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GRADIENT ALTERNATING-DIRECTION METHODS

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1. Introduction

We shall be concerned with iterative methods for the solution of the system of equations

$$(1) \qquad Ax = \bar{f},$$

where A is a symmetric square matrix and x, f are N-dimensional real vectors. We suppose that the eigenvalues λ_k of the matrix A are non-negative, $0 \leq \alpha \leq \lambda_1 \leq \lambda_2 \leq \ldots \leq \lambda_N \leq \beta < \infty$, and that A may be expressed as a sum of positive semi-definite matrices which are easily invertible, $A = \sum_{i=1}^{p} A_i$, $(A_i x, x) \geqq 0$, $i = 1,2$. The alternating-direction iterative methods were introduced in the papers by Peaceman, Rachford and Douglas in 1955. These methods, which have passed extensive development since then, use the inversion of matrices of the form $I + \tau A_i$, where I is the identity matrix and $0 < \tau < \infty$, in the intermediate stages [1]. Such methods may be understood to be based on the preliminary multiplication of the equation (1) by the matrix H_τ^{-1},

$$(2) \qquad H_\tau = \frac{1}{\tau}(I + \tau A_1)(I + \tau A_2) \ldots (I + \tau A_p),$$

where the iteration parameter τ is found in such a way that the condition number of the matrix $H_\tau^{-1} A$ be minimum. We shall not dwell on various versions of the algorithms studied in papers by Janenko, Kellogg, Samarskiĭ, Marčuk, D'jakonov, the author, and others (see e.g. the surveys in [2] - [4]), which differ in the ways of realization in the main. Instead, we give attention to the following form of the alternating-direction iterative methods:

$$(3) \qquad x = x^{n-1} - \omega_n H_n^{-1} (Ax^{n-1} - f).$$

For $p = 2$ scheme (3) is equivalent to the Douglas-Rachford method if $w_n \equiv 1$ and to that of Peaceman-Rachford if $w_n \equiv 2$ [4] .

The algorithms of alternating directions have found their principal application in the finite difference methods for solving elliptic equations with $p \geqq 2$ independent variables. If, e.g., A_i is a difference analogue of the operator of the second derivative with respect to one variable then H_τ is a product of easily invertible tridiagonal matrices (the so-called alternating-direction implicit methods, ADI). On the other hand, defining A_1 and A_2

as a lower and upper triangular matrix, respectively, (i.e. $A_1 + A_2 = A$, $A_1 = A_2'$), we obtain alternating-direction explicit methods (ADE) or point-triangular methods, studied by A.A. Samarskiǐ and the author. Some versions of these point-triangular methods coincide with particular realizations of the symmetric successive over-relaxation method (SSOR), see [2], [4] and the references quoted there.

The basic results on the optimization of iterative methods of the form (3) consist in the minimization of the spectral radius of the matrix

$$T_n = \sum_{s=1}^{n} (I - \omega_s H_{\tau_s}^{-1} A) \tag{4}$$

under the hypothesis that its spectrum is real. For example, if $\alpha > 0$, $p = 2$, $\omega_n \equiv 2$, and the matrices A_1, A_2 are commutative then the sequences τ_s of iteration parameters are known such that the number $n(\varepsilon)$ of iterations necessary for reducing the norm of the error $y^n = x - x^n$ ε^{-1}-times satisfies the inequality

$$n(\varepsilon) \leq C|\ln \varepsilon| . \ln \frac{\beta}{\alpha} , \tag{5}$$

where C is a constant independent of the bounds of the spectrum of A. Another approach is connected with the use of constant $\tau_n \equiv \tau$ and the selection of ω_n according to the Chebyshev acceleration method. In this case, supposing $\alpha > 0$, $p = 2$, commutative A_1 and A_2, and the optimum value of τ, we obtain the inequality [5]

$$n(\varepsilon) \leq \ln \frac{1-\sqrt{1-\varepsilon^2}}{\varepsilon} / \ln \frac{1-\sqrt{\gamma}}{1+\sqrt{\gamma}} , \tag{6}$$

where $\gamma = 2(\alpha/\beta)^{1/2}(1+\alpha/\beta)^{-1}$. For $\varepsilon \ll 1$, $\alpha/\beta \ll 1$ the inequality (6) may be written as

$$n(\varepsilon) \leq |\ln \varepsilon| / 2\sqrt{2\sqrt{\alpha/\beta}} . \tag{6a}$$

A number of papers present the convergence conditions for the iterative processes and estimates of $n(\varepsilon)$ for non-commutative matrices A_i and $p > 2$. However, these estimates prove to be weaker than (5), (6) (cf. [1] - [4] and the references quoted there).

In the present paper we discuss the optimization of iteration parameters connected with minimizing certain functionals which characterize the suppression of errors in successive approximations. In other words, we shall investigate the application of the method of steepest descent, of the minimum residual method and the conjugate gradient method to the alternating-direction algorithms. The above methods have been introduced and studied by Kantorovič, Krasnosel'skiǐ, Kreǐn, Hestenes, Stiefel and others ([6] - [9]). We note that it seems that such an approach has been investigated for the first time in the papers by Godunov and Prokopov, Marčuk and Kuznecov, see [3], [10].

2. The method of steepest descent and the minimum residual method

Putting $\tau_n \equiv \tau$ in (3) and defining ω_n from the minimum condition of the functional

(7) $$\Phi(x^{n+1}) = (Ax^{n+1}, x^{n+1}) - 2(f, x^{n+1}) = (Ay^{n+1}, y^{n+1}) - (f, x^{n+1})$$

as

(8) $$\omega_n = \frac{(r^n, H_\tau^{-1} r^n)}{(AH_\tau^{-1} r^n, H_\tau^{-1} r^n)}, \quad r_n = f - Ax^n,$$

we come to the method of steepest descent, for which the relation

(9) $$\frac{\Phi(x^{n+1})}{\Phi(x^n)} = \frac{(Ay^{n+1}, y^{n+1})}{(Ay^n, y^n)} = q_n = 1 - \frac{(r^n, H_\tau^{-1} r^n)^2}{(A^{-1} r^n, r^n)(AH_\tau^{-1} r^n, H_\tau^{-1} r^n)}$$

holds [3]. If the matrix $H^{1/2} A H^{-1/2}$ is positive definite and the bounds of its spectrum are $0 < m < M < \infty$, then the inequality

(10) $$q_n \leq q = \left(\frac{M-m}{M+m}\right)^2$$

holds. In particular, if $p = 2$ and A_i are symmetric, commutative, and satisfy the condition $\delta(x,x) \leq (A_i x, x) \leq \Delta(x,x)$, $i = 1,2$, $\delta > 0$ then we have

(11) $$m = 2\sqrt{\delta/\Delta} / (1 + \sqrt{\delta/\Delta})^2,$$
$$M = (1 + \delta/\Delta)/(1 + \sqrt{\delta/\Delta})^2,$$
$$q = (1 - \sqrt{\delta/\Delta})^4 (1 + \sqrt{\delta/\Delta})^4$$

for $\tau = (\delta\Delta)^{-1/2}$. This means that the method (3), (8) with a constant optimal value of τ converges no worse that the Peaceman--Rachford method (formula (5) with $\omega_n \equiv 2$).

Under the assumptions stated before (10) we can obtain an estimate of another kind for the method of steepest descent. Putting $k_n = (Ay^n, y^n)$ from (9) we have (see [5]):

(12) $$k_n - k_{n+1} = \frac{(r^n, H_\tau^{-1} r^n)}{(AH_\tau^{-1} r^n, H^{-1} r^n)} \geq \frac{(r^n, H_\tau^{-1} r^n)}{M} \geq \frac{(r^n, y^n)^2}{M(H_\tau y^n, y^n)} \geq$$

$$\geq \frac{k_n^2}{Mq^n(H_\tau y^0,y^0)} .$$

From this it follows immediately that

$$(13) \qquad (Ay^{n+1},y^{n+1}) \leq (Ay^0,y^0)/\left[1+(Ay^0,y^0)M^{-1}(Hy^0,y^0)^{-1}\sum_{s=1}^{n} q^{-s}\right].$$

The inequality (13) leads to the bound

$$(14) \qquad (Ay^{n+1},y^{n+1}) \leq \frac{1-q^{-1}}{1-q^{-n}} M(H_\tau y^0,y^0)$$

for $q<1$. If we do not require the positive definitness of A (i.e. we admit $m = 0$, $q = 1$) then (13) implies the inequality

$$(15) \qquad (Ay^{n+1},y^{n+1}) \leq M(H_\tau y^0,y^0)/n$$

obtained in [10] and for $H_\tau = I$ even earlier by Kantorovič [6]. In the practically most important case $q = 1 - \gamma$, $\gamma << 1$ the bound (14) gives a rather better result than (15):

$$(Ay^{n+1},y^{n+1}) \leq M(H_\tau y^0,y^0)/n(1+n\gamma).$$

The minimum residual method is defined by (3) with $\tau_n = \tau$ and computing ω_n from the condition of minimum value of the functional (r^{n+1},r^{n+1}):

$$(16) \qquad \omega_n = \frac{(AH_\tau^{-1}r^n,r^n)^2}{(AH_\tau^{-1}r^n,AH_\tau^{-1}r^n)} .$$

In this case the residual r^n satisfies the relation

$$(17) \qquad \frac{\|r^{n+1}\|^2}{\|r^n\|^2} = \frac{(r^{n+1},r^{n+1})}{(r^n,r^n)} = \bar{q}_n = 1 - \frac{(AH_\tau^{-1}r^n,r^n)^2}{(r^n,r^n)(AH_\tau^{-1}r^n,AH_\tau^{-1}r^n)}$$

and bounds for $\bar{q}_n$ analogous to (10), (11) can be easily obtained. Since, under the above assumptions, the relation

$$\|r^n\| - \|r^{n+1}\| = \frac{(AH_\tau^{-1}r^n,r^n)^2}{\|AH_\tau^{-1}r^n\|(\|r^n\|+\|r^{n+1}\|)} \geq \frac{(AH_\tau^{-1}r^n.r^n)}{2M\|r^n\|}$$

follows from (17) we obtain

$$(18) \qquad \|r^n\| - \|r^{n+1}\| \geq \frac{\|r^n\|^2}{2M\cdot\|H_\tau y^0\|\bar{q}^{-n}}$$

with the help of the inequalities

$$(r^n,r^n) \leq (AH^{-1}r^n,r^n) \, \| H_\tau y^n \| \cdot \| r^n \| \, , \; \| Hy^n \| \leq \bar{q}_n \| Hy^0 \| .$$

From this estimate

$$(19) \qquad \| r^{n+1} \| \leq \frac{1-\bar{q}^{-1}}{1-\bar{q}^{-n}} \, 2M \, \| H_\tau y^0 \|$$

follows for $\bar{q}<1$. Analogously to the previous case, the inequality

$$(20) \qquad (r^{n+1},r^{n+1}) \leq 4M^2(H_\tau y^0,H_\tau y^0)/n^2$$

is a consequence of (18) in the case of a singular matrix $A(\bar{q} \leq 1)$. The inequality (20) is obtained in [11].

Let us consider the problem of the choice of parameters τ in (3) for $p = 2$ based on the condition of minimum value of functionals. This problem is studied in [11]. In the method of steepest descent, calculating ω_n from the formula (8), we come to the nonlinear equation

$$(21) \qquad \tau_n = \left[\frac{(H_{\tau_n} r^n,r^{n+1})}{(H^{-1}_{\tau_n} A_1A_2H^{-1}_{\tau_n} r^n,r^{n+1})} \right]^{1/2},$$

which follows from the condition $\frac{d\,\Phi(x^{n+1})}{d\tau} = 0$. Similarly in the minimum residual method we obtain

$$(22) \qquad \tau_n = \left[\frac{(AH^{-1}_{\tau_n} r^n,r^{n+1})}{(H^{-1}_{\tau_n} A_1A_2H^{-1}_{\tau_n} r^n,r^{n+1})} \right]^{1/2}$$

from the equation $\frac{d(r^{n+1},r^{n+1})}{d\tau} = 0$. ($\omega_n$ in (22) is calculated from (16.) It can be easily seen that for these τ_n the functionals $\Phi(x^{n+1})$ and (r^{n+1},r^{n+1}) attain its minimum if $AH^{-1}_{\tau_n}$ is a symmetric positive definite matrix. Notice that if now r^n possesses one dominant component in the expansion with respect to the eigenfunctions of the matrix $AH^{-1}_{\tau_n}$, then (21) and (22) become

$$(23) \qquad \tau_n \approx \left[\frac{(r^n,r^n)}{(A_1A_2r^n,r^n)} \right]^{1/2},$$

i.e., one approximate formula which under the assumptions made above is true even for $\omega_n \equiv 2$ particularly (see [11]).

It is possible to propose algorithms with the computation of iteration parameters using a posteriori information on the basis of the above considerations. We carry out the iterations by formula (3) with fixed values $\omega_n = 2$, $\tau_n = \tau_0$ (e.g., $\tau_0 = (\delta\Delta)^{-1/2}$ if δ and Δ are known) at first. If the condition

$$(24) \qquad \left| \frac{\| r^{n_k+1} \|}{\| r^{n_k} \|} - \frac{\| r^{n_k} \|}{\| r^{n_k-1} \|} \right| \leq \varepsilon$$

with a sufficiently small ε is satisfied for some n_k (this characterizes the isolation of the dominant harmonics in r^{n_k}) then we compute τ_n using formula (23) and ω_n using (8) or (16) in the next iteration. The following iterations are performed with $\omega_n = 2$ and $\tau_n = \tau_0$ again until the condition (24) is satisfied etc.

For the methods under consideration we present the results of experiments with alternating-direction implicit methods for the five-point approximation of the Laplace equation $\Delta u = 0$ on a square grid in a square domain with the boundary condition $u|_\Gamma = 1$. The iterations were performed on the grids $m \times m$ $(m = 10, 20, 40)$ with $u^0_{ij} = 0$ till the condition $\max\limits_{i,j} | u^{n+1}_{ij} - u^n_{ij} | \leq 10^{-5}$ was satisfied. For comparison we present the numbers of iterations for the Peaceman-Rachford method in Table 1 $(\omega_n = 2)$. The first column corresponds to constant parameters close to their optimum values ($\tau = \tau_0 = 2.25, 4.75, 10$ for $m = 10, 20, 40$ respectively) and the second one to the optimum sequence τ_n "of Wachspress" [1]. The numbers of iterations with $\tau = \tau_0$ and ω_n calculated by the minimum residual method (16) are given in the third column while those with ω_n and τ_n calculated from (16), (23) and the condition (24) satisfied for $\varepsilon = 10^{-2}$ are presented in the fourth column. Finally the numbers of iterations in the fifth column correspond to ω_n and τ_n calculated from the formulae (16), (22) for each n. Although these last results seem to be best their character is purely illustrative since finding τ_n is here a very time-consuming process involving the solution of a nonlinear equation.

m \ N	1	2	3	4	5
10	17	9	17	13	9
20	31	13	28	15	11
40	60	16	54	18	13

Table 1.

The computations performed show that with ω_n calculated by the method of steepest descent (8) we obtain roughly the same results for the problems under consideration.

3. Conjugate gradient methods

Defining the conjugate gradient methods, as applied to the equation (1) multiplied by the matrix H_τ^{-1}, in accord with [9], we obtain the following class of iteration algorithms [5]

$$(25)\qquad \begin{aligned} &x_{n+1}=x_n+a_n p_n, \quad p_{n+1}=Kq_{n+1}+b_n p_n, \quad q_{n+1}=AH^{-1}Br_{n+1},\\ &r_{n+1}=H^{-1}(f-Ax_{n+1}), \quad a_n=\frac{(q_n,p_n)}{(p_n,Rp_n)}, \quad b_n=\frac{(q_{n+1},Kq_{n+1})}{(q_n,Kq_n)},\\ &q_0=AH^{-1}Br_0, \quad r_0=H^{-1}(f-Ax_0), \quad p_0=Kq_0 \end{aligned}$$

where $R = AH_\tau^{-1}BH_\tau^{-1}A$, B and K are certain symmetric positive definite matrices, and H_τ is supposed to be symmetric for the sake of simplicity. The process given is optimal in the following sense: The vector x_n minimizes the functional $\Phi(x) = (r,Br)$ on an $(n+1)$-dimensional hyperplane passing through the points $x_0,\ldots,x_n$. As is shown in [8], [9], [5] it is valid that

$$(26)\qquad y_{n+1} = y_0 - TP_n(T)y_0 ,$$

where $T = KR$ and $P_n(\nu)$ is a certain polynomial of degree n, holds for the error vectors. If ν_k and z_k, $k = 1,2,\ldots,N$, are the eigenvalues and the corresponding orthogonal eigenvectors of the matrix T and $\varphi(\nu_k)$ are the eigenvalues of the matrix R, which will be considered to be a function of ν_k, then we arrive at

$$(27)\qquad \Phi(x_{n+1}) = \sum_{k=1}^{\nu} \varphi(\nu_k)\,[1-\nu_k p_n(\nu_k)]^2(y_0,z_k).$$

If $0<\nu_1 \leq \nu_k \leq \nu_N$ and $\varphi(\nu)$ is a polynomial it is possible to estimate the rate of the decrease of the functional $\Phi(x_{n+1})$ constructing a polynomial of the form

$$(28)\qquad t(\nu) = \varphi(\nu)\,[1-\nu P_n(\nu)]^2 = \varphi(\nu)F_{n+1}^2(\nu)$$

that satisfies the condition $F_{n+1}(0) = 1$ and possesses the least deviation from zero on the interval $[\nu_1,\nu_N]$.

Choosing the matrices B and K in various ways, we come to different versions of conjugate gradient methods. E.g., for a symmetric matrix $H_\tau A$ we obtain the following algorithms.

A. An analogue of the multistep method of steepest descent is obtained by putting $B = A^{-1}H_\tau$, $K = I$, $R = T = H_\tau^{-1}A$, $\Phi(x_n) = (A^{-1}H_\tau r_n, r_n) = (H_\tau^{-1}Ay_n, y_n)$:

(29) $$p_0 = r_0, \quad x_{n+1} = x_n + p_n(r_n,r_n)/(p_n, H_\tau^{-1}AP_n),$$

$$r_{n+1} = H^{-1}(f-Ax_{n+1}), \quad p_{n+1} = r_{n+1} - p_n(H_\tau^{-1}Ap_n, r_{n+1})/(p_n, H_\tau^{-1}Ap_n).$$

B. Choosing $B = I$, $K = A^{-1}H_\tau$, $R = AH_\tau^{-2}A$, $T = H_\tau^{-1}A$, $\Phi(x_n) = (r_n, r_n)$, we arrive at an analogue of the multistep minimum residual method:

(30) $$p_0 = r_0, \quad r_n = H_\tau^{-1}(f-Ax_n),$$

$$x_{n+1} = x_n + \frac{H_\tau^{-1}Ar_n, p_n)}{(H_\tau^{-1}Ap_n, H_\tau^{-1}Ap_n)} p_n, \quad p_{n+1} = r_{n+1} - \frac{(H_\tau^{-1}Ap_n, H_\tau^{-1}Ap_{n+1})}{(H_\tau^{-1}p_n, H_\tau^{-1}p_n)}.$$

If the matrix $H_\tau^{-1}A$ is not symmetric, analogous but somewhat more time-consuming algorithms can be constructed. We shall not study them here (see [5]).

Since the inequality

(31) $$\Phi(x_n \le \max_{\nu \in [\nu_1, \nu_N]} [1-\nu P_{n-1}(\nu)]^2 \Phi(x_0)$$

follows immediately from (27), it is apparent that, on the assumptions made in deriving (6), (6a) for the Čebyšev acceleration method, these bounds remain true also for any of the conjugate gradient methods. Now $n(\varepsilon)$ denotes the number of iterations necessary for satisfying the condition $\Phi(x_n) \le \varepsilon^2 \Phi(x_0)$.

Inequalities of another kind can be constructed with the help of special polynomials employed for estimating the functionals $\Phi(x_n)$. E.g. if $F_n(\nu)$ is the Lanczos polynomial

(32) $$F_n(\nu) = \frac{1-\cos[(n+1)\arccos(1-2\nu)]}{2(n+1)^2\nu}$$

we have

(33) $$|\nu F_n(\nu)| \le (n+1)^{-2}$$

for $\nu \in [0,1]$. Analogously, using the polynomial

(34) $$\hat{F}_n(\nu) = \frac{(-1)^n \cos[(2n+1)\arccos(1-\sqrt{\lambda})]}{2(n+1)\sqrt{\lambda}}$$

of degree n (cf. [10]), we come to the inequality

$$(35) \qquad |\nu \hat{F}_n^2(\nu)| \leq (2n+1)^{-2}, \qquad \nu \in [0,1] .$$

Since $\rho(\nu) = \nu$ in the method A and $\varphi(\lambda) = \lambda^2$ in the method B we immediately obtain from (33), (35) that the bounds

$$(36) \qquad (H_\tau^{-1}Ay_n, y_n) \leq \frac{(y_0, y_0)}{(2n+1)^2} ,$$

$$(37) \qquad (r_n, r_n) \leq \frac{(y_0, y_0)}{(n+1)^4}$$

hold for the multistep method of steepest descent (29) and for the multistep minimum residual method (30), respectively.

These bounds are obviously independent of the condition of the matrix $H_\tau^{-1}A$ and hold, in particular, also for A singular. The inequalities (36) and (37) give fast convergence for small n and a slower one for large n (this convergence is worse than ensured by (6) for $n \to \infty$).

It is possible to find estimates of the decrease of the functional $\Phi(x_n)$, which are - in a sense - a compromise. To this end we substitute a product of the Lanczos polynomial of degree k and the Čebyšev polynomial of the first kind of degree $n - k$, which possesses the least deviation from zero on the interval $[\nu_1, \nu_N]$, for $F_n(\lambda)$ instead of (32). Then we arrive at

$$(38) \qquad (r_n, r_n) \leq \min_k \left[\frac{2\gamma_0^{n-k}}{(k+1)^2(1+\gamma_0^{2(n-k)})}\right]^2 (y_0, y_0), \qquad \gamma_0 = \frac{1-\gamma^{1/2}}{1+\gamma^{1/2}}$$

instead of (37). An analogous approach allows us to obtain the bound

$$(39) \qquad (Ay_n, y_n) \leq \min_k \left[\frac{2\gamma_0^{n-k}}{(2k+1)(1+\gamma_0^{2(n-k)})}\right]^2 (y_0, y_0)$$

instead of (36).

4. Conclusion

The gradient methods considered are not better than the algorithms based on the minimization of the spectral radius of the transition operator as far as the asymptotic rate of convergence is concerned. At the same time they are somewhat worse as concerns the economy of computation. On the other hand, our opinion is that the bounds and illustrative numerical experiments presented indicate that their efficiency is sufficiently good. Gradient methods possess suitable relaxation properties for small values of n (including also singular matrices). Apparently the nonlinear problem of the choice of parameters τ_n from variational considerations needs further investigation.

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