

Superlinear convergence of conjugate gradient method

by

ZENON FORTUNA

Technical University of Warsaw
Institute of Automatic Control

For the case of minimizing a quadratic functional in a real Hilbert space with Hessian $A = A_1 + A_2$, where A_1 is an algebraic operator and A_2 is a compact operator, superlinear convergence of the Conjugate Gradient Method is obtained. An example of a functional of such a type is encountered in an optimal control problem for a linear dynamic system with delays.

The Conjugate Gradient Method (CGM) has been used since its introduction by Hestenes [3] in many algorithms of numerical optimization. It was soon noticed that CGM is considerably better than the Steepest Descent Method (SDM). The theoretical evaluation, however, of the rate of convergence ($q_n = (Q_{n+1} - \hat{Q}) / (Q_n - \hat{Q})$, Q_n is suboptimal value of functional at the n -th step of iterations) for CGM remained no better than for SDM, i.e. when $\text{sp } A \subset [m, M]$, $m > 0$, then

$$q_n \leq \left(\frac{M-m}{M+m} \right)^2, \quad n=0, 1, \dots$$

In [1] can be found a better evaluation

$$q_n \leq \left(\frac{\sqrt{M} - \sqrt{m}}{\sqrt{M} + \sqrt{m}} \right)^2 + \varepsilon_n, \quad \varepsilon_n \rightarrow 0, \quad n=0, 1, \dots$$

but this is still linear convergence.

In this paper we show that for a wide class of minimized functionals we have, in fact, superlinear convergence of CGM, i.e., $\sqrt[n]{Q_n - \hat{Q}} \rightarrow 0$.

Problem. Let us have the following process:

$$\begin{aligned} \dot{x}(t) &= Dx(t) + Ex(t-h) + Fu(t), \\ x(t) &= \varphi(t) \text{ for } t \in [t_0 - h, t_0]. \end{aligned} \quad (1)$$

We want to find a control function \hat{u} which minimizes the functional

$$Q(u) = \frac{1}{2} \int_{t_0}^{t_1} [(x(t), Nx(t)) + (u(t), Ru(t))] dt \quad (2)$$

$N \geq 0$, $R > 0$, D, E, F — constant matrices.

Under these assumptions \hat{u} exists and is unique.

If we want to find the actual solution, we have to solve the two-point boundary-value problem. Usually we use iterative algorithms for this problem. It is easy to compute the gradient of functional (2) with constraints (1) so it is reasonable to choose the Conjugate Gradient Method. In the case of a problem with delays ($E \neq 0$) the numerical procedures typically converge more slowly than without delays. We want to show that these numerical difficulties decrease with the number of iterations, because in the general case of process (1), the CGM assures superlinear convergence.

In [2] we find the solution of equation (1)

$$x(t) = x_0(t) + \int_{t_0}^t K(t, \tau) Fu(\tau) d\tau,$$

where $x_0(t)$ is the trajectory generated by $u(t) = 0$ and $K(t, \tau)$ is a continuous function matrix. Let us denote $x(t)$ by the shorter notation

$$x = x_0 + Lu \quad (3)$$

where L is above-defined compact linear operator in space U of piece-wise continuous function $u(t)$ (Volterra's operator with continuous kernel). After substituting (3) into (2) we obtain

$$\begin{aligned} Q(u) &= \frac{1}{2} [\langle u, (R + L^* NL) u \rangle + \langle x_0, NLu \rangle + \langle u, L^* Nx_0 \rangle + \langle x_0, Nx_0 \rangle] = \\ &= \frac{1}{2} \langle u - \hat{u}, A(u - \hat{u}) \rangle + \hat{Q} \end{aligned}$$

where $\langle \dots \rangle$ denotes inner product in $L^2(t_1, t_2, R^n)$

$$A = R + L^* NL, u = -A^{-1} L^* Nx_0, \hat{Q} = Q(\hat{u}).$$

It is sufficient then to prove the following theorem:

We use CGM for minimization of the quadratic functional

$$Q(u) = \frac{1}{2} \langle u - \hat{u}, A(u - \hat{u}) \rangle, \quad (*)$$

$u \in H$ — real Hilbert space,

$A \in L(H)$ — set of linear bounded operators on H

sp $A \subset [m, 1]$, $m > 0$

$A = A_1 + A_2$

$A_1 > 0$, selfadjoint, $I + a_1 A_1 + a_2 A_1^2 + \dots + a_N A_1^N = 0$

$A_2 \geq 0$, compact, selfadjoint

(such an operator A_1 is called the algebraic operator).

The algorithm is the following

- (a) $\left\{ \begin{array}{l} 0. \text{ Choose } u_0 \text{ — start point; } i=0. \\ 1. \text{ Compute } g_i \text{ — gradient of } Q \text{ in point } u_i. \\ 2. \text{ Find } s_i = g_i + \alpha_{i-1} s_{i-1}; \alpha_{-1}=0, \text{ for } i>0 \alpha_{i-1} \text{ is such, that } \langle s_i, A s_{i-1} \rangle = 0. \\ 3. \text{ Find } u_{i+1} = u_i + \eta_i s_i \text{ where } \eta_i \text{ minimizes the function } f(\eta) = Q(u_i + \eta s_i). \\ 4. i := i+1, \text{ go to 1.} \end{array} \right.$

Let us denote $Q_i = Q(u_i)$.

THEOREM. $\sqrt[n]{Q_n} \rightarrow 0$ (superlinear convergence).

The theorem is proved with two lemmas.

LEMMA 1. $\lim_{k \rightarrow \infty} \frac{Q_{k+N}}{Q_k} = 0$.

Proof. It is a well known fact [1] that if we have directions s_0, s_1, \dots, s_{k-1} , then $Q_k = \frac{1}{2} \min_{z \in S_{k-1}} \langle g_0 - z, A^{-1}(g_0 - z) \rangle$ for $S_{k-1} = \text{lin} \{A s_0, A s_1, \dots, A s_{k-1}\}$. (Q_k is a suboptimal value of Q on subspace S_{k-1}).

From algorithm (a) it is easily seen that

$$S_{k-1} = \text{lin} \{A g_0, A^2 g_0, \dots, A^k g_0\}$$

and

$$\begin{aligned} Q_k &= \frac{1}{2} \min_{l_1 \dots l_k} \langle g_0 + l_1 A g_0 + \dots + l_k A^k g_0, A^{-1}(g_0 + \dots + l_k A^k g_0) \rangle = \\ &= \langle g_0 + c_1^{(k)} A g_0 + c_2^{(k)} A^2 g_0 + \dots + c_k^{(k)} A^k g_0, A^{-1}(\dots) \rangle = \langle g_k, A^{-1} g_k \rangle. \end{aligned}$$

When we change the coefficients $c_i^{(k)}$ in any way, the value of Q_k will increase, so

$$\begin{aligned} \frac{Q_{k+N}}{Q_k} &= \frac{\langle g_0 + c_1^{(k+N)} A g_0 + \dots + c_{k+N}^{(k+N)} A^{k+N} g_0, A^{-1}(\dots) \rangle}{\langle g_0 + c_1^{(k)} A g_0 + \dots + c_k^{(k)} A^k g_0, A^{-1}(\dots) \rangle} \leq \\ &\leq \frac{\langle (I + a_1 A + a_2 A^2 + \dots + a_N A^N)(g_0 + c_1^{(k)} A g_0 + \dots + c_k^{(k)} A^k g_0), A^{-1}(\dots) \rangle}{\langle g_0 + c_1^{(k)} A g_0 + \dots + c_k^{(k)} A^k g_0, A^{-1}(\dots) \rangle} = \\ &= \frac{\langle C g_k, A^{-1} C g_k \rangle}{\langle g_k, A^{-1} g_k \rangle} \end{aligned}$$

where

$$\begin{aligned} C &= I + a_1 A + \dots + a_N A^N = I + a_1 (A_1 + A_2) + a_2 (A_1 + A_2)^2 + \dots + a_N (A_1 + A_2)^N = \\ &= [I + a_1 A_1 + \dots + a_N A_1^N] + [a_1 A_2 + a_2 A_1 A_2 + a_2 A_2 A_1 + a_2 A_2^2 + \dots]. \end{aligned}$$

The first bracket is equal $\mathbf{0}$ because of the assumption on operator A_1 . The second bracket is a linear, selfadjoint and compact operator (because A_2 is compact). So C is compact operator.

Because $\text{sp } A \subset [m, 1]$, then

$$\frac{1}{\langle g_k, A^{-1} g_k \rangle} \leq \frac{1}{\langle g_k, g_k \rangle}$$

and

$$\frac{Q_{k+N}}{Q_k} \leq \langle C \bar{g}_k, A^{-1} C \bar{g}_k \rangle, \bar{g}_k = \frac{g_k}{\|g_k\|}.$$

The sequence $(\bar{g}_k)_0^\infty$ is weakly convergent to $\mathbf{0}$ (because $\langle \bar{g}_i, \bar{g}_j \rangle = \delta_{ij}$).

Thus $C \bar{g}_k \rightarrow 0$ and $\frac{Q_{k+N}}{Q_k} \rightarrow 0$.

Q.E.D.

LEMMA 2. If $\frac{Q_{k+N}}{Q_k} \rightarrow 0$, then $\sqrt[n]{Q_n} \rightarrow 0$.

Proof. Let $n = rN + s$, $0 \leq s < N$. Then

$$\sqrt[n]{Q_n} = \sqrt[n]{Q_0} \sqrt[n]{\frac{Q_n}{Q_0} \frac{Q_{2N}}{Q_N} \cdots \frac{Q_{rN}}{Q_{(r-1)N}}} \sqrt[n]{\frac{Q_n}{Q_{rN}}}.$$

For sufficiently large n we have $\sqrt[n]{Q_0} \leq 2$.

By assumption $\frac{Q_{rN}}{Q_{(r-1)N}} \xrightarrow{r \rightarrow \infty} 0$, so for any $\varepsilon \in (0, 1]$ there exists an integer r_0

such that for all $k \geq r_0$, $\frac{(Q)_{kN}}{Q_{(k-1)N}} \leq \varepsilon^N$.

Because

$$\frac{Q_n}{Q_{rN}} \leq 1, \frac{Q_{iN}}{Q_{(i-1)N}} \leq 1, i = 1, 2, \dots, r_0,$$

then

$$\sqrt[n]{Q_n} \leq 2 \sqrt[n]{\frac{Q_{(r_0+1)N}}{Q_{r_0N}} \frac{Q_{(r_0+2)N}}{Q_{(r_0+1)N}} \cdots \frac{Q_{rN}}{Q_{(r-1)N}}} \leq 2 \sqrt[n]{\varepsilon^{N(r-r_0)}} = \frac{2}{\sqrt[n]{\varepsilon^{Nr_0+s}}} \varepsilon.$$

For sufficiently large n

$$\sqrt[n]{\varepsilon^{Nr_0+s}} \geq \sqrt[n]{\varepsilon^{N(r_0+1)}} \geq \frac{1}{2}.$$

Finally, there exists such n_0 that for every $n \geq n_0$.

$$\sqrt[n]{Q_n} \leq 4\varepsilon.$$

This means $\sqrt[n]{Q_n} \rightarrow 0$.

Q.E.D.

Convergence with property $\sqrt[n]{Q_n} \rightarrow 0$ is, surely, weaker than with $\frac{Q_{k+N}}{Q_k} \rightarrow 0$.

But the first property has a clearer interpretation. Namely, for any $\varepsilon > 0$ exists a n_0 , such that for $n \geq 0$

$$\sqrt[n]{Q_n} < \varepsilon \sqrt[n]{Q_0} \quad (\text{because } \sqrt[n]{Q_0} \rightarrow 1).$$

This means $Q_n < Q_0 \varepsilon^n$, i.e., starting from $n \geq n_0$ the sequence Q_n converges to 0 faster than a geometrical progression with ratio ε . So, we have superlinear convergence ($(Q_n)_0^\infty$ converges to 0 faster than any geometrical progression).

Remark 1. The property of superlinear convergence is not general. It is possible to show an operator A and gradient g_0 such that $(Q_n)_0^\infty$ has only linear convergence. An example

$(e_i)_0^\infty$ — orthonormal basis in H

$$Ae_k \stackrel{\Delta}{=} b_{k-1} e_{k-1} + a_k e_k + b_k e_{k+1}, \quad b_{-1} = 0, \quad b_i = \frac{1-m}{4},$$

$$a_i = \frac{1+m}{2}, \quad i=0, 1, \dots$$

$g_0 = e_0$.

It is possible to prove that the closure \bar{A} of A is a positive, selfadjoint, linear operator such that when we minimize (*) we obtain $\frac{Q_{n+1}}{Q_n} \geq \left(\frac{1-m}{4}\right)^2, n=0, 1, \dots$

For details see [5].

Remark 2. When $A = I + A_2$ where A_2 is compact, then $\frac{Q_{n+1}}{Q_n} \rightarrow 0$ (because $N=1$). If we can invert the operator A_1 (for problem (1) and (2) $A_1 = R$ is a known matrix) we can obtain the above case by modifying the algorithm (a): we put

$$s_i = A_1^{-1} g_i + \alpha_{i-1} s_{i-1}.$$

In this way we shall have stronger superlinear convergence.

References

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Superliniowa zbieżność metody gradientu sprzężonego

Dla przypadku minimalizacji funkcjonału kwadratowego w rzeczywistej przestrzeni Hilberta, w którym Hessian ma postać $A = A_1 + A_2$, gdzie A_1 jest operatorem algebraicznym, a A_2 jest operatorem zwartym otrzymano superliniową zbieżność metody gradientu sprzężonego. Przykładem takiego funkcjonału jest układ liniowy z opóźnieniem.

Суперлинейная сходимость метода сопряженного градиента

Для случая минимизации квадратического функционала в действительном гильбертовом пространстве, в котором определитель Гессе имеет вид $A=A_1+A_2$, где A_1 является оператором алгебраическим, а A_2 является компактным оператором, получена суперлинейная сходимость метода сопряженного градиента. Примером такого функционала является линейная система с запаздыванием.

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