Recent Advances in Krylov Subspace Spectral Methods

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Abstract

This paper describes a reformulation of Krylov Subspace Spectral (KSS) Methods, which build on Gene Golub's many contributions pertaining to moments and Gaussian quadrature to produce high-order accurate approximate solutions to variable-coefficient time-dependent PDE. Because KSS methods rely on perturbations of Krylov subspaces in the direction of the data, they can be reformulated in terms of derivatives of nodes and weights of Gaussian quadrature rules, which can be computed analytically. Because these derivatives allow KSS methods to be described in terms of operator splittings, they facilitate stability analysis. Under reasonable assumptions on the coefficients of the problem, certain KSS methods are unconditionally stable.

1 Introduction

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

$$u_t + Lu = 0 \quad \text{on } (0, 2\pi) \times (0, \infty), \tag{1}$$

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

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with periodic boundary conditions

$$u(0,t) = u(2\pi,t), \quad t > 0. \tag{3}$$

The operator L is a second-order differential operator of the form

$$Lu = -(pu_x)_x + qu, \tag{4}$$

where p 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 [4] 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 [1], originally for the purpose of computing elements of the inverse of a matrix, to elements of the matrix exponential of an operator. This paper summarizes recent advances in the development of these methods.

2 Krylov Subspace Spectral Methods

Let $S(t) = \exp[-Lt]$ represent the exact solution operator of the problem (1), (2), (3). Krylov subspace spectral methods, introduced in [4], use Gaussian quadrature on the spectral domain to compute the Fourier components of the solution. These methods are time-stepping algorithms that compute the solution at time $t_1, t_2, \ldots$, where $t_n = n\Delta t$ for some choice of Δt. We briefly review how these methods work.

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 can be approximated by an $N \times N$ matrix L_N that represents a linear operator on the space of grid functions. Then, each Fourier component of the solution at time t_{n+1} can be approximated by a bilinear form

$$\hat{u}(\omega, t_{n+1}) \approx \hat{\mathbf{e}}_\omega^H e^{-L_N \Delta t} \mathbf{u}(t_n), \tag{5}$$

where

$$[\hat{\mathbf{e}}_\omega]_j = \frac{1}{\sqrt{2\pi}} e^{i\omega j \Delta x}, \quad [\mathbf{u}(t_n)]_j = u(j\Delta x, t_n). \tag{6}$$

In [1] Golub and Meurant describe a method for computing quantities of the form

$$\mathbf{u}^T f(A)\mathbf{v}, \tag{7}$$

where $\mathbf{u}$ and $\mathbf{v}$ are N-vectors, A is an $N \times N$ symmetric positive definite matrix, and f is a smooth function. Our goal is to apply this method with $A = L_N$, $f(\lambda) = \exp(-\lambda t)$ for some t, and the vectors $\mathbf{u}$ and $\mathbf{v}$ are derived from $\hat{\mathbf{e}}_\omega$ and $\mathbf{u}(t_n)$. The quantity (7) can be viewed as a Riemann-Stieltjes integral

$$\mathbf{u}^T f(A)\mathbf{v} = I[f] = \int_a^b f(\lambda)\, d\alpha(\lambda), \tag{8}$$

provided that the measure $\alpha(\lambda)$, which is defined in terms of the spectral decomposition of A, is positive and increasing.

As discussed in [1], the integral $I[f]$ can be bounded using either Gauss, Gauss-Radau, or Gauss-Lobatto quadrature rules, whose nodes, as well as the weights, can be obtained using the symmetric Lanczos algorithm if $\mathbf{u} = \mathbf{v}$, and the unsymmetric Lanczos algorithm if $\mathbf{u} \neq \mathbf{v}$.

Employing these quadrature rules yields the following basic process (for details see [4]) for computing the Fourier coefficients of $\mathbf{u}(t_{n+1})$ from $\mathbf{u}(t_n)$.

for $\omega = -N/2 + 1, \ldots, N/2$
  Choose a scaling constant δ_ω
  Compute $u_1 \approx \hat{\mathbf{e}}_\omega^H \exp[-L_N \Delta t]\hat{\mathbf{e}}_\omega$
    using the symmetric Lanczos algorithm
  Compute $u_2 \approx \hat{\mathbf{e}}_\omega^H \exp[-L_N \Delta t](\hat{\mathbf{e}}_\omega + \delta_\omega \mathbf{u}^n)$
    using the unsymmetric Lanczos algorithm
  $[\hat{\mathbf{u}}^{n+1}]_\omega = (u_2 - u_1)/\delta_\omega$
end

This algorithm has high-order temporal accuracy, as indicated by the following theorem. Let $BL_N([0, 2\pi]) = \text{span}\{\ e^{-i\omega x}\ \}_{\omega=-N/2+1}^{N/2}$ denote a space of bandlimited functions with at most N nonzero Fourier components.

Theorem 2.1 *Let L be a self-adjoint m-th order positive definite differential operator on $C_p([0, 2\pi])$ with coefficients in $BL_N([0, 2\pi])$.*

Let $f \in BL_N([0, 2\pi])$. Then the preceding algorithm, applied to the problem (1), (2), (3) using K-node Gaussian quadrature rules, is consistent; i.e.

$$[\hat{\mathbf{u}}^1]_\omega - \hat{u}(\omega, \Delta t) = O(\Delta t^{2K}),$$

for $\omega = -N/2 + 1, \ldots, N/2$.

Proof. See [4, Lemma 2.1, Theorem 2.4]. □

Because the parameter δ_ω should be small, catastrophic cancellation can result, as it does with the approximation of derivatives by finite differences. A reformulation of KSS methods, presented in Section 3, not only alleviates this problem, but also facilitates stability analysis, the results of which are presented in Sections 4 and 5.

3 Reformulation

From the algorithm given in the preceding section, we see that each Fourier component $[\hat{\mathbf{u}}^{n+1}]_\omega$ approximates the derivative

$$\frac{d}{d\delta_\omega} \left[\hat{\mathbf{e}}_\omega^H (\hat{\mathbf{e}}_\omega + \delta_\omega \mathbf{u}^n) \mathbf{e}_1^T \exp[T_\omega(\delta_\omega)\Delta t] \mathbf{e}_1 \right] \Bigg|_{\delta_\omega = 0} \tag{9}$$

where $T_\omega(\delta_\omega)$ is the tridiagonal matrix output by the unsymmetric Lanczos algorithm applied to the matrix L_N with starting vectors $\hat{\mathbf{e}}_\omega$ and $(\hat{\mathbf{e}}_\omega + \delta_\omega \mathbf{u}^n)$ (which reduces to the symmetric Lanczos algorithm for $\delta_\omega = 0$).

For a given δ_ω, let $\lambda_{\omega,j}$, $j = 1, \ldots, K$, be the nodes of the K-point Gaussian rule obtained by applying the unsymmetric Lanczos algorithm to L_N with starting vectors $\hat{\mathbf{e}}_\omega$ and $(\hat{\mathbf{e}}_\omega + \delta_\omega \mathbf{u}^n)$. Let $w_{\omega,j}$, $j = 1, \ldots, K$, be the corresponding weights. Then, letting $\delta_\omega \to 0$, we obtain the following, assuming all required derivatives exist:

$$[\hat{\mathbf{u}}^{n+1}]_\omega \;=\; \sum_{j=1}^{K} w_{j,\omega} e^{-\lambda_{j,\omega}\Delta t} \left[\hat{\mathbf{e}}_\omega^H \mathbf{u}^n + \frac{w'_{j,\omega}}{w_{j,\omega}} - \Delta t \lambda'_{j,\omega} \right] \tag{10}$$

where the $'$ denotes differentiation with respect to δ_ω, and evaluation of the derivative at $\delta_\omega = 0$. Efficient algorithms for obtaining the derivatives of the nodes and weights from those of the recursion coefficients, which are themselves computed using a Lanczos-like iteration introduced in [5], are presented in [3].

4 Convergence Analysis

When $K = 1$, we simply have

$$\mathbf{u}^{n+1} = e^{-C_N \Delta t} P_N [I - \Delta t \, \mathrm{diag}(\tilde{\mathbf{q}})] \mathbf{u}^n, \tag{11}$$

where $\tilde{\mathbf{q}} = \mathbf{q} - \mathrm{Avg}\, q$ and $L = C + V$ is a splitting of L such that C is the constant-coefficient operator obtained by averaging the coefficients of L, and the variation of the coefficients is captured by V. The operator P_N is the orthogonal projection onto $BL_N([0, 2\pi])$.

Let $p(x)$ be constant and let $q(x)$ in (4) belong to $BL_M([0, 2\pi])$ for a fixed integer M. In [3], it is shown that for the problem (1), (2), (3), KSS with a one-node Gaussian rule is unconditionally stable. Also, in the two-node case, there exists a constant C such that

$$\|\tilde{S}_N(\Delta t)\|_\infty \leq C, \tag{12}$$

where $\tilde{S}_N(\Delta t)$ is the matrix such that $\mathbf{u}^{n+1} = \tilde{S}_N(\Delta t)\mathbf{u}^n$ for given N and Δt, and the constant C is independent of N and Δt. It should be emphasized that this result is not sufficient to conclude unconditional stability, as in the 1-node case, but it does demonstrate the scalability of KSS methods with respect to the grid size.

5 Application to the Wave Equation

In this section we apply KSS methods to the problem

$$\begin{cases} \frac{\partial^2 u}{\partial t^2} + Lu = 0 & \text{in } (0, 2\pi) \times \mathbb{R}\,, \\ u(0, t) = u(2\pi, t) & \text{on } \mathbb{R}\,, \end{cases} \tag{13}$$

with the initial conditions

$$u(x, 0) = f(x), \quad u_t(x, 0) = g(x), \quad x \in (0, 2\pi), \tag{14}$$

where, as before, the operator L is as described in (4).

A spectral representation of the operator L allows us the obtain a representation of the solution operator (the *propagator*) in terms of the sine and cosine families generated by L by a simple functional calculus. The entries of the propagator, as functions of L, indicate which functions are the integrands in the Riemann-Stieltjes integrals used to compute the Fourier components of the solution.

We first recall a result concerning the accuracy of each component of the approximate solution.

Theorem 5.1 *Assume that $f(x)$ and $g(x)$ satisfy (3), and let $u(x, \Delta t)$ be the exact solution of (13), (14) at $(x, \Delta t)$, and let $\tilde{u}(x, \Delta t)$ be the approximate solution computed by a KSS method that uses K-node Gaussian quadrature rules to compute each Fourier components. Then*

$$|\langle \hat{\mathbf{e}}_\omega, u(\cdot, \Delta t) - \tilde{u}(\cdot, \Delta t) \rangle| = O(\Delta t^{4K}). \tag{15}$$

Proof. See [2]. □

Let $p(x)$ be constant and let $q(x)$ in (4) belong to $BL_M([0, 2\pi])$ for some integer M. In [3], it is shown that for the problem (1), (2), (3), the one-node KSS method is unconditionally stable and exhibits 3rd-order convergence in time.

References

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