Enhancement of Krylov Subspace Spectral Methods by Block Lanczos Iteration

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Abstract. This paper presents a modification of Krylov Subspace Spectral (KSS) Methods, which build on the work of Golub, Meurant and others pertaining to moments and Gaussian quadrature to produce high-order accurate approximate solutions to variable-coefficient time-dependent PDE. Whereas KSS methods currently use Lanczos iteration to compute the needed quadrature rules, the modification uses block Lanczos iteration in order to avoid the need to compute two quadrature rules for each component of the solution, or use perturbations of quadrature rules. It will be shown that under reasonable assumptions on the coefficients of the problem, a 1-node KSS method is unconditionally stable, and methods with more than one node are shown to possess favorable stability properties as well. Numerical results suggest that block KSS methods are significantly more accurate than their non-block counterparts.

Keywords: spectral methods, Gaussian quadrature, variable-coefficient, block Lanczos method, stability, heat equation
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INTRODUCTION

Consider the following initial-boundary value problem in one space dimension,

$$u_t + Lu = 0, \quad 0 < x < 2\pi, \quad t > 0, \tag{1}$$

$$u(x,0) = f(x), \quad 0 < x < 2\pi, \tag{2}$$

with periodic boundary conditions. The operator L is a second-order differential operator of the form

$$Lu = -(p(x)u_x)_x + q(x)u, \tag{3}$$

where $p(x)$ is a positive function and $q(x)$ is a nonnegative (but nonzero) smooth function. It follows that L is self-adjoint and positive definite.

In [1] a class of methods, called Krylov subspace spectral (KSS) methods, was introduced for the purpose of solving time-dependent, variable-coefficient problems such as this one. These methods are based on the application of techniques developed by Golub and Meurant in [2], originally for the purpose of computing elements of the inverse of a matrix, to elements of the matrix exponential of an operator.

It has been shown in these references that KSS methods, by employing different approximations of the solution operator for each Fourier component of the solution, achieve higher-order accuracy in time than other Krylov subspace methods (see, for example, [3]) for stiff systems of ODE, and, as shown in [4], they are also quite stable, considering that they are explicit methods.

In this paper, we consider whether these methods can be enhanced, in terms of accuracy, stability or any other measure, by using a single block Gaussian quadrature rule to compute each Fourier component of the solution, instead of two standard Gaussian rules where one is obtained from the other by perturbing the initial vector of a Krylov subspace in the direction of the solution from the previous time step.

BLOCK KRYLOV SUBSPACE SPECTRAL METHODS

We discretize functions defined on $[0,2\pi]$ on an N-point uniform grid with spacing $\Delta x = 2\pi/N$. With this discretization, the operator L and the solution operator $S(\Delta t) = \exp[-L\Delta t]$ can be approximated by $N \times N$ matrices that represent

linear operators on the space of grid functions. Given a vector $\mathbf{u}^n$ that represents the approximate solution at time $t_n = n\Delta t$ for some choice of Δt, we approximate each Fourier component of the solution at time t_{n+1} by a bilinear form

$$\hat{u}(\omega, t_{n+1}) \approx \hat{\mathbf{e}}_\omega^H S_N(\Delta t)\mathbf{u}^n, \tag{4}$$

where

$$[\hat{\mathbf{e}}_\omega]_j = \frac{1}{\sqrt{2\pi}} e^{i\omega j\Delta x}, \quad [\mathbf{u}^n]_j = u(j\Delta x, t_n), \tag{5}$$

and

$$S_N(t) = \exp[-L_N t], \quad [L_N]_{jk} = -p(j\Delta x)[D_N^2]_{jk} + q(j\Delta x), \tag{6}$$

where D_N is a discretization of the differentiation operator that is defined on the space of grid functions.

We are now ready to describe block KSS methods. For each wave number $\omega = -N/2+1, \ldots, N/2$, we define

$$R_0(\omega) = \begin{bmatrix} \hat{\mathbf{e}}_\omega & \mathbf{u}^n \end{bmatrix}$$

and then compute the QR factorization $R_0(\omega) = X_1(\omega)B_0(\omega)$, which yields

$$X_1(\omega) = \begin{bmatrix} \hat{\mathbf{e}}_\omega & \mathbf{u}_\omega^n / \|\mathbf{u}_\omega^n\|_2 \end{bmatrix}, \quad B_0(\omega) = \begin{bmatrix} 1 & \hat{\mathbf{e}}_\omega^H \mathbf{u}^n \\ 0 & \|\mathbf{u}_\omega^n\|_2 \end{bmatrix},$$

where

$$\mathbf{u}_\omega^n = \mathbf{u}^n - \hat{\mathbf{e}}_\omega \hat{\mathbf{e}}_\omega^H \mathbf{u}^n.$$

We then carry out K iterations of the block Lanczos algorithm described in [5], with $K \ll N$ and initial block $X_1(\omega)$ to obtain a block tridiagonal $2K \times 2K$ matrix of recursion coefficients,

$$\mathscr{T}_K(\omega) = \begin{bmatrix} M_1(\omega) & B_1(\omega)^H & & & \\ B_1(\omega) & M_2(\omega) & B_2(\omega)^H & & \\ & \ddots & \ddots & \ddots & \\ & & B_{K-2}(\omega) & M_{K-1}(\omega) & B_{K-1}(\omega)^H \\ & & & B_{K-1}(\omega) & M_K(\omega) \end{bmatrix}, \tag{7}$$

where each block $M_j(\omega)$ and $B_j(\omega)$ is 2×2. Then, we can express each Fourier component of the approximate solution at the next time step as

$$[\hat{\mathbf{u}}^{n+1}]_\omega = \left[B_0^H E_{12}^H \exp[-\mathscr{T}_K(\omega)\Delta t] E_{12} B_0\right]_{12} \tag{8}$$

where $E_{12} = \begin{bmatrix} \mathbf{e}_1 & \mathbf{e}_2 \end{bmatrix}$, the matrix of the first two standard basis vectors in $\mathbb{R}^{2K}$. The computation of $E_{12}^H \exp[-\mathscr{T}_K(\omega)\Delta t] E_{12}$ consists of computing the eigenvalues and eigenvectors of $\mathscr{T}_K(\omega)$ in order to obtain the nodes and weights for block Gaussian quadrature, and then applying the block quadrature rule as described in [2].

In [6], it was demonstrated that recursion coefficients for all wave numbers $\omega = -N/2+1, \ldots, N/2$ can be computed simultaneously, by regarding them as functions of ω and using symbolic calculus to apply differential operators analytically, as much as possible. As a result, KSS methods require $O(N \log N)$ floating-point operations per time step, which is comparable to other time-stepping methods. The same approach can be applied to block KSS methods. For both types of methods, it can be shown that for a K-node Gaussian rule or block Gaussian rule, K applications of the operator L_N to the previous solution $\mathbf{u}^n$ are needed.

CONVERGENCE ANALYSIS

We now examine the convergence of block KSS methods by first investigating their consistency and stability. As shown in [1], [4], the original KSS methods are high-order accurate in time, but are also explicit methods that possess stability properties characteristic of implicit methods, so it is desired that block KSS methods share both of these traits. For convenience, we define $BL_N([0,2\pi]) = \text{span}\{\, e^{-i\omega x} \,\}_{\omega=-N/2+1}^{N/2}$, the space of bandlimited 2π-periodic functions with at most N nonzero Fourier components. The following theorems were stated and proved in [7].

Theorem 1 *Let L be a self-adjoint mth-order positive definite differential operator on $C_p([0,2\pi])$ with coefficients in $BL_N([0,2\pi])$, and let $f \in BL_N([0,2\pi])$. Assume that for each $\omega = -N/2+1, \ldots, N/2$, the recursion coefficients in*

(7) are computed on a $2^K N$-point uniform grid. Then a block KSS method that uses a K-node block Gaussian rule to compute each Fourier component $[\hat{\mathbf{u}}^1]_\omega$, for $\omega = -N/2+1,\ldots,N/2$, of the solution to (1), (2) satisfies

$$\left|[\hat{\mathbf{u}}^1]_\omega - \hat{u}(\omega,\Delta t)\right| = O(\Delta t^{2K}), \quad \omega = -N/2+1,\ldots,N/2,$$

where $\hat{u}(\omega,\Delta t)$ is the corresponding Fourier component of the exact solution at time Δt.

The simple form of the approximate solution operator in the case of $K = 1$ yields the following result. For convenience, we denote by $\tilde{S}_N(\Delta t)$ the matrix such that $\mathbf{u}^{n+1} = \tilde{S}_N(\Delta t)\mathbf{u}^n$, for given N and Δt.

Theorem 2 *Let $q(x)$ in (3) belong to $BL_M([0,2\pi])$ for a fixed integer M. Then, for the problem (1), (2), the block KSS method with $K = 1$ is unconditionally stable. That is, given $T > 0$, there exists a constant C_T, independent of N and Δt, such that*

$$\left\| \left[\tilde{S}_N(\Delta t)\right]^n \right\|_2 \leq C_T, \tag{9}$$

for $0 \leq n\Delta t \leq T$.

It is important to note that although stability has only been shown for the case where the leading coefficient $p(x)$ is constant, it has been demonstrated that KSS methods exhibit similar stability on more general problems, such as in [4] where it was applied to a second-order wave equation with time steps that greatly exceeded the CFL limit. Furthermore, [4] also introduced homogenizing similarity transformations that can be used to extend the applicability of theoretical results concerning stability that were presented in that paper, as well as the one given here. In [7], numerical results are given that support the conjecture that under appropriate assumptions concerning the regularity of the coefficients, unconditional stability also holds for $K > 1$.

NUMERICAL RESULTS

In this section, we will present numerical results for comparisons between the original KSS method (as described in [4]) and the new block KSS method, applied to parabolic problems. For convenience, we denote by KSS(K) the original KSS method with K Gaussian nodes, and by KSS-B(K) the block KSS method with K block Gaussian nodes.

First, we solve parabolic problems in one and two space dimensions, fully defined in [7], in which the leading coefficient $p(x)$ in (3) is constant, and the coefficient $q(x)$ is smoothly varying. The results are shown in Figure 1, and compared to those obtained using the original KSS method, and the MATLAB stiff ODE solver `ode23s`, described in [8], as it is suitable for parabolic problems such as these.

In the 2-D case, the variable coefficient of the PDE is smoothed to a greater extent than in the 1-D case, because the prescribed decay rate of the Fourier coefficients is imposed in both the x- and y-directions. This results in greater accuracy in the 2-D case, which is consistent with the result proved in [1] that the local truncation error varies linearly with the variation in the coefficients. We see that significantly greater accuracy is obtained with block KSS methods, in both one and two space dimensions.

In an attempt to understand why the block KSS method is significantly more accurate, we examine the nodes for both methods, which reveals that for the original KSS method, all of the nodes used to compute $[\hat{\mathbf{u}}^{n+1}]_\omega$ tend to be clustered around $\hat{\mathbf{e}}_\omega^H L_N \hat{\mathbf{e}}_\omega$, whereas with the block KSS method, half of the nodes are clustered near this value, and the other half are clustered near $[\mathbf{u}_\omega^n]^H L_N \mathbf{u}_\omega^n$, so the previous solution plays a much greater role in the construction of the quadrature rules.

In [7], similar results are obtained on two other problems of interest: a hyperbolic system of two coupled first-order PDE, using basis functions described in [9], and computing $e^{-A\Delta t}\mathbf{v}$, where $\mathbf{v}$ is a given vector and A is a symmetric positive definite matrix with entries randomly generated in such a way as to impose strong diagonal dominance.

SUMMARY

We have demonstrated that for parabolic variable-coefficient PDE, block KSS methods are capable of computing Fourier components of the solution with greater accuracy than the original KSS methods, and they possess similar stability properties. By pairing the solution from the previous time step with each trial function in a block and applying the Lanczos algorithm to them together, we obtain a block Gaussian quadrature rule that is better suited to approximating a bilinear form involving both functions than the approach of perturbing Krylov subspaces in the direction of the solution.

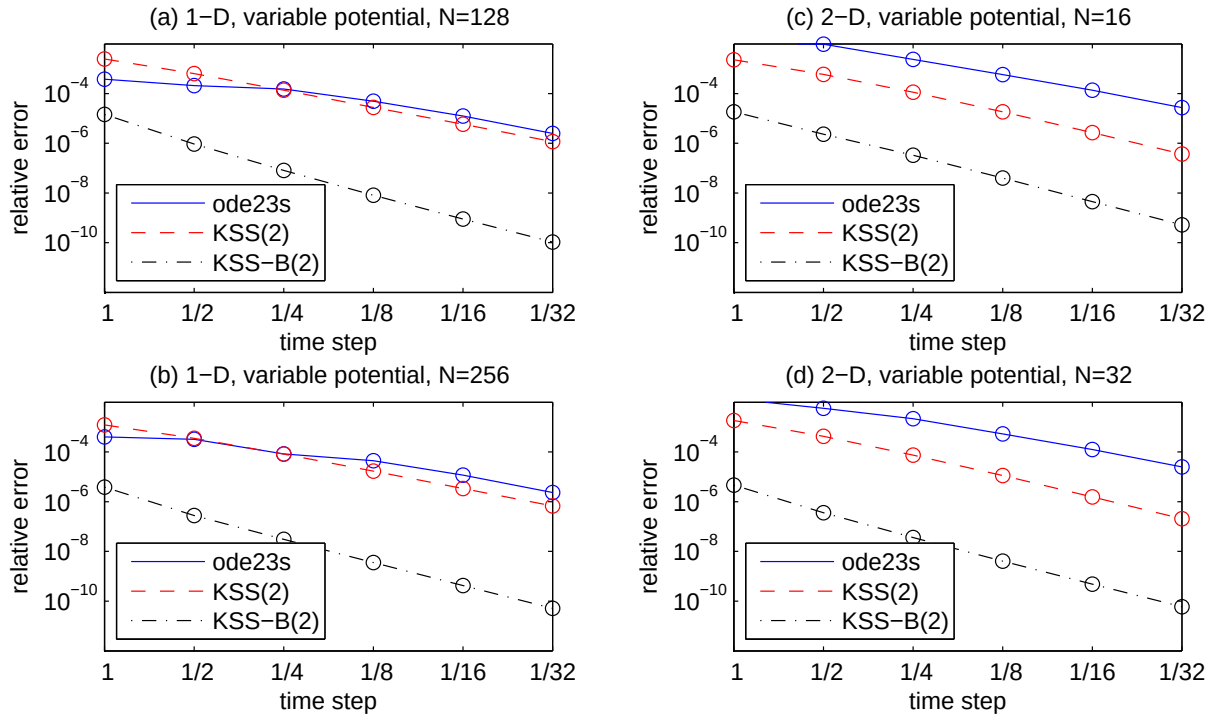

FIGURE 1. (a) Upper left plot: Estimates of relative error in the approximate solution of (1), (2), with $p(x)$ constant, at $T = 1$. Solutions are computed using the MATLAB solver `ode23s` (solid curve), the original 2-node KSS method (dashed curve), and a 2-node block KSS method (dotted-dashed curve), with $N = 128$ grid points. (b) Lower left plot: Estimates of relative error in the approximate solution of the same problem, using the same methods, with $N = 256$ grid points. (c) Upper right plot: Estimates of relative error in the approximate solution of a 2-D analogue of (1), (2) at $T = 1$. Solutions are computed with $N = 16$ grid points per dimension. (b) Lower right plot: Estimates of relative error in the approximate solution of the same problem, using the same methods, with $N = 32$ grid points per dimension. In all cases, all methods use time steps $\Delta t = 2^{-j}$, $j = 0, \ldots, 5$.

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