JOURNAL OF COMPUTATIONAL AND APPLIED MATHEMATICS

ELSEVIER

Journal of Computational and Applied Mathematics 50 (1994) 255-262

On application of the Lanczos method to solution of some partial differential equations

Vladimir Druskin [a,*], Leonid Knizhnerman [b]

[a] *Schlumberger-Doll Research, Old Quarry Road, Ridgefield, CT 06877-4108, United States*
[b] *Central Geophysical Expedition, Narodnogo Opolcheniya St., House 40, Building 3, Moscow 123298, Russia*

Received 20 May 1992; revised 25 March 1993

Abstract

Let A be a square symmetric $n \times n$ matrix, ϕ be a vector from $\mathbb{R}^n$, and f be a function defined on the spectral interval of A. The problem of computation of the vector $u = f(A)\phi$ arises very often in mathematical physics.

We propose the following method to compute u. First, perform m steps of the Lanczos method with A and ϕ. Define the *spectral Lanczos decomposition method* (SLDM) solution as $u_m = \|\phi\| Qf(H)e_1$, where Q is the $n \times m$ matrix of the m Lanczos vectors and H is the $m \times m$ tridiagonal symmetric matrix of the Lanczos method. We obtain estimates for $\|u - u_m\|$ that are stable in the presence of computer round-off errors when using the simple Lanczos method.

We concentrate on computation of $\exp(-tA)\phi$, when A is nonnegative definite. Error estimates for this special case show superconvergence of the SLDM solution. Sample computational results are given for the two-dimensional equation of heat conduction. These results show that computational costs are reduced by a factor between 3 and 90 compared to the most efficient explicit time-stepping schemes. Finally, we consider application of SLDM to hyperbolic and elliptic equations.

Key words: Spectral Lanczos decomposition method; Numerical methods; Partial differential equations

1. Introduction

Let A be a symmetric $n \times n$ matrix. The Lanczos method has become accepted as a powerful tool for finding the eigenpairs (eigenvalues and eigenvectors) of A, when A is large and sparse. Here we demonstrate another use of the Lanczos method. Let f be a function defined on the spectral interval of A and ϕ a vector in $\mathbb{R}^n$. Consider the problem of computing the vector

$$u = f(A)\phi. \tag{1}$$

Solving a system of linear equations is a problem of this kind, where $f(A) = A^{-1}$. Such

* Corresponding author. e-mail: druskin@sdr.slb.com.

SSDI 0377-0427(93)E0120-B

problems with different forms of f also appear in mathematical physics when solving semidiscrete approximations of partial differential equations whose coefficients do not depend on one of the variables

$$f(A)=\exp(-tA), \quad \text{for parabolic equations,}$$
$$f(A)=\cos(+tA^{1/2}), \quad \text{for hyperbolic equations,}$$
$$f(A)=\exp(-tA^{1/2}), \quad \text{for elliptic equations.}$$

In the well-known explicit methods for computing u, $f(A)$ is approximated by a polynomial function of A. We can study the common properties of such methods through the eigenvalues and eigenvectors of A. Denote these eigenvalues by λ_i, $i=1,\dots,n$, and the corresponding eigenvectors by z_i. If ϕ is expanded in terms of z_i,

$$\phi=\sum_{i=1}^{n}\phi_i z_i, \tag{2}$$

then

$$u=\sum_{i=1}^{n}\phi_i f(\lambda_i) z_i.$$

Take the vector $p(A)\phi$ with p a polynomial of degree $\leqslant m-1$ as an approximate value of u. Then the error norm is

$$\|u-p(A)\phi\|=\left\|\sum_{i=1}^{n}\phi_i(f-p)(\lambda_i)z_i\right\|=\left[\sum_{i=1}^{n}\phi_i^2(f-p)^2(\lambda_i)\right]^{1/2}. \tag{3}$$

Thus, the problem has been reduced to the discrete polynomial approximation of f with the nodes λ_i and the weights ϕ_i^2.

Most of the computation in polynomial methods is connected with multiplying A with vectors; thus, the most important characteristic of such a method is the degree of the polynomial (measured by m) needed to achieve a given accuracy. It can be shown that for any fixed m, the minimum in (3) is achieved if and only if p consists of the initial m terms in the Fourier series expansion of f in the (λ_i, ϕ_i^2)-orthogonal polynomials. The Lanczos process, which initially was intended for the computation of the spectrum of A, also allows one to build up the discrete orthogonal polynomials whose weight function approximates the generalized weight (λ_i, ϕ_i^2) in a certain sense.

The Lanczos process was first applied to solving linear systems [13,15,16], then to solving one-dimensional [8,9] and multi-dimensional [2] parabolic equations. The general scheme of applying the Lanczos process to solving problem (1) was suggested in [1,3] and in another form in [17]. Error bounds for the computation of (1) in general and for the most common specific forms of f are given below. In the final section, we extend our results to the case of finite computer arithmetic.

2. The spectral Lanczos decomposition method

We first review the results of applying m steps of the Lanczos method for generating the eigenvectors of A [14, Chapter 13]. In the Krylov subspace $\mathscr{K}^m=\operatorname{span}\{\phi, A\phi,\dots,A^{m-1}\phi\}$, generate the basis $q_1, \ldots, q_m$ by Gram–Schmidt orthogonalization of the vectors ϕ, $A\phi, \ldots, A^{m-1}\phi$. The orthogonalization can be carried out by the following three-term recurrence:

$$Aq_i = \beta_{i-1}q_{i-1} + \alpha_i q_i + \beta_i q_{i+1}, \quad i = 1, \ldots, m-1,$$

where $\beta_0 q_0$ is assumed to be 0, $q_1 = \phi / \|\phi\|$, and $\beta_i \geqslant 0$. Denote by H the tridiagonal symmetric matrix

$$\begin{bmatrix} \alpha_1 & \beta_1 & \cdots & 0 \\ \beta_1 & \alpha_2 & \beta_2 & \\ \vdots & & \ddots & \vdots \\ 0 & \cdots & \beta_{m-1} & \alpha_m \end{bmatrix},$$

with θ_i, $s_i = (s_{1i}, \ldots, s_{mi})^{\mathrm{T}}$, $i = 1, \ldots, m$, the eigenvalues and normalized eigenvectors of H. Define e_i as the ith unit m vector, Q the matrix of basis vectors q_i, $Q = [q_1 \mid q_2 \mid \ldots \mid q_m]$, and $y_i = Qs_i$. Then (θ_i, y_i) are the approximate eigenpairs of the matrix A that would be obtained by the Ritz method applied to $\mathscr{K}^m$.

In view of (2) and the orthonormality of the matrix $[s_1 \mid s_2 \mid \ldots \mid s_m]$, we have

$$\phi = \|\phi\| q_1 = \|\phi\| Q e_1 = \|\phi\| Q \sum_{i=1}^{m} s_{1i} s_i = \|\phi\| \sum_{i=1}^{m} s_{1i} y_i,$$

which is why it is natural to take the vector

$$u_m = \|\phi\| \sum_{i=1}^{m} s_{1i} f(\theta_i) y_i = \|\phi\| Q f(H) e_1$$

as an approximation to u. This definition is correct because the spectrum of H is contained in the spectral segment of A. We call the method just described the *spectral Lanczos decomposition method* or SLDM.

3. The general SLDM error bound

We will assume that A is not scalar; that is, $\lambda_n = \max_i \lambda_i > \min_i \lambda_i = \lambda_1$. Assign

$$B = \frac{\lambda_n + \lambda_1}{\lambda_n - \lambda_1} I - \frac{2}{\lambda_n - \lambda_1} A, \qquad g(x) = f\{\tfrac{1}{2}[(\lambda_n + \lambda_1) - (\lambda_n - \lambda_1)x]\};$$

then $-I \leqslant B \leqslant I$ and the function g is defined on the segment $[-1, 1]$. Consider the Chebyshev series of the first kind

$$g(x) = \sum_{k=0}^{\infty} g_k T_k(x). \tag{4}$$

Theorem 1 (Druskin and Knizhnerman [3, §3]). *If series* (4) *converges absolutely on* $[-1, 1]$, *the inequality*

$$\|u - u_m\| \leqslant 2\|\phi\| \sum_{k=m}^{\infty} |g_k|$$

holds.

Theorem 1 cannot, in general, be noticeably improved. There has been found an example where the error is greater than the right-hand side of Theorem 1's inequality multiplied by $\frac{3}{8}^{1/2}$.

4. The computation of $\exp(-tA)$

Assume that $A \geqslant 0$. Evidently,

$$u(t) = \exp(-tA)\phi = \exp[-\tfrac{1}{2}t\lambda_n(I - B)]\phi = \exp(-\tfrac{1}{2}t\lambda_n)\exp(\tfrac{1}{2}\lambda_n B)\phi,$$

with $B = I - 2A/\lambda_n$, $-I \leqslant B \leqslant I$. Using the expansion

$$e^{ax} = I_0(a) + 2\sum_{k=1}^{\infty} I_k(a)T_k(x),$$

where I_k is the Bessel function, one easily finds that

$$u(t) = e^{-t\lambda_n/2}\left[I_0(\tfrac{1}{2}t\lambda_n)\phi + 2\sum_{k=1}^{\infty} I_k(\tfrac{1}{2}t\lambda_n)T_k(B)\phi\right].$$

Thus,

$$g_k = 2I_k(\tfrac{1}{2}t\lambda_n), \quad \text{for } k \geqslant 1. \tag{5}$$

Theorem 2 (Druskin and Knizhnerman [3, §4]). *Let* $a = \frac{1}{2}t\lambda_n$ *and* $m \leqslant a$. *Then the error bound*

$$\frac{\|u - u_m\|}{\|\phi\|} \leqslant \left[\sqrt{2\pi} + O\left(\frac{m}{a}\right)\right]\frac{a^{0.5}}{m}\exp\left[-0.5\frac{m^2}{a} + O\left(\frac{m^4}{a^3}\right)\right]$$

holds.

The proof uses (5) and the asymptotics for I_k. In [3], there is also a proof of an estimate for small a.

Numerical example. Consider the model problem

$$-\Delta u + \frac{\partial u}{\partial t} = 0, \quad (x, y) \in \Omega =]0, 1[^2, \qquad t > 0,$$

$$u(x, y, t)|_{t=0} = x(1 - x)y(1 - y), \qquad u(x, y, t)|_{(x,y)\in\partial\Omega} = 0.$$

Table 1

t	Exact solution differential equation	Exact solution semi-discrete equation	SLDM	LIM
0.001	$0.61456\cdot10^{-1}$	$0.61456\cdot10^{-1}$	$0.61456\cdot10^{-1}$	$0.61458\cdot10^{-1}$
0.002	$0.60469\cdot10^{-1}$	$0.60469\cdot10^{-1}$	$0.60469\cdot10^{-1}$	$0.60471\cdot10^{-1}$
0.004	$0.58517\cdot10^{-1}$	$0.58517\cdot10^{-1}$	$0.58516\cdot10^{-1}$	$0.58523\cdot10^{-1}$
0.008	$0.54711\cdot10^{-1}$	$0.54711\cdot10^{-1}$	$0.54689\cdot10^{-1}$	$0.54722\cdot10^{-1}$
0.016	$0.47507\cdot10^{-1}$	$0.47508\cdot10^{-1}$	$0.47392\cdot10^{-1}$	$0.47534\cdot10^{-1}$
0.032	$0.35155\cdot10^{-1}$	$0.35160\cdot10^{-1}$	$0.34955\cdot10^{-1}$	$0.35218\cdot10^{-1}$
0.064	$0.18794\cdot10^{-1}$	$0.18801\cdot10^{-1}$	$0.18657\cdot10^{-1}$	$0.18871\cdot10^{-1}$
0.128	$0.53158\cdot10^{-2}$	$0.53201\cdot10^{-2}$	$0.52767\cdot10^{-2}$	$0.53598\cdot10^{-2}$
0.256	$0.42489\cdot10^{-3}$	$0.42557\cdot10^{-3}$	$0.42189\cdot10^{-3}$	$0.43196\cdot10^{-3}$
0.512	$0.27145\cdot10^{-5}$	$0.27231\cdot10^{-5}$	$0.26969\cdot10^{-5}$	$0.28059\cdot10^{-5}$
1.024	$0.11078\cdot10^{-9}$	$0.11150\cdot10^{-9}$	$0.11020\cdot10^{-9}$	$0.11839\cdot10^{-9}$
	Number of matrix–vector multiplications:		15	3192
	Number of operations per step:		$10n$	$6n$

Approximating the Laplacian as usual on a rectangular grid with the spacing $h = \frac{1}{51}$, we get the second-order semi-discrete scheme with a spatial operator A. This scheme has been solved by the method described above and by the local iteration method [7]. Table 1 gives results of the comparison for the point $(\frac{25}{51}, \frac{25}{51})$.

Use of SLDM has also shown a noticeable effect on splitting (alternating direction) methods for parabolic equations [5]. In addition, SLDM has been implemented for solving the three-dimensional parabolic system that arises when displacement currents are neglected in Maxwell's equations. The computational time for the impulse response of the electromagnetic field in an inhomogeneous, conductive earth, on a $40 \times 40 \times 75$ grid, was several hours on a microVax or Vax computer [6]. For these examples, $\|A\| t$ was up to 10^9.

5. Other matrix functions

We will assume here that $\|\phi\| = 1$.

(a) $u(t) = \cos(t\sqrt{A})\phi$, $A \geqslant 0$ [3, §5]. This vector function satisfies the hyperbolic Cauchy problem

$$Au + \frac{\mathrm{d}^2 u}{\mathrm{d}t^2} = 0, \quad u(0) = \phi, \quad \frac{\mathrm{d}u}{\mathrm{d}t}(0) = 0.$$

If $\tau = 2/\sqrt{\lambda_n}$, $x = 2t/\tau$, $\xi = 2m/x - 1$, for all $0 < \xi \leqslant 1$, then

$$\|u - u_m\| \leqslant \frac{\exp\left[-\frac{1}{3}x(2\xi)^{1.5}\right]}{2(\pi\xi)^{1/2}(4m^2 - x^2)^{1/4}}$$

(some O-terms have been thrown away).

(b) $u(z)=\exp(-z\sqrt{A})\phi$, $\lambda_1>0$ [3, §6]. This vector function satisfies the elliptical Dirichlet problem

$$Au-\frac{\mathrm{d}^2u}{\mathrm{d}z^2}=0,\quad z>0,\ u(0)=\phi,\ u(+\infty)=0.$$

If $c=(\lambda_n+\lambda_1)/(\lambda_n-\lambda_1)$, then

$$\|u-u_m\|\leqslant\frac{2\Phi(c)^{-m}}{1-\Phi(c)^{-1}}.$$

(c) $u=A^{-1}\phi$, $\lambda_1>0$ (SSLE [3, §7]).

$$\|u-u_m\|\leqslant\|u\|\frac{2\delta}{1-\delta},$$

with $\delta=T_m[(\lambda_n+\lambda_1)(\lambda_n-\lambda_1)]^{-1}$.

6. Computer arithmetic

The previous results assume that all computations are done in exact arithmetic. The Lanczos method, however, has been avoided in the past because of its instability. This instability shows up in loss of orthogonality of y_k's and in the appearance of parasitic counterparts to θ_i's.

In [11,12], Paige clarified the behavior of the simple (without re-orthogonalization) Lanczos method with finite computer arithmetic. He also pointed out that, in spite of the instability, there appear among the θ's approximations to the λ's as m increases (the so-called Lanczos phenomenon).

Using Paige's well-known theorems, we have proved that finite computer arithmetic does not change a number of the results given here. The sense of these proofs is roughly as follows. The Lanczos process is unstable by itself, but the error bounds remain stable in the presence of roundoff errors.

Let ϵ be the elementary computer rounding error, c_1 the maximal number of nonzero elements in rows of A, and define the following auxiliary quantities:

$$\epsilon_1=\left(7+c_1\frac{\|\|A\|\|}{\|A\|}\right)\epsilon,\qquad \epsilon_2=\sqrt{2}\max[12(n+4)\epsilon,\ \epsilon_1],\qquad \eta=m^{2.5}\|A\|\epsilon_2.$$

Also, let f be defined on $[\lambda_1-\eta,\ \lambda_n+\eta]$,

$$B=\frac{(\lambda_n+\lambda_1)I-2A}{\lambda_n-\lambda_1+2\eta},\qquad g(x)=f\{\tfrac{1}{2}[(\lambda_n+\lambda_1)-(\lambda_n-\lambda_1+2\eta)x]\},$$

and g_k be defined by (4).

Theorem 3 (Druskin and Knizhnerman [4, §2]). *If*

$$m[6(n+4)\epsilon+\epsilon_1]\leqslant1,\quad (n+4)\epsilon<\tfrac{1}{24},$$

and series (4) *converges absolutely on* $[-1, 1]$, *then the error bound*

$$\frac{\|u-u_m\|}{\|\phi\|} \leqslant 4\sqrt{\frac{2}{\pi}}\,\|g\|_{L_2(]-1,1[,(1-x^2)^{-0.5})}\|A\|m^3\frac{\epsilon_1}{\lambda_n-\lambda_1}+\frac{10}{\sqrt{24}}m^{0.5}\sum_{k=m}^{\infty}|g_k|$$

is valid for the computation of (1) *by means of the simple Lanczos method.*

Evidently, Theorem 3 is an analog of Theorem 1 for finite computer arithmetic. Theorem 3 shows that the simple Lanczos method produces an approximate solution of (1) with a stable error estimate. One can obtain results on the convergence of the eigenvalues of the simple Lanczos method by taking for f in Theorem 3 a "cap-like" polynomial picking out the particular eigenvalue [4, §§5, 6].

Acknowledgements

We thank A. Kashik for support and M. Oristaglio for helpful discussions and review of the manuscript.

References

[1] V. Druskin and L. Knizhnerman, Using operational series in orthogonal polynomials for computation of functions of self-adjoint operators and background of Lanczos phenomenon, Dept. at VINITI No. 1535-B87, 1987 (in Russian).

[2] V. Druskin and L. Knizhnerman, A spectral semi-discrete method for the numerical solution of 3-D non-stationary problems in electrical prospecting, *Izv. Acad. Sci. USSR Phys. Solid Earth* (8) (1988) 63–74 (in Russian; translated into English).

[3] V. Druskin and L. Knizhnerman, Two polynomial methods to compute functions of symmetric matrices, *U.S.S.R. Comput. Math. and Math. Phys.* **29** (12) (1989) 112–121.

[4] V. Druskin and L. Knizhnerman, Error bounds in the simple Lanczos procedure when computing functions of symmetric matrices and eigenvalues, *U.S.S.R. Comput. Math. and Math. Phys.* **31** (7) (1991) 20–30.

[5] V. Druskin and L. Knizhnerman, The Lanczos optimization of a splitting-up method to solve homogeneous evolutionary equations, *J. Comput. Appl. Math.* **42** (2) (1992) 221–231.

[6] A. Hördt, V. Druskin, L. Knizhnerman and K.-M. Strack, Interpretation of 3-D effects in deep transient electromagnetic soundings in the Münsterland area (Germany), *Geophys.* **57** (9) (1992) 1127–1137.

[7] V.O. Lokutsievskiy and O.V. Lokutsievskiy, Using the Chebyshev parameters for the numerical solution of some evolutionary problems, preprint No. 99, Inst. Appl. Math., Acad. Sci. USSR, Moscow, 1984 (in Russian).

[8] B. Nour-Omid, Lanczos method for heat conduction analysis, *Internat. J. Numer. Methods Engrg.* **24** (1) (1987) 251–262.

[9] B. Nour-Omid and R.W. Clough, Dynamic analysis of structure using Lanczos co-ordinates, *Earthquake Engrg. and Structural Dynamics* **12** (4) (1984) 565–577.

[10] C.C. Paige, The computation of eigenvalues and eigenvectors of very large sparse matrices, Ph.D. Thesis, Univ. London, 1971.

[11] C.C. Paige, Error analysis of the Lanczos algorithm for tridiagonalizing a symmetric matrix, *J. Inst. Math. Appl.* **18** (3) (1976) 341–349.

[12] C.C. Paige, Accuracy and effectiveness of the Lanczos algorithm for the symmetric eigenproblem, *Linear Algebra Appl.* **34** (1980) 235–258.

[13] C.C. Paige and M.A. Saunders, Solution of sparse indefinite systems of linear equations, *SIAM J. Numer. Anal.* **12** (4) (1975) 617–629.
[14] B.N. Parlett, *The Symmetric Eigenvalue Problem* (Prentice-Hall, Englewood Cliffs, NJ, 1980).
[15] B.N. Parlett, A new look at the Lanczos algorithm for solving symmetric systems of linear equations, *Linear Algebra Appl.* **29** (1980) 323–346.
[16] H.D. Simon, The Lanczos algorithm for solving linear systems, Ph.D. Thesis, Univ. California, Berkeley, CA, 1982.
[17] H.A. van der Vorst, An iterative solution method for solving $f(A)x = b$, using Krylov subspace information obtained for the symmetric positive definite matrix A, *J. Comput. Appl. Math.* **18** (2) (1987) 249–263.