JOURNAL OF OPTIMIZATION THEORY AND APPLICATIONS: Vol. 14, No. 4, 1974

TECHNICAL NOTE

Least-Square Acceleration of Iterative Methods for Linear Equations

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Communicated by A. V. Balakrishnan

Abstract. Ordinary iteration schemes for solving linear algebraic equations are one-step, i.e., only the last iterant is used in order to compute the following one. This note advocates the use of several iterants by means of least-square acceleration. The resulting scheme is easy to implement and is very effective in cases where the basic iteration matrix is close to symmetric. The note provides theoretical estimates for the rate of convergence as well as a numerical example. The example deals with the numerical solution of Poisson's equation in a rectangular annulus, by five-point formulae, using the alternating-direction method.

Key Words. Linear systems, iterative methods, least-square methods, acceleration methods.

1. Acceleration Scheme

The purpose of this note is to advocate the use of an acceleration scheme for some iterative methods used for the solution of large linear systems.

Suppose that the solution of the equation $Ax = f$ is computed by the iteration scheme

$$x_{i+1} = Hx_i + g. \tag{1}$$

Then, the suggested acceleration scheme is as follows: start with x_0,

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an initial approximation to x. Compute, for some n, the vectors $x_1, \ldots, x_n, x_{n+1}$. Then, solve for constants α_i, $i = 0, \ldots, n$, the minimum problem

$$\left\| \sum_{i=0}^{n} \alpha_i (x_{i+1} - x_i) \right\|_2^2 = \min, \tag{2}$$

$$\sum_{i=0}^{n} \alpha_i = 1. \tag{3}$$

The vector

$$\bar{y} = \sum_{i=0}^{n} \alpha_i x_{i+1}$$

is, in certain cases, a much better approximation to x than x_{n+1}. n is usually much smaller than the order of the matrix, so the resulting linear equation is quite simple to solve. Actually, most of the work done at this stage is in the computation of the scalar products (x_i, x_j). Observe also that A or H do not enter explicitly into the computation and that Eq. (1) does not necessarily represent an explicit iteration scheme.

We exhibit here two types of such schemes, to be considered later. One is the general linear iteration, i.e., if $A = A_1 + A_2$, then

$$A_1 x_{i+1} = -A_2 x_i + f. \tag{4}$$

If $A_1 = L + \omega^{-1} D$, where D is some block diagonal matrix and L is the lower diagonal part, then $A_2 = U + (1 - \omega^{-1})D$, where U is the upper diagonal part. This is the familiar overrelaxation technique. For some matrices A and for the optimal ω, the corresponding $H = A_1^{-1} A_2$ will have all the (complex) eigenvalues on some circle (Ref. 1).

The other method is an alternating direction method, namely,

$$\begin{aligned} (A_1 + \lambda)\, x_{2i} &= -(A_2 - \lambda)\, x_{2i-1} + f, \\ (A_2 + \lambda)\, x_{2i+1} &= -(A_1 - \lambda)\, x_{2i} + f. \end{aligned} \tag{5}$$

For the iteration cycle $x_{2i} \to x_{2i+2}$, H is

$$H = (A_1 + \lambda)^{-1} (A_2 - \lambda)(A_2 + \lambda)^{-1} (A_1 - \lambda). \tag{6}$$

It is known that, for the analysis of convergence, one may use the matrix

$$\tilde{H} = (A_1 - \lambda)(A_1 + \lambda)^{-1} (A_2 - \lambda)(A_2 + \lambda)^{-1}. \tag{7}$$

In the case that A_1 and A_2 are symmetric, it follows that $\tilde{H}$ is a product of two symmetric matrices (not necessarily symmetric).

Analysis and estimates for the suggested scheme are given by the following propositions:

Proposition 1.1. The minimization problem (2)–(3) is equivalent to the following procedure. Find

$$y_1 = \sum_{i=0}^{n} \alpha_i x_i$$

for which the residual is minimal:

$$\| y_1 - Hy_1 - g \| = \min. \tag{8}$$

Proof. Multiply Eq. (1) by α_i and add for $i = 0,..., n$. One has

$$\sum_{i=0}^{n} \alpha_i x_{i+1} = \sum_{i=0}^{n} \alpha_i (Hx_i + g) = g + H \sum_{i=0}^{n} \alpha_i x_i .$$

It is clear that (2) and (8) are equivalent. Observe, also, that the suggested combination $\bar{y}$ is better than y_1, since $\bar{y} = Hy_1 + g$.

Proposition 1.2. If H is symmetric, $\| H \| = 1 - \epsilon$, then

$$\begin{aligned} \| y_1 - Hy_1 - g \| &\leqslant T_n^{-1}[1/(1-\epsilon)] \cdot \| x_0 - Hx_0 - g \| \\ &\sim 2[1 + \epsilon + \sqrt{(2\epsilon)}]^{-n} \cdot \| x_0 - Hx_0 - g \|, \end{aligned} \tag{9}$$

where $T_n(t)$ is Tchebisheff's polynomial of order n.

Proof. This estimate is actually proved in Ref. 2 for $A = I - H$, $\lambda_{\min} \geqslant \epsilon$, $\lambda_{\max} \leqslant 2 - \epsilon$ (the notations coincide with that of Ref. 2). For the sake of completeness, we sketch the proof here. Since

$$x_i - x = H^i(x_0 - x), \qquad (I - H)x = g,$$

it follows that

$$\begin{aligned} \| y_1 - Hy_1 - g \| &= \left\| \sum_{i=0}^{n} \alpha_i (x_{i+1} - x_i) \right\| \\ &= \left\| \sum_{i=0}^{n} \alpha_i [(x_{i+1} - x) - (x_i - x)] \right\| \\ &= \left\| \sum_{i=0}^{n} \alpha_i (H^{i+1} - H^i)(x_0 - x) \right\| = \left\| \sum_{i=0}^{n} \alpha_i H^i (I - H)(x_0 - x) \right\| \\ &= \left\| \left(\sum_{i=0}^{n} \alpha_i H^i \right) (x_0 - Hx_0 - g) \right\|. \end{aligned} \tag{10}$$

The α_i minimize the last expression on the right. Thus,

$$\left\|\left(\sum_i \alpha_i H^i\right)(x_0 - Hx_0 - g)\right\| \leqslant \left\|\sum_{i=0}^{n} \beta_i H^i\right\| \cdot \| x_0 - Hx_0 - g \|, \tag{11}$$

where $\| \sum_{i=0}^{n} \beta_i H^i \|$ is minimal among all combinations $\| \sum_{i=0}^{n} \gamma_i H^i \|$ for which $\sum_{i=0}^{n} \gamma_i = 1$.

The quantity $\| \sum \beta_i H^i \|$ can be estimated by the following minimum problem. Consider all polynomials

$$g(t) = \sum_{i=0}^{n} \gamma_i t^i$$

for which

$$g(1) = \sum_{i=0}^{n} \gamma_i = 1.$$

Then, the polynomial that comes closest to zero on the interval $[-1 + \epsilon, 1 - \epsilon]$ (the interval containing the spectrum of H) is

$$p(t) = T_n[t/(1 - \epsilon)],$$

where T_n is the Tchebisheff polynomial of order n. The distance to zero on $[-1 + \epsilon, 1 - \epsilon]$ is given by $T_n^{-1}[1/(1 - \epsilon)]$. It follows then, by standard arguments, that

$$\left\|\sum_{i=0}^{n} \beta_i H^i\right\| \leqslant T_n^{-1}[1/(1 - \epsilon)]. \tag{12}$$

The estimate (9) follows now from (11), (12), and the identity

$$T_k(t) = \tfrac{1}{2}\{[t + \sqrt{(t^2 - 1)}]^k + [t - \sqrt{(t^2 - 1)}]^k\}, \tag{13}$$

from which the estimate

$$T_n[1/(1 - \epsilon)] \sim T_n(1 + \epsilon) \sim \tfrac{1}{2}\{1 + \epsilon + \sqrt{[(1 + \epsilon)^2 - 1]}\}^n \sim \tfrac{1}{2}[1 + \epsilon + \sqrt{(2\epsilon)}]^n \tag{14}$$

is obtained easily.

One should compare (9) with the asymptotic rate of convergence of (1), which is $\| H \|^n$, that is,

$$\begin{aligned} \| x_n - Hx_n - g \| &= \| H^n(x_0 - Hx_0 - g \| \sim \| H^n \| \cdot \| x_0 - Hx_0 - g \| \\ &= (1 - \epsilon)^n \| x_0 - g \|. \end{aligned} \tag{15}$$

For $\epsilon = 0.1$, $n = 10$, we get $(1 - \epsilon)^n \sim e^{-1}$, whereas

$$2[1 + \epsilon + \sqrt{(2\epsilon)}]^{-n} \sim e^{-4},$$

which means that the number of iterations using accelerations is reduced by a factor of four.

Consider now the second case, that is, H is a multiple of a unitary matrix:

$$H = (1 - \epsilon)U.$$

We may proceed here by trying to find the minimum of $\| \sum_{i=0}^{n} \gamma_i H^i \| \cdot$ where

$$\sum_{i=0}^{n} \gamma_i = 1.$$

Now, the spectrum of H is on a circle. The corresponding polynomial $p(z)$ will be closest to zero on the circle $| t | = 1 - \epsilon$ [while satisfying $p(1) = 1$]. It is well known that $p(z) = z^n$. This means that the method of estimation used in Proposition 1.2 can guarantee only that $\| H^n \| \cdot \| x_0 - g \|$, which is the rate of convergence without any acceleration. There is no hope to get a better estimate by a different method, since it is possible to construct an example where x_n actually minimizes (2)–(3). We will not do it here.

In the numerical solution of boundary value problems for elliptic equations, one has, generally, a choice between overrelaxation and the alternating directions method (Ref. 1). The former is optimized by a matrix H for which the eigenvalues are on a circle. The latter uses a product of symmetric matrices, which is *close* to a symmetric matrix. The two methods have about the same effectiveness. On the basis of the analysis above, it is better to use alternating directions and to accelerate it.

2. Numerical Example

The acceleration method was used for the solution of Poisson's equation in the rectangular annulus bounded on the outside by the unit square and on the inside by a square having the length of 1. The resulting 5-point difference scheme was solved by the following alternating direction method:

$$\begin{aligned} u^{(2n)}(i+1,j) + u^{(2n)}(i-1,j) - 2u^{(2n)}(i,j) + \lambda h^2 u^{(2n)}(i,j) \\ = -[u^{(2n-1)}(i,j+1) + u^{(2n-1)}(i,j-1) - 2u^{(2n-1)}(i,j) - \lambda h^2 u^{(2n-1)}(1,j)] \\ + h^2 f(i,j), \end{aligned} \tag{16}$$

$$\begin{aligned} u^{(2n+1)}(i,j+1) + u^{(2n+1)}(i,j-1) - 2u^{(2n+1)}(i,j) + \lambda h^2 u^{(2n+1)}(i,j) \\ = -[u^{(2n)}(i+1,j) - u^{(2n)}(i-1,j) - 2u^{(2n)}(i,j) - \lambda h^2 u^{(2n)}(i,j)] + h^2 f(i,j) \end{aligned} \tag{17}$$

Table 1. Results for the example.

λ	Initial residue	40 iterations without acceleration	40 iterations with acceleration
$-\pi h/8$	93.556	0.15498	0.000149
$-\pi h/4$	55.006	0.028599	0.0000086
$-\pi h/2$	30.146	0.002044	0.000000026
$-\pi h$	15.444	0.001064	2×10^{-9} *
$-2\pi h$	7.236	0.000048	**
$4\pi h$	3.381	0.000871	**

* After acceleration following 30 iterations.
** Residual much smaller than 10^{-9} after acceleration following 30 iterations.

for $h = 0.1$ (21 points on the side, 240 internal points). Note that $u(i, j)$ stands for $u(ih, jh)$.

Various parameters λ_k were chosen. The function $f(i, j)$ was taken to be identically equal to 4. Boundary values of $u(i, j)$ were taken to be that of the function $x^2 + y^2$.

For each parameter, we computed $u(i, j)$ by direct iteration and also by acceleration. There, we used 10 (double) cycles, thus taking combinations of 10 vectors at a time. In each case, the iteration was terminated when the residual was smaller than 10^{-9}, provided that this occurred before 40 (double) iterations. The results are summarized in Table 1.

Further information is given in Table 2. Here, we exhibit the gain in each least-square computation. It is shown that the computed combination of the ten iterants is indeed much better than the last one.

Table 2. Results for the example.

	Ratio of residues before and after acceleration			
λ	1	2	3	4
$-\pi h/8$	10	7	7	3
$\pi h/4$	14	13	9	4
$\pi h/2$	38	25	24	15
$-\pi h$	127	61	40	*
$-2\pi h$	240	200	*	*
$-4\pi h$	150	128	*	*

* The computation had been terminated before.

References

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