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Enveloping an Iteration Scheme

Abstract: The problem of determining the optimal values of relaxation parameters for a linear iteration is solved. The optimal iteration scheme is achieved by a second-order linear iteration method.

Introduction

In this paper we discuss two procedures for accelerating iterative methods for solving the Nth order linear system

$$Au = b\,, \tag{1}$$

where A is a given real nonsingular $N \times N$ matrix, and b (which is given) and the solution u are N-vectors. One procedure is the class of semi-iterative methods and the other is the class of relaxation methods. Both of these methods are described by R. S. Varga [1]. Both methods deal with an iteration scheme of the form

$$u_{n+1} = Gu_n + f\,. \tag{2}$$

The iteration scheme has the property that its fixed point v, where

$$v = Gv + f\,, \tag{3}$$

is the solution, u, of (1).

Both acceleration methods employ an additional set of parameters, one for each iteration for adjusting the value of the newly arrived at iterate. For a specified number of iterations, say m, we consider the problem of optimally determining these parameters, i. e., determining them so that the error between the mth iterate and the exact solution is minimized. For semi-iterative methods this problem has been solved [2] and the parameters are characterized as the coefficients of an appropriately normalized Chebyshev polynomial of degree m. In this paper we show that the optimization problem for the class of relaxation methods is solved by choosing parameters which are the roots of an appropriately determined mth degree orthogonal polynomial.

For semi-iterative methods, the optimal iteration scheme is achievable by an appropriate iteration method of second degree, i.e., one of the form

$$v_{n+1} = (\alpha_n G + \beta_n)v_n + \gamma_n v_{n-1} + k_n\,. \tag{4}$$

By this we mean that for appropriate choices of α_n, β_n, γ_n, and k_n, v_n coincides with the nth iterate of the optimal semi-iterative method of n steps, for any n.

We will show that the same is true for the optimal relaxation method. We refer to this method of second degree as the *envelope* of the class of relaxation methods. We use this terminology for the following reason. For a given choice, say $u_0 = 0$, consider the polygonal path joining the points $(i\,, \|u_i - u\|)$, $i = 0, 1, \cdots, n$, where $\|\cdot\|$ denotes the norm of the vector u. This polygonal path characterizes the iteration scheme for each n and each choice of n relaxation parameters. The totality of all such polygonal paths corresponding to all possible relaxation schemes has a lower envelope that is yet another polygonal path. This envelope is described by the second-degree method.

Our solution consists in adapting to this more general case a special case that has been solved by E. Stiefel [3], where $Gu + k$ is the gradient of a quadratic form. In this case the iteration scheme is a relaxation version of the method of steepest descent and the envelope is the method of conjugate gradients.

The optimal method

Consider the linear system

$$Au = b\,. \tag{1}$$

Let the iteration scheme

$$u_{n+1} = Gu_n + f, \qquad n = 0, 1, \cdots \tag{5}$$

where G is an $N \times N$ matrix and f an N-vector have a unique fixed point that coincides with the solution of (1). We write (5) as

$$\Delta u_\nu = r_\nu, \qquad \nu = 0, 1, \cdots, \tag{6}$$

where

$$\Delta u_\nu = u_{\nu+1} - u_\nu, \tag{7}$$

$r_\nu = f - Mu_\nu$, and

$M = I - G$.

where I is the identity matrix.

We now introduce the first acceleration procedure for (5).

• *Semi-iterative methods*

Let $\alpha_{n,k}$, $\quad k = 0, 1, \cdots, n, \quad n = 0, 1, \cdots$ be a sequence of real constants with the property

$$\sum_{k=0}^{n} \alpha_{n,k} = 1, \qquad n = 0, 1, \cdots \tag{8}$$

and let

$$v_n = \sum_{k=0}^{n} \alpha_{n,k} u_k, \qquad n = 0, 1, \cdots \tag{9}$$

The v_n define a semi-iterative method of successive approximations to u. The error $e_n \equiv v_n - u$ satisfies

$$e_n = P_n(G)e_0, \qquad n = 1, 2, \cdots, \tag{10}$$

$$P_n(x) = \sum_{k=0}^{n} \alpha_{n,k} x^k. \tag{11}$$

in which $P_n(1) \equiv 1$.

Let the eigenvalues λ of G be real and suppose that they lie in the interval $[\alpha, \beta]$ with $\alpha < \beta < 1$. Then for the eigenvalues $P_n(\lambda)$ of $P_n(G)$, we see that the

$$\max_{\alpha \leq \lambda \leq \beta} |P_n(\lambda)| \tag{12}$$

is minimized under the constraint $P_n(1) = 1$ for

$$P_n(x) = T_n\left(\frac{2x - (\beta + \alpha)}{\beta - \alpha}\right) \Big/ T_n(\gamma), \tag{13}$$

where

$$\gamma = \frac{2 - \beta - \alpha}{\beta - \alpha} \tag{14}$$

and the T_n are the Chebyshev polynomials of degree n defined by

$$T_n(x) = \cos(n \cos^{-1} x), \qquad n = 0, 1, \cdots, \tag{15}$$

if $|x| \leq 1$.

Moreover from the property

$$T_{n+1}(x) = 2xT_n(x) - T_{n-1}(x) \tag{16}$$

of the Chebyshev polynomials, it can be deduced that the v_n of Eq. (9) for the choice of P_n in (13) obey the following second-order recurrence relation:

$$v_{n+1} = (\alpha_n G + \beta_n I)v_n + \gamma_n v_{n-1} + f_n, \qquad n = 1, 2, \cdots, \tag{17}$$

where

$$\alpha_n = \frac{2}{(\beta - \alpha)\gamma w_{n+1}}$$

$$\beta_n = \frac{\beta + \alpha}{(\alpha - \beta)\gamma w_{n+1}}$$

$$\gamma_n = 1 - w_{n+1}$$

$$f_n = \frac{2\, w_{n+1}}{\gamma\, (\beta - \alpha)} f$$

$$w_1 = 1$$

$$w_2 = \frac{1}{1 - 1/2\gamma^2}$$

$$w_{n+1} = \frac{1}{1 - w_n/4\gamma^2}, \qquad n = 2, 3, \cdots. \tag{18}$$

The choice of the $\alpha_{n,k}$ gives the optimal acceleration to the semi-iterative scheme and the property (16) enables one to avoid using the coefficients of the Chebyshev polynomials and resumming for every change in n, by use of the second-order method (17).

Now let us consider the second acceleration procedure.

• *Relaxation methods*

Let t_n, $n = 0, 1, \cdots$ be a sequence of positive constants. Let x_n, $n = 0, 1, \cdots$ define a relaxed iterative method corresponding to (5), where

$$x_{n+1} - x_n = (1/t_n)(f - Mx_n). \tag{19}$$

We write this as

$$\Delta x_n = r_n/t_n, \tag{20}$$

where $\Delta x_n = x_{n+1} - x_n$ and $r_n = f - Mx_n$.

The error $e_n = x_n - u$ satisfies

$$e_n = -M^{-1}r_n, \tag{21}$$

if M is nonsingular.

Suppose that M is positive definite and Hermitian. Then if $(u, v) = u^*v$ denotes the usual inner product in N-space, (u, Mu) defines a metric in this space which we denote by $\mu(u)$. In particular for the N-vector $e = -M^{-1}r$, we have

$$\mu(e) = (M^{-1}r, r) \tag{22}$$

For each n, we consider the problem of choosing the

t_j, $j=0, 1, \cdots, n$ so that $\mu(e_n)$ is a minimum. Of course the optimal relaxation parameters will depend on n, but for convenience we suppress displaying this dependence. Following Stiefel, we may formulate the solution to this problem as follows.

Let $R_n(\lambda)$, $n=1, 2, \cdots$, be a sequence of polynominals given by

$$R_n(\lambda)=\prod_{j=1}^{n}(1-\lambda/t_{j-1}). \tag{23}$$

If the initial iterate is $x_0=0$, then

$$x_1=\frac{f}{t_0}=M^{-1}\Big[I-\Big(I-\frac{M}{t_0}\Big)\Big]f=M^{-1}[I-R_1(M)]f.$$

Then

$$x_n=M^{-1}[I-R_n]f, \tag{24}$$

since by induction

$$\begin{aligned} x_{n+1}&=M^{-1}\Big[I-R_n+\frac{M}{t_n}-\frac{M}{t_n}\Big(I-R_n\Big)\Big]f\\ &=M^{-1}[I-R_{n+1}]f. \end{aligned}$$

Similarly

$$r_n=R_n(M)f \tag{25}$$

so that from (22)

$$\mu(e_n)=(M^{-1}R_n(M)f, R_n(M)f). \tag{26}$$

Let M have distinct eigenvalues $0<\lambda_1<\lambda_2<\cdots<\lambda_N<1$ and let T be the matrix whose jth column is the eigenvector of M with eigenvalue λ_j, $j=1, \cdots, N$. Then

$$\begin{aligned} \mu(e_n)&=(M^{-1}T\,T^{-1}R_n(M)T\,T^{-1}f, T\,T^{-1}R_n(M)T\,T^{-1}f)\\ &=(\Lambda^{-1}R_n(\Lambda)\bar f, R_n(\Lambda)\bar f). \end{aligned} \tag{27}$$

Here Λ is the $N\times N$ diagonal matrix, $\Lambda=(\lambda_j\delta_{ij})$ and $\bar f=T^{-1}f$.

Then

$$\mu(e_n)=\sum_{j=1}^{N}\bar f_j^2\ [R_n^{\,2}(\lambda_j)]/\lambda_j, \tag{28}$$

where $\bar f_j$, $j=1, \cdots, N$ are the components of $\bar f$. Thus if we introduce the density

$$\rho(\lambda)=\sum_{j=1}^{N}\bar f_j^2\delta(\lambda-\lambda_j), \tag{29}$$

we may write

$$\mu(e_n)=\int_0^1[\rho(\lambda)/\lambda]R_n^{\,2}(\lambda)d\lambda. \tag{30}$$

In the case that the eigenvalues of M are not distinct this representation for $\mu(e_n)$ will in general involve $R_n(\lambda)$ and some of its derivatives. We do not treat this more involved case further.

Now the problem of optimal choice of the relaxation parameters corresponds to finding the polynomial $R_n(\lambda)$ which solves the polynomial least-squares problem with respect to the weight $\rho(\lambda)/\lambda$. Of course we must impose the additional constraint

$$R_n(0)=1, \qquad n=0, 1, \cdots$$

if we are to recover polynomials of the type (23). Denoting the class of polynomial of degree n as Π_n, the problem to be solved is explicitly

$$\min_{\substack{R_n\epsilon\Pi_n\\R(0)=1}}\mu(e_n)=\min_{\substack{R_n\epsilon\Pi_n\\R(0)=1}}\int_0^1[\rho(\lambda)/\lambda]R_n^{\,2}(\lambda)d\lambda.$$

The solution to this constrained least-squares problem is the set of polynomials $P_n(\lambda)$, orthonormal on (0,1) with respect to the weight $\rho(\lambda)$ (see [4]), i.e.,

$$\int_0^1P_\nu(\lambda)P_\mu(\lambda)\rho(\lambda)d\lambda=0, \qquad \mu\neq\nu. \tag{31}$$

Thus the optimal relaxation parameters are $t_{j,n}$, $j=1, \cdots, n$, $n=1, 2, \cdots$, where for each n, the $t_{j,n}$ are the roots of $P_n(\lambda)$.

As in the case for the optimal semi-iterative method, the optimal relaxation method may be replaced by a second-order iteration method that frees the method from use of the roots $t_{j,n}$ as well as recomputing for each n change. This second-order method emerges from the second-order recurrence relation

$$\lambda R_i(\lambda)=-q_iR_{i+1}(\lambda)+(p_i+q_i)R_i(\lambda)-p_iR_{i-1}(\lambda), \qquad i=1, 2, \cdots \tag{32}$$

obeyed by the $R_i(\lambda)$, which we henceforth assume to satisfy (31). We take

$$R_0=1, p_0=0, q_{-1}=0,$$

and

$$\begin{aligned} q_i&=(1/N_i)(r_i, Mr_i)-p_i\\ &=(1/N_i)\int_0^1\lambda R_i^{\,2}(\lambda)\rho(\lambda)d\lambda-p_i \end{aligned}$$

$$p_i=(N_i/N_{i-1})q_{i-1}$$

$$N_i=(r_i, r_i)=\int_0^1R_i^{\,2}(\lambda)\rho(\lambda)d\lambda, \qquad i=0, 1, 2, \cdots. \tag{33}$$

Note that the p_i and q_i may be computed without any use of the orthogonal polynomials.

The second-order scheme is

$$\Delta z_i=(1/q_i)(r_i+p_i\Delta z_{i-1}), \qquad z_0=0. \tag{34}$$

We claim that this scheme envelopes the optimal relaxation scheme for each n, i.e., $z_i=M^{-1}[I-R_i(M)]f$ [see (24)]. This may be seen as follows.

Since $z_0 = 0$, $r_0 = f = R_0(M)f$. Suppose by induction that $r_i = R_i(M)f$. Now since $r_i = f - Mz_i$, we have

$$r_{i+1} - r_i = -M\Delta z_i . \tag{35}$$

Then, from Eq. (34),

$$\begin{aligned} r_{i+1} - r_i &= -\frac{M}{q_i}(r_i + p_i\Delta z_{i-1}) \\ &= -\frac{Mr_i}{q_i} + \frac{p_i}{q_i}(r_i - r_{i-1}) \\ &= \left[\left(\frac{p_i}{q_i} - \frac{M}{q_i}\right)R_i(M) - \frac{p_i}{q_i}R_{i-1}(M)\right]f. \end{aligned} \tag{36}$$

Using (32) this becomes

$$r_{i+1} = R_{i+1}(M)f. \tag{37}$$

Then having completed the induction we may write

$$z_i = M^{-1}(f - r_i) = M^{-1}[I - R_i(M)]f, \tag{38}$$

which is what was to be proved.

Remark: Notice that the three-step recurrence scheme (34) must theoretically terminate after N steps. This follows from the fact that since $\rho(\lambda)$ as given in Eq. (29) has N jumps, then only N orthogonal polynomials $P_n(\lambda)$ can be generated by (31).*

Examples

From $Au = b$, certain iteration schemes are obtained by splitting A

$$A = P - N \tag{39}$$

where N is nonsingular. Then writing

$$Nu_{n+1} = Pu_n - b . \tag{40}$$

*The author is grateful to R. Varga for urging him to include this remark.

Then

$$f = -N^{-1}b$$

$$G = N^{-1}P$$

$$M = I - N^{-1}P \tag{41}$$

1) The Jacobi method corresponds to $N = \text{diag}\, A$.
2) The Gauss-Seidel method corresponds to $N = L$ (which equals the lower triangular portion of A up to and including the main diagonal, with all other elements of L taken as zero).
3) The method of steepest descent corresponds to $M = -A$ and $f = b$.

In each of these three cases we must take care that the associated matrix M has the properties required in the section on the optimal method, i.e., Hermitian and positive definite.

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References

1. R. S. Varga, *Matrix Iterative Analysis*, Prentice-Hall, N.J., 1962, Chs. 4 and 5.
2. *Ibid.*, p. 132ff.
3. E. Stiefel, "Relaxationsmethoden bester Strategie zur Lösung linearer Gleichungssystems," *Commentarii Mathematici Helvetici* **29,** 157–179 (1955).
4. I. P. Natanson, *Constructive Function Theory*, Vol. II, p. 60, Frederick Ungar, New York, 1965.

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