.3}$$

Note that the definition of β_i is equivalent to "restarting" the procedure after every $q \ge n$ iterations. Typically q is chosen to be n. However since precise minimization of f along $x_i + \alpha p_i$ usually requires infinite subprocedure computationally, the above algorithm must be modified to be *implementable*. In the sequel two ways to accomplish this are proposed and their properties shown. In Section II it is shown that, under the assumptions made above, the Fletcher–Reeves method with reset remains convergent for certain finite terminations of the one-dimensional search. In Section III it is shown that with an additional assumption n-step quadratic convergence can be preserved for a finite termination of increasing accuracy.

II. A Convergent Implementation of the Conjugate Gradient Reset Method

To describe the process of conducting the one-dimensional search we suppose the existence of an algorithm that generates for each i a sequence $\gamma_{i0}, \gamma_{i1}, \cdots$, with the properties

$$f(x_i + \gamma_{ij} p_i) \le f(x_i + \gamma_{ij-1} p_i), \qquad j \ge 1 \tag{2.1}$$

and $\gamma_{ij} \to \gamma_i^*$ where γ_i^* is the least positive zero of $(d/d\gamma) f(x_i + \gamma p_i)$.

Let $S(x_0) = \{x \in E_n : f(x) \le f(x_0)\}$ be bounded and Θ and c be scalars such that $0 < \Theta < 1$ and $0 < c < 1/\lambda$. Furthermore, let

$$\epsilon_{ij} = \frac{\langle -g_{ij}, p_i\rangle}{\|g_{ij}\|\,\|p_i\|}, \qquad g_{ij} = g(x_i + \gamma_{ij} p_i) \tag{2.2}$$

and

$$\delta_i = c\,\frac{\langle -g_i, p_i\rangle}{\|p_i\|^2}. \tag{2.3}$$

Here δ_i gives a lower bound for the step size α_i. Note that $\epsilon_{ij} = 0$ if one-dimensional search is performed exactly.

First, we modify the procedure to calculate the step size α_i as follows. The one-dimensional search is stopped when the following conditions are satisfied:

$$\gamma_{ij} \ge \delta_i \tag{2.4}$$

$$f(x_i + \gamma_{ij} p_i) \le f(x_i + \delta_i p_i) \tag{2.5}$$

$$\epsilon_{ij} \le \frac{\Theta\|g_i\|^2}{\|g_{ij}\|\,\|p_i\|}. \tag{2.6}$$

In this case we set $\alpha_i = \gamma_{ij}$. Then $g_{i+1} = g_{ij}$. These conditions imply that the ith step size α_i must be at least as large as δ_i and that the one-dimensional search is stopped when $|\cos\phi|$, where ϕ is the angle between p_i and g_{ij}, becomes smaller than $\Theta\|g_i\|^2/\|g_{ij}\|\,\|p_i\|$. Note that (2.6) is equivalent to

$$|\langle -g_{i+1}, p_i\rangle| = |\langle -g_{ij}, p_i\rangle| \le \Theta\|g_i\|^2, \tag{2.7}$$

which is similar to the proposal by Daniel [3]. This modified algorithm is well defined (e.g., [5, pp. 59–60]), and can be shown to be convergent. To do this we first need two lemmas.

Lemma 2.1: For $i = 0,1,2,\cdots$, there exist scalars k_1, k_2, k_3, and k_4 in $(0,\infty)$ such that

$$\langle -g_i, p_i\rangle \ge k_1\|g_i\|^2 \tag{2.8}$$

$$\beta_i \le k_2 \tag{2.9}$$

$$k_3\|g_i\| \le \|p_i\| \le k_4\|g_i\|. \qquad \square \tag{2.10}$$

Proof: Let the index set I_q be $I_q = \{i \in \{0, q, 2q, \cdots\}\}$. Then for $i \in I_q$,

$$\langle -g_i, p_i\rangle = \|g_i\|^2. \tag{2.11}$$

For $i \notin I_q$, $p_i = -g_i + \beta_{i-1} p_{i-1}$.

$$\begin{aligned} \therefore\ \langle -g_i, p_i\rangle &= \|g_i\|^2 + \beta_{i-1}\langle -g_i, p_{i-1}\rangle \\ &\ge \|g_i\|^2 - \beta_{i-1}\Theta\|g_{i-1}\|^2 \quad \text{by (2.7)} \\ &= (1-\Theta)\|g_i\|^2. \end{aligned} \tag{2.12}$$

Equations (2.11) and (2.12) imply that $\langle -g_i, p_i\rangle \ge k_1\|g_i\|^2$, $k_1 = 1 - \Theta$. Next by construction, $f(x_i + \delta_i p_i) < f(x_i)$. Therefore $f(x_{i+1}) < f(x_i)\ \forall i$. By Taylor's theorem, then,[1]

$$\begin{aligned} 0 > f(x_{i+1}) - f(x_i) &= f(x_i + \alpha_i p_i) - f(x_i) \\ &= \alpha_i\langle g_i, p_i\rangle + \tfrac{1}{2}\alpha_i^2\langle p_i, Q(\xi_i) p_i\rangle, \qquad \xi_i \in L(x_i, x_{i+1}) \\ &\ge -\alpha_i\|g_i\|\,\|p_i\| + \tfrac{1}{2}\alpha_i^2\mu\|p_i\|^2. \end{aligned}$$

Hence

$$\alpha_i \le \frac{2}{\mu}\frac{\|g_i\|}{\|p_i\|}. \tag{2.13}$$

Now by Taylor's formula,

$$g_{i+1} = g_i + \int_0^1 Q(x_i + t\alpha_i p_i)\alpha_i p_i\, dt.$$

[1] $L(x_i, x_{i+1})$ denotes the linear segment connecting x_i and x_{i+1}.

$$\therefore \|g_{i+1}\| \le \|g_i\| + \lambda\alpha_i\|p_i\|. \tag{2.14}$$

Equations (2.13) and (2.14) imply that

$$\|g_{i+1}\| \le \left(1 + \frac{2\lambda}{\mu}\right)\|g_i\|. \tag{2.15}$$

$$\therefore \beta_i \le k_2 = \left(1 + \frac{2\lambda}{\mu}\right)^2.$$

Finally define $w(i): E_1 \to E_1$ such that $w(i) = 0$ if $i \in I_q$, and $w(i) = 1$ otherwise.

Then

$$\|p_{i+1}\| \le \|g_{i+1}\| + \beta_i\|p_i\| = \|g_{i+1}\| + w(i+1)\frac{\|g_{i+1}\|^2}{\|g_i\|^2}\|p_i\|$$

$$\le \cdots$$

$$\le \|g_{i+1}\|\left[1 + \sum_{k=i_0}^{i}\left(\prod_{j=k}^{i} w(j+1)\right)\frac{\|g_{i+1}\|}{\|g_k\|}\right],$$

where i_0 is the largest number not exceeding i that is congruent to zero modulo q. But $\prod_{j=k}^{i} w(j+1)$ is 0 if $i+1 \in I_q$ and is 1 otherwise, and

$$\frac{\|g_{i+1}\|}{\|g_k\|} \le \left(1 + \frac{2\lambda}{\mu}\right)^{i+1-k} \le \left(1 + \frac{2\lambda}{\mu}\right)^q \text{ by (2.15).}$$

Hence

$$\|p_{i+1}\| \le k_4\|g_{i+1}\|, \qquad k_4 = 1 + \left(1 + \frac{2\lambda}{\mu}\right)^q q.$$

If $i + 1 = 0$ (modulo q), the result is immediate. The left-hand side of (2.10) is the immediate consequence of (2.8). Clearly $k_3 = k_1 = 1 - \Theta$. Q.E.D.

It is easy to show that $S(x_0)$ is compact from the assumptions. Hence $f(x)$ achieves its minimum on $S(x_0)$. Let z be the unique minimizer. Then the following lemma can be stated.

Lemma 2.2: For $i = 0,1,2,\cdots$,

$$\|g_i\| \ge \mu\|x_i - z\|$$
$$\|g_i\|^2 > \mu(f(x_i) - f(z)) \;\forall\; x_i \in S(x_0). \qquad \square$$

This lemma holds regardless of the accuracy of one-dimensional search. For a proof, see e.g., [5, pp. 37–38].

Now we state a convergence theorem for this algorithm.

Theorem 2.1:

1) The sequence $\{f(x_i)\}$ converges downward to $f(z)$.
2) The sequence $\{x_i\}$ converges to z. $\square$

Proof: Suppose that $f(x_i)$ does not converge to $f(z)$. Then by Lemma 2.2, $\|g_i\|$ is bounded away from zero for all i, i.e., there exists an $m > 0$ such that $\|g_i\| \ge m \;\forall\; i$.

$$\therefore \langle -g_i, p_i\rangle \ge (1 - \Theta)\|g_i\|^2 \ge k_1 m^2. \tag{2.16}$$

Let $M = \max\{\|g(x)\| : x \in S(x_0)\}$. Clearly M is bounded. From (2.10), then,

$$\|p_i\| \le k_4 M. \tag{2.17}$$

Substituting (2.16) and (2.17) into (2.3), we get

$$\delta_i = c\frac{\langle -g_i, p_i\rangle}{\|p_i\|^2} \ge \frac{ck_1m^2}{(k_4M)^2}. \tag{2.18}$$

Then

$$f(x_i + \delta_i p_i) = f(x_i) + \delta_i\langle g_i, p_i\rangle + \frac{\delta_i^2}{2}\langle p_i, Q(\xi_i)p_i\rangle,$$
$$\xi_i \in L(x_i, x_i + \delta_i p_i)$$
$$\le f(x_i) - \tfrac{1}{2}\delta_i\langle -g_i, p_i\rangle$$
$$\le f(x_i) - \tfrac{1}{2}R, \qquad R = ck_1^2m^4/k_4^2M^2. \tag{2.19}$$
$$\therefore f(x_{i+1}) \le f(x_i + \delta_i p_i) \le f(x_i) - \tfrac{1}{2}R,$$

which implies that $f(x_i) \to -\infty$ as $i \to \infty$. This is a contradiction. Hence $f(x_i) \to f(z)$.

Next, since $f(x_i)$ converges to $f(z)$, given any $\epsilon > 0$, there exists an integer $N > 0$ such that

$$f(x_i) - f(z) < \epsilon \;\forall\; i > N. \tag{2.20}$$

By Taylor's theorem,

$$f(x_i) = f(z) + \langle g(z), x_i - z\rangle + \tfrac{1}{2}\langle x_i - z, Q(\xi)(x_i - z)\rangle,$$
$$\xi \in L(x_i, z)$$
$$\ge f(z) + \tfrac{1}{2}\mu\|x_i - z\|^2. \tag{2.21}$$

Equations (2.20) and (2.21), then, imply that

$$\epsilon > \tfrac{1}{2}\mu\|x_i - z\|^2 \;\forall\; i > N,$$

i.e.,

$$\|x_i - z\| < \sqrt{\frac{2}{\mu}\epsilon} \;\forall\; i > N.$$

This holds for all ϵ. Hence x_i converges to z. Q.E.D.

Now we state a theorem on the rate of convergence.

Theorem 2.2—(Linear Convergence): The modified conjugate gradient reset method converges to z at least linearly, i.e., there exist scalars K_1 and $K_2 \in (0, \infty)$ and t_1 and $t_2 \in (0,1)$ such that for $i = 0,1,2,\cdots$,

$$f(x_i) - f(z) \le K_1 t_1^{\,i};$$
$$\|x_i - z\| \le K_2 t_2^{\,i}. \qquad \square$$

Proof: Let $\Delta_i = f(x_i + \alpha_i p_i) - f(x_i)$. Then by (2.3), (2.4), (2.5), and (2.19),

$$\Delta_i \le -c\langle -g_i, p_i\rangle^2/2\|p_i\|^2$$
$$\le -ck_1^2\|g_i\|^2/2k_4^2 \text{ by (2.8) and (2.10).}$$

Therefore, by Lemma 2.2,

$$f(x_{i+1}) - f(x_i) \le -ck_1^2\mu^2\|x_i - z\|^2/2k_4^2. \tag{2.22}$$

Now from Taylor's theorem and the assumption on $Q(x)$, it is easily shown that

$$\mu\|x_i - z\|^2 \le 2(f(x_i) - f(z)) \le \lambda\|x_i - z\|^2. \tag{2.23}$$

Equations (2.22) and (2.23), then, imply that

$$f(x_{i+1}) - f(x_i) \leq -ck_1{}^2\mu^2(f(x_i) - f(z))/k_4{}^2\lambda$$
$$= -t(f(x_i) - f(z)),$$
$$t = ck_1{}^2\mu^2/k_4{}^2\lambda. \quad (2.24)$$

Hence

$$f(x_i) - f(z) \leq K_1t_1{}^i, \quad (2.25)$$

where $K_1 = f(x_0) - f(z)$, and $t_1 = 1 - t$. It is easily shown that $t_1 \in (0,1)$. Finally (2.25) and (2.23) imply that

$$\|x_i - z\|^2 \leq \frac{2}{\mu}(f(x_i) - f(z)) \leq \frac{2}{\mu}K_1t_1{}^i.$$
$$\therefore \|x_i - z\| \leq K_2t_2{}^i, \quad (2.26)$$

where $K_2 = \sqrt{2K_1/\mu}$ and $t_2 = \sqrt{t_1}$. Q.E.D.

III. An n-Step Quadratic Convergent Implementation of the Conjugate Gradient Reset Method

The convergent implementation of the previous section has the very nice feature that it maintains, within a fixed limit, the precision with which the minimization of $|\langle -g(x_i + \alpha p_i),p_i\rangle/\|g_i\|^2|$ is carried out at each step. However, it can only be shown to converge linearly. If we wish to ensure a faster convergence, then we must make the one-dimensional search progressively more precise. In the sequel we propose one such modification.

In addition to the earlier assumptions, we assume that $f(\cdot)$ is three times continuously differentiable and we modify the conjugate gradient reset method so that the one-dimensional search is stopped when the following conditions are satisfied:

$$\gamma_{ij} \geq \delta_i \quad (3.1)$$

$$f(x_i + \gamma_{ij}p_i) \leq f(x_i + \delta_ip_i) \quad (3.2)$$

$$\epsilon_{ij} \leq \frac{\Theta_i\|g_i\|^2}{\|g_{ij}\|\,\|p_i\|}, \quad (3.3)$$

where $0 < \Theta_i < \min\{1,\|p_i\|\}$. As before, when a j is found satisfying (3.1)–(3.3), we set $\alpha_i = \gamma_{ij}$ and g_{ij} becomes g_{i+1}. Note that these are very similar to (2.4)–(2.6). The only difference is the condition (3.3), in which Θ_i goes to zero as i goes to infinity. Again this method is well defined.

To establish an n-step quadratic convergence, we use a procedure similar to that of Cohen's [1] for the conjugate gradient algorithm with the exact one-dimensional search. Basically, the approach consists of establishing the rate of convergence of our algorithm by means of a suitable comparison with the Newton–Raphson method, a pattern of proof first used by Daniel [2].

Definition: Let $\{x_i\}$ be a sequence generated by the modified conjugate gradient reset method with α_i determined by (3.1)–(3.3). For each $i \in I_q$, define the quadratic function $f_i(x)$ by

$$f_i(x) = f(x_i) + \langle g(x_i), x - x_i\rangle + \tfrac{1}{2}\langle x - x_i, Q(x_i)(x - x_i)\rangle. \quad (3.4)$$

Then for each $i \in I_q$, we shall denote by $\overset{j}{x}_i$, $\overset{j}{g}_i$, $\overset{j}{p}_i$, $\overset{j}{\alpha}_i$, and $\overset{j}{\beta}_i$, $j = 0,1,2,\cdots,v(i)$, the quantities constructed by the conjugated gradient reset algorithm with the exact one-dimensional search when applied to the problem $\min\{f_i(z): z \in E_n\}$ with $\overset{0}{x}_i = x_i$ and with $v(i)$ determined so that $\overset{v(i)}{g}_i = 0$ and $\overset{v(i)-1}{g}_i \neq 0$. Since $q \geq n$ and $f_i(\cdot)$ quadratic, $v(i) \leq n$ and $\overset{i}{x}_i \equiv \overset{v(i)}{x}_i$ and $\overset{j}{g}_i = \overset{j}{p}_i = 0$ for $j > v(i)$.

We shall denote by $0_k(\cdot):E_1 \to E_1$, $k = 1,2,\cdots,13$, functions with the property that for each k, there exist an $\epsilon_k > 0$ and an $r_k > 0$ such that

$$|0_k(t)/t| \leq r_k \text{ for all } |t| < \epsilon_k. \quad (3.5)$$

First the following three lemmas are needed.

Lemma 3.1: For $i = 0,1,2,\cdots$, there exist scalars c_1 through c_7 in $(0,\infty)$ such that

$$\langle -g_i,p_i\rangle \geq c_1\|g_i\|^2 \quad (3.6)$$

$$\beta_i \leq c_2 \quad (3.7)$$

$$c_3\|g_i\| \leq \|p_i\| \leq c_4\|g_i\| \quad (3.8)$$

$$\alpha_i \leq c_5 \quad (3.9)$$

$$\|g_{i+1}\| \leq c_6\|p_i\| \quad (3.10)$$

$$\|p_{i+1}\| \leq c_7\|p_i\|. \quad \square \quad (3.11)$$

Proof: Equations (3.6)–(3.8) are proved exactly the same as before by replacing Θ by Θ_i. Now by (2.13) and (3.8), we obtain

$$\alpha_i \leq \frac{2}{\mu}\frac{\|g_i\|}{\|p_i\|} \leq c_5, \qquad c_5 = \frac{2}{\mu c_3}.$$

Next,

$$\|g_{i+1}\| \leq \|g_{i+1} - g_i\| + \|g_i\| \leq c_5\lambda\|p_i\| + \frac{1}{c_3}\|p_i\| = c_6\|p_i\|.$$

Finally,

$$\|p_{i+1}\| \leq \|g_{i+1}\| + \beta_i\|p_i\| \leq c_6\|p_i\| + c_2\|p_i\| = c_7\|p_i\|.$$

Q.E.D.

Lemma 3.2: For $i \in I_q$ and $j = 0,1,\cdots,n-1$,

$$\|\overset{j+1}{g}_i\| \leq \left(1 + \frac{\lambda}{\mu}\right)\|\overset{j}{p}_i\|. \quad \square \quad (3.12)$$

This is the immediate consequence of the inequality

$$\|\overset{j+1}{g}_i\| \leq \left(1 + \frac{\lambda}{\mu}\right)\|\overset{j}{g}_i\|. \quad (3.13)$$

Lemma 3.3: Let $Q_i = \int_0^1 Q(x_i + t\alpha_i p_i)\, dt$. For $i \in I_q$ and $j = 0,1,\cdots,n-1$,

$$\|Q(x_{i+j}) - Q(x_i)\| \le 0_1(\|p_i\|) \tag{3.14}$$

$$\|Q_{i+j} - Q(x_i)\| \le 0_2(\|p_i\|) \tag{3.15}$$

$$\|p_{i+j+1} - \overset{j+1}{p_i}\| \le 0_3(\|p_{i+j} - \overset{j}{p_i}\|) + 0_4(\|g_{i+j+1} - \overset{j+1}{g_i}\|) + 0_5(\|g_{i+j} - \overset{j}{g_i}\|) + 0_6(\|p_i\|^2) \tag{3.16}$$

$$\|g_{i+j+1} - \overset{j+1}{g_i}\| \le \|g_{i+j} - \overset{j}{g_i}\| + 0_7(\|p_i\|^2) + \lambda\|\alpha_{i+j}p_{i+j} - \overset{j}{\alpha_i}\overset{j}{p_i}\| \tag{3.17}$$

$$\|\alpha_{i+j}p_{i+j} - \overset{j}{\alpha_i}\overset{j}{p_i}\| \le 0_8(\|g_{i+j} - \overset{j}{g_i}\|) + 0_9(\|p_{i+j} - \overset{j}{p_i}\|) + 0_{10}(\|p_i\|^2) \tag{3.18}$$

$$\|g_{i+j} - \overset{j}{g_i}\| \le 0_{11}(\|p_i\|^2) \tag{3.19}$$

$$\|p_{i+j} - \overset{j}{p_i}\| \le 0_{12}(\|p_i\|^2) \tag{3.20}$$

$$\|\alpha_{i+j}p_{i+j} - \overset{j}{\alpha_i}\overset{j}{p_i}\| \le 0_{13}(\|p_i\|^2). \quad \square \tag{3.21}$$

The proof is similar to that in Polak's book [8, pp. 263–267]. First note that since f is three times continuously differentiable and the sequence $\{x_i\}$ converges strongly to z, there exists a scalar B in $(0,\infty)$ such that

$$\|g''(x_{i+k} + t\alpha_{i+k}p_{i+k})\| \le B \tag{3.22}$$

for $i = 0,1,2,\cdots$, and all t in $[0,1]$, where $g''(\cdot)$ is the second derivative of $g(\cdot)$ with respect to t.

Now the first inequality (3.14) can be proved by using (3.11), (3.22), and the two inequalities

$$\|Q(x_{i+j}) - Q(x_i)\| \le \sum_{k=0}^{j-1} \|Q(x_{i+k+1}) - Q(x_{i+k})\| \tag{3.23}$$

and

$$\|Q(x_{i+k+1}) - Q(x_{i+k})\| \le d_1\|p_{i+k}\|. \tag{3.24}$$

Next, (3.15) can be proved by (3.11), (3.14), and the inequality

$$\|Q_{i+j} - Q(x_{i+j})\| < d_2\|p_{i+j}\|. \tag{3.25}$$

Equation (3.16) is the most complicated. First note that for $i \in I_q$, $j = n-1$ and $q = n$,

$$\|p_{i+n} - \overset{n}{p_i}\| = \|-g_{i+n} + \overset{n}{g_i}\|. \tag{3.26}$$

And for either $q > n$ and $j \in \{1,2,\cdots,n-1\}$ or $q = n$ and $j \in \{0,1,2,\cdots,n-2\}$,

$$\|p_{i+j+1} - \overset{j+1}{p_i}\| \le \|-g_{i+j+1} + \overset{j+1}{g_i}\| + \|\beta_{i+j}p_{i+j} - \overset{j}{\beta_i}\overset{j}{p_i}\|. \tag{3.27}$$

Now for $j = 0,1,\cdots,v(i)-1$, it is easily shown (e.g., [2]) that

$$\overset{j}{\beta_i} = 1 + \frac{\langle \overset{j+1}{g_i} + \overset{j}{g_i}, Q(x_i)\overset{j}{p_i}\rangle}{\langle \overset{j}{p_i}, Q(x_i)\overset{j}{p_i}\rangle}. \tag{3.28}$$

Next,

$$\beta_{i+j} = \frac{\|g_{i+j+1}\|^2}{\|g_{i+j}\|^2} = \frac{\langle g_{i+j+1} - g_{i+j}, g_{i+j+1}\rangle + \langle g_{i+j+1}, g_{i+j}\rangle}{\|g_{i+j}\|^2}. \tag{3.29}$$

But

$$g_{i+j+1} = g_{i+j} + \alpha_{i+j}Q_{i+j}p_{i+j}$$

and

$$\alpha_{i+j} = \langle g_{i+j+1} - g_{i+j}, p_{i+j}\rangle / \langle p_{i+j}, Q_{i+j}\, p_{i+j}\rangle.$$

Therefore,

$$\frac{\langle g_{i+j+1} - g_{i+j}, g_{i+j+1}\rangle}{\|g_{i+j}\|^2} = S_{i+j} - U_{i+j} + \frac{\langle g_{i+j+1}, Q_{i+j}\, p_{i+j}\rangle}{\langle p_{i+j}, Q_{i+j}\, p_{i+j}\rangle}, \tag{3.30}$$

where

$$S_{i+j} \triangleq \langle g_{i+j+1}, Q_{i+j}\, p_{i+j}\rangle \langle g_{i+j+1}, p_{i+j}\rangle / \|g_{i+j}\|^2 \langle p_{i+j}, Q_{i+j}\, p_{i+j}\rangle$$

$$U_{i+j} \triangleq \beta_{i+j-1} \langle g_{i+j+1}, Q_{i+j}\, p_{i+j}\rangle \langle g_{i+j}, p_{i+j-1}\rangle / \|g_{i+j}\|^2 \langle p_{i+j}, Q_{i+j}\, p_{i+j}\rangle, \tag{3.31}$$

and

$$\frac{\langle g_{i+j+1}, g_{i+j}\rangle}{\|g_{i+j}\|^2} = 1 + \alpha_{i+j}\frac{\langle g_{i+j}, Q_{i+j}\, p_{i+j}\rangle}{\|g_{i+j}\|^2} = 1 + S'_{i+j} - U'_{i+j} + \frac{\langle g_{i+j}, Q_{i+j}\, p_{i+j}\rangle}{\langle p_{i+j}, Q_{i+j}\, p_{i+j}\rangle}, \tag{3.32}$$

where

$$S'_{i+j} \triangleq \langle g_{i+j}, Q_{i+j}\, p_{i+j}\rangle \langle g_{i+j+1}, p_{i+j}\rangle / \|g_{i+j}\|^2 \langle p_{i+j}, Q_{i+j}\, p_{i+j}\rangle$$

$$U'_{i+j} \triangleq \beta_{i+j-1} \langle g_{i+j}, Q_{i+j}\, p_{i+j}\rangle \langle g_{i+j}, p_{i+j-1}\rangle / \|g_{i+j}\|^2 \langle p_{i+j}, Q_{i+j}\, p_{i+j}\rangle. \tag{3.33}$$

Hence from (3.28), (3.29), (3.30), and (3.32), we obtain

$$\|\beta_{i+j}\, p_{i+j} - \overset{j}{\beta_i}\overset{j}{p_i}\| \le \|p_{i+j} - \overset{j}{p_i}\| + \|(S_{i+j} + S'_{i+j})p_{i+j}\| + \|(U_{i+j} + U'_{i+j})\, p_{i+j}\| + \|V_{i+j}\|, \tag{3.34}$$

where

$$V_{i+j} \triangleq \frac{\langle g_{i+j+1} + g_{i+j}, Q_{i+j}\, p_{i+j}\rangle}{\langle p_{i+j}, Q_{i+j}\, p_{i+j}\rangle} p_{i+j} - \frac{\langle \overset{j+1}{g_i} + \overset{j}{g_i}, Q(x_i)\overset{j}{p_i}\rangle}{\langle \overset{j}{p_i}, Q(x_i)\, \overset{j}{p_i}\rangle} \overset{j}{p_i}. \tag{3.35}$$

Using (3.3), (3.10), and (3.11), we can then show that $\|S_{i+j}\, p_{i+j}\|$, $\|S'_{i+j}\, p_{i+j}\|$, $\|U_{i+j}\, p_{i+j}\|$, and $\|U'_{i+j}\, p_{i+j}\|$ are all bounded above by $d_1\|p_i\|^2$ for some $d_1 < \infty$. As for $\|V_{i+j}\|$, let $C_{i+j} = \langle p_{i+j}, Q_{i+j}\, p_{i+j}\rangle\langle \overset{j}{p_i}, Q(x_i)\, \overset{j}{p_i}\rangle$.

Then

$$\begin{aligned}\|V_{i+j}\| \le \frac{1}{C_{i+j}} [&\|\langle g_{i+j+1}, Q_{i+j}(p_{i+j} - \overset{j}{p}_i)\rangle \\ &\cdot \langle \overset{j}{p}_i, Q(x_i)\, \overset{j}{p}_i\rangle p_{i+j}\| \\ &+ \|\langle g_{i+j+1}, Q_{i+j}\overset{j}{p}_i\rangle\langle \overset{j}{p}_i - p_{i+j}, Q(x_i)\overset{j}{p}_i\rangle p_{i+j}\| \\ &+ \|\langle g_{i+j+1} - \overset{j+1}{g}_i, Q_{i+j}\overset{j}{p}_i\rangle\langle p_{i+j}, Q(x_i)\overset{j}{p}_i\rangle p_{i+j}\| \\ &+ \|\langle \overset{j+1}{g}_i, Q_{i+j}\overset{j}{p}_i\rangle\langle p_{i+j}, Q(x_i)(\overset{j}{p}_i - p_{i+j})\rangle p_{i+j}\| \\ &+ \|\langle \overset{j+1}{g}_i, (Q_{i+j} - Q(x_i))\,\overset{j}{p}_i\rangle\langle p_{i+j}, Q(x_i)\, p_{i+j}\rangle p_{i+j}\| \\ &+ \|\langle \overset{j+1}{g}_i, Q(x_i)\,\overset{j}{p}_i\rangle\langle p_{i+j}, (Q(x_i) - Q_{i+j})\, p_{i+j}\rangle p_{i+j}\| \\ &+ \|\langle \overset{j+1}{g}_i, Q(x_i)\,\overset{j}{p}_i\rangle\langle p_{i+j}, Q_{i+j}\, p_{i+j}\rangle(p_{i+j} - \overset{j}{p}_i)\| \\ &+ \|\langle g_{i+j}, Q_{i+j}\,(p_{i+j} - \overset{j}{p}_i)\rangle\langle \overset{j}{p}_i, Q(x_i)\,\overset{j}{p}_i\rangle p_{i+j}\| \\ &+ \|\langle g_{i+j}, Q_{i+j}\,\overset{j}{p}_i\rangle\langle \overset{j}{p}_i - p_{i+j}, Q(x_i)\,\overset{j}{p}_i\rangle p_{i+j}\| \\ &+ \|\langle g_{i+j} - \overset{j}{g}_i, Q_{i+j}\,\overset{j}{p}_i\rangle\langle p_{i+j}, Q(x_i)\,\overset{j}{p}_i\rangle p_{i+j}\| \\ &+ \|\langle \overset{j}{g}_i, Q_{i+j}\,\overset{j}{p}_i\rangle\langle p_{i+j}, Q(x_i)(\overset{j}{p}_i - p_{i+j})\rangle p_{i+j}\| \\ &+ \|\langle \overset{j}{g}_i, (Q_{i+j} - Q(x_i))\overset{j}{p}_i\rangle\langle p_{i+j}, Q(x_i)\, p_{i+j}\rangle p_{i+j}\| \\ &+ \|\langle g_i, Q(x_i)\, p_i\rangle\langle p_{i+j}, (Q(x_i) - Q_{i+j})\, p_{i+j}\rangle p_{i+j}\| \\ &+ \|\langle \overset{j}{g}_i, Q(x_i)\,\overset{j}{p}_i\rangle\langle p_{i+j}, Q_{i+j}\, p_{i+j}\rangle(p_{i+j} - \overset{j}{p}_i)\|\,].\end{aligned} \tag{3.36}$$

Noting that $C_{i+j} \ge \mu^2\|p_{i+j}\|^2\|\overset{j}{p}_i\|^2$ and using (3.10), (3.11), and Lemma 3.2, we obtain

$$\begin{aligned}\|V_{i+j}\| \le\ & d_2\|p_{i+j} - \overset{j}{p}_i\| + d_3\|g_{i+j+1} - \overset{j+1}{g}_i\| \\ &+ d_4\|Q_{i+j} - Q(x_i)\|\,\|p_{i+j}\| + d_5\|g_{i+j} - \overset{j}{g}_i\|.\end{aligned} \tag{3.37}$$

Hence (3.16) holds for all $i \in I_q$ and $j = 0,1,\cdots,v(i) - 1$. For $j = v(i), v(i) + 1,\cdots,n - 1$, $\overset{j}{p}_i = \overset{j}{g}_i = 0$. Hence (3.16) becomes

$$\|p_{i+j+1}\| \le 0_3(\|p_{i+j}\|) + 0_4(\|g_{i+j+1}\|) + 0_5(\|g_{i+j}\|) + 0_6(\|p_i\|^2).$$

This obviously is true since from (3.11), we have

$$\|p_{i+j+1}\| \le 0_3(\|p_{i+j}\|).$$

Hence (3.16) holds for all $i \in I_q$ and $j = 0,1,\cdots,n - 1$.

The proof of (3.17) follows exactly that of [8, lemma 4, p. 265]. Next, for $j = 0,1,\cdots,v(i) - 1$,

$$\|\alpha_{i+j}\, p_{i+j} - \overset{j}{\alpha}_i\overset{j}{p}_i\| \le \|a_{i+j}\| + \|b_{i+j}\|, \tag{3.38}$$

where

$$\begin{aligned} a_{i+j} &\triangleq (\langle g_{i+j+1}, p_{i+j}\rangle/\langle p_{i+j}, Q_{i+j}p_{i+j}\rangle)\, p_{i+j} \\ b_{i+j} &\triangleq (\langle -g_{i+j}, p_{i+j}\rangle/\langle p_{i+j}, Q_{i+j}p_{i+j}\rangle)p_{i+j} \\ &\quad - (\langle -\overset{j}{g}_i, \overset{j}{p}_i\rangle/\langle \overset{j}{p}_i, Q(x_i)\,\overset{j}{p}_i\rangle)\overset{j}{p}_i.\end{aligned} \tag{3.39}$$

But

$$\|a_{i+j}\| \le \frac{\|g_{i+j}\|\,\|p_{i+j}\|}{\mu\|p_{i+j}\|^2}\|p_{i+j}\| \le d_6\|p_i\| \tag{3.40}$$

by (3.10) and (3.11) and, by proceeding similarly as in (3.36), we obtain

$$\|b_{i+j}\| \le d_7\|p_{i+j} - \overset{j}{p}_i\| + d_8\|g_{i+j} - \overset{j}{g}_i\| + d_9 0_2(\|p_i\|)\,\|p_i\|. \tag{3.41}$$

Equations (3.38), (3.40), and (3.41), then, imply (3.18). For $j = v(i), v(i) + 1,\cdots,n - 1$, (3.18) becomes

$$\|\alpha_{i+j}p_{i+j}\| \le 0_8(\|g_{i+j}\|) + 0_9(\|p_{i+j}\|) + 0_{10}(\|p_i\|^2).$$

This obviously holds since from (3.9), we have

$$\|\alpha_{i+j}\, p_{i+j}\| \le 0_9(\|p_{i+j}\|).$$

Therefore (3.18) holds for all $i \in I_q$ and $j = 0,1,\cdots,n - 1$.

Inequalities (3.19)–(3.21) can now be proved by induction. Clearly they hold for $j = 0$ and for any $i \in I_q$ from (3.18) and because $\overset{0}{g}_i = g_i$ and $\overset{0}{p}_i = p_i$.

Now suppose that (3.19)–(3.21) hold for any $j' \in \{0,1,\cdots,n - 2\}$ and $i \in I_q$. Then, replacing j' by $j' + 1$ in (3.17), we get

$$\begin{aligned}\|g_{i+j'+1} - \overset{j'+1}{g}_i\| \le\ & \|g_{i+j'} - \overset{j'}{g}_i\| + 0_7(\|p_i\|^2) \\ &+ \lambda\|\alpha_{i+j'}p_{i+j'} - \overset{j'}{\alpha}_i\overset{j'}{p}_i\|.\end{aligned} \tag{3.42}$$

Equation (3.42) with (3.19) and (3.21) for $j = j'$ implies that (3.19) must be true for $j = j' + 1$.

Next, using (3.16) for $j = j'$, we get

$$\begin{aligned}\|p_{i+j'+1} - \overset{j'+1}{p}_i\| \le\ & 0_3(\|p_{i+j'} - \overset{j'}{p}_i\|) + 0_4(\|g_{i+j'+1} - \overset{j'+1}{g}\|) \\ &+ 0_5(\|g_{i+j'} - \overset{j'}{g}_i\|) + 0_6(\|p_i\|^2).\end{aligned} \tag{3.43}$$

Making use of (3.20) for $j = j'$ and of (3.19) for $j = j'$ and $j = j' + 1$, we find that (3.43) implies (3.20) for $j = j' + 1$. Finally, setting $j = j' + 1$ in (3.18) and making use of (3.19) and (3.20) for $j = j' + 1$, we find that (3.21) must be true for $j = j' + 1$. Q.E.D.

Now we can state a theorem on the rate of convergence.

Theorem 3.1—(n-Step Quadratic Convergence): Suppose that the function $f(\cdot)$ is three times continuously differentiable and that the spectrum of $Q(\cdot) = \partial^2 f(\cdot)/\partial x^2$ is bounded below and above by $\mu > 0$ and λ respectively. Consider the sequence $\{x_i\}$ generated by the modified conjugate gradient reset method with α_i determined by (3.1)–(3.3) when applied to the problem $\min\{f(z) : z \in E_n\}$. Then there exists an integer $N' > 0$ and $h \in (0,\infty)$ such that

$$\|x_{i+n} - z\| \le h\|x_i - z\|^2 \tag{3.44}$$

for all $i \ge N'$, $i \in I_q$. □

Proof: By Taylor's formula,

$$g(x_i) = g(z) + \int_0^1 Q(x_i + t(x_i - z)\, dt.$$

$$\therefore \|g_i\| = \lambda\|x_i - z\|. \tag{3.45}$$

Since $x_i \to z$, $\|g_i\| \to 0$. Hence by (3.8), $\|p_i\| \to 0$. Therefore (3.21), (3.5), (3.8), and (3.45) imply that there must exist an integer $N'' > 0$ and $h' \in (0, \infty)$ such that

$$\|\alpha_{i+j} p_{i+j} - \alpha_i p_i\| \le h'\|x_i - z\|^2 \tag{3.46}$$

holds for $j \in \{0, 1, \cdots, n-1\}$ and all $i \in I_q$ greater than or equal to N''. The remainder of the proof follows exactly that of [1, theorem 8, p. 67].

IV. Conclusion

Two modifications of the Fletcher–Reeves conjugate gradient reset method were proposed that provide for finite termination of the one-dimensional search at each iteration. It was shown that linear convergence is retained for the first and n-step quadratic for the second. Since it is not possible, in general, to perform the one-dimensional minimization exactly, these results give an indication of how one can specify an implementable algorithm.

There are two apparent difficulties with the proposed algorithm, the apparent need to know an upper bound on the Hessian matrix of $f(x)$ and the need to evaluate the gradient for each trial step size in the one-dimensional search. δ_i, however, is used only to guarantee sufficient reduction at each step to assure convergence, and in Section II, to assist in determining a linear rate. Its only function in achieving n-step quadratic convergence is to assure convergence. As noted by one of the reviewers, any other method of assuring sufficient improvement at each step would also suffice. There are several that would work without requiring knowledge of bounds on the Hessian. For example, a variation of the method by Armijo [9] will work. In this case it is possible to make the comparison on α_i directly, and parameters can be loosely chosen so that this will seldom cause more of a restriction than (3.3).

The need to evaluate the gradient for each trial step size is more serious. For high-dimensional problems this can be very costly, as usually several trials are required to find an acceptable step size. One ad hoc improvement would be to impose some easily performed subsidiary test that must be met at each iteration before the test of (3.3) is begun. One possibility would be to proceed with a fixed number of trials first, say three. Clearly, however, this is an area in which further work is needed.

References

[1] A. I. Cohen, "Rate of convergence of several gradient algorithms," *SIAM J. Numer. Anal.*, vol. 9, pp. 248–259, 1972.

[2] J. W. Daniel, "The conjugate gradient method for linear and nonlinear operator equations," *SIAM J. Numer. Anal.*, vol. 41, pp. 10–26, 1967.

[3] ——, "Convergence of the conjugate gradient method with computationally convenient modifications," *Numer. Math.*, vol. 10, pp. 125–131, 1967.

[4] R. Fletcher and C. M. Reeves, "Function minimization by conjugate gradients," *Comput. J.*, pp. 149–154, 1964.

[5] K. Kawamura, "Study of the conjugate gradient method and its application to the constrained minimization problems," Ph.D. dissertation, Univ. Mich., Ann Arbor, 1972.

[6] R. Klessig and E. Polak, "Efficient implementations of the Polak–Ribière conjugate gradient algorithm," *SIAM J. Contr.*, vol. 10, pp. 524–549, 1972.

[7] J. M. Ortega and W. C. Rheinboldt, *Iterative Solution of Nonlinear Equations in Several Variables.* New York: Academic, 1970.

[8] E. Polak, *Computational Methods in Optimization, A Unified Approach.* New York, Academic, 1971.

[9] L. Armijo, "Minimization of functions having continuous partial derivatives," *Pac. J Math.*, vol. 16, pp. 1–3, 1966.

Kazuhiko Kawamura (S'73–M'73) was born in Nagoya, Japan, in 1939. He received the B.E. degree in electrical engineering from Waseda University, Tokyo, Japan, in 1963, the M.S.E.E. degree from the University of California, Berkeley, in 1966, and the Ph.D. degree in electrical engineering from the University of Michigan, Ann Arbor, in 1972.

He was a Research Assistant both in the Electronics Research Laboratory at the University of California and in the Systems Engineering Laboratory at the University of Michigan. From 1968 to 1971, he was associated with the Institute for Burn Medicine, Ann Arbor, Mich., as a system analyst. Presently he is a Lecturer in Electrical Engineering at the University of Michigan-Dearborn, and has taught courses in modern control theory and nonlinear control systems. His research interests include control, optimization, and the application of system theory to social science.

Dr. Kawamura is a member of Eta Kappa Nu, Sigma Xi, and the Society of Instrument and Control Engineers of Japan.

Richard A. Volz (M'60) was born in Woodstock, Ill., on July 10, 1937. He received the B.S. degree in electrical engineering from Northwestern University, Evanston, Ill., in 1960, and pursued his graduate studies there under a National Science Foundation Fellowship, receiving the M.S. and Ph.D. degrees in 1961 and 1964, respectively.

In 1964 he joined the staff at the University of Michigan, Ann Arbor, where he has worked on optimal discrete control, radio navigation, multipath problems in high-frequency radar systems, computer-aided design, and hybrid computation. His current interests include computational methods of optimization and hybrid computation. He is currently an Associate Professor in the Department of Electrical and Computer Engineering and Chairman of the Systems Engineering Laboratory at the University of Michigan, Ann Arbor.