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Iterative across-time solution of linear differential equations: Krylov subspace versus waveform relaxation☆

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ABSTRACT

The aim of this paper is two-fold. First, we propose an efficient implementation of the continuous time waveform relaxation (WR) method based on block Krylov subspaces. Second, we compare this new WR–Krylov implementation against Krylov subspace methods combined with the shift and invert (SAI) technique. Some analysis and numerical experiments are presented. Since the WR–Krylov and SAI–Krylov methods build up the solution simultaneously for the whole time interval and there is no time stepping involved, both methods can be seen as iterative across-time methods. The key difference between these methods and standard time integration methods is that their accuracy is not directly related to the time step size.

1. Introduction

An important sub-task frequently arising in the numerical solution of partial differential equations (PDEs) is the solution of the following initial value problem (IVP):

$$y'(t) = -Ay(t), \qquad y(0) = v, \quad t \in [0, T],\ A \in \mathbb{R}^{n\times n}. \tag{1}$$

Here A is typically very large and sparse. Note that (1) is equivalent to the problem of computing the action of the matrix exponential [1,2]:

$$y(t) = \exp(-tA)v, \quad t \in [0, T]. \tag{2}$$

Krylov subspace methods have been successfully used for the evaluation of the matrix exponential and for the numerical solution of various time dependent problems since the late 80s. We mention in chronological order some early pa-

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pers [3–10]. For a more recent work see the surveys in [11] and in corresponding chapters of [2,12]. These methods are based on a projection of the original IVP (1) onto the Krylov subspace

$$\mathcal{K}_m(A, w) = \mathrm{span}(w, Aw, A^2w, \ldots, A^{m-1}w),$$

where usually $w = v$ or $w = Av$ holds. A significant part of the computational work in Krylov subspace methods is spent for building up a basis of $\mathcal{K}_m(A, w)$, which is usually done by the Arnoldi or Lanczos process [13,14]. The process computes the columns $v_1, v_2, \ldots, v_m$ of $V_m \in \mathbb{R}^{n\times m}$ which form an orthonormal basis of $\mathcal{K}_m(A, w)$ and $v_1 = w/\|w\|$. The matrix V_m satisfies the so-called Arnoldi decomposition [13,14], namely,

$$AV_m = V_{m+1}H_{m+1,m} = V_mH_{m,m} + v_{m+1}h_{m+1,m}e_m^T, \quad \mathbb{R}^m \ni e_m = (0, \ldots, 0, 1)^T,$$

where $H_{m+1,m} = V_{m+1}^TAV_m \in \mathbb{R}^{(m+1)\times m}$ and $H_{m,m} = V_m^TAV_m \in \mathbb{R}^{m\times m}$ are upper Hessenberg and $h_{m+1,m}$ is the only nonzero entry in the last row of $H_{m+1,m}$. Furthermore, if the Krylov subspace method converges successfully then for some $m \ll n$ it holds

$$AV_m \approx V_mH_{m,m},$$

i.e., the colspan of V_m is an approximate invariant subspace of A.

An attractive feature of the method is that in some situations it suffices to build up just a single Krylov basis for the whole time interval of interest $t \in [0, T]$. Indeed, with $w = v$ an approximate solution $y_m(t)$ to problem (1) can be computed as

$$y(t) = \exp(-tA)v = \exp(-tA)V_m\beta e_1 \approx \underbrace{V_m \exp(-tH_{m,m})\beta e_1}_{y_m(t)}, \quad t \in [0, T], \tag{3}$$

where $\beta = \|w\|$ and $\mathbb{R}^m \ni e_1 = (1, 0, \ldots, 0)^T$. The approximation y_m in (3) should satisfy

$$\|y(t) - y_m(t)\| \leqslant \text{tolerance}, \quad t \in [0, T],$$

which can be checked in practice by some error estimates, for example, with the help of the exponential residual defined as [15–17]

$$r_m(t) \equiv -Ay_m(t) - y_m'(t). \tag{4}$$

The property of having a single Krylov basis for the whole time interval makes the methods computationally efficient. In some cases this property can be extended [18] to a more general IVP

$$y'(t) = -Ay(t) + g(t), \qquad y(0) = v, \quad t \in [0, T], \ A \in \mathbb{R}^{n\times n} \tag{5}$$

where $g : [0, T] \to \mathbb{R}^n$ is a given function. Furthermore, this property allows one to regard the Krylov subspace methods applied in this setting as, to some extent, *time stepping free* methods.

Remark 1. Here we use the term "time stepping free" to indicate that the accuracy does not depend on a time step Δt, as is the case for the standard time integration solvers such as Runge–Kutta or multistep methods. One should emphasize that this independence on the time step is partial, i.e., the efficiency does depend on the length of the time interval (typically, the smaller T, the smaller Krylov dimension m suffices [19,9]).

If A is close to a symmetric positive definite matrix with a stiff spectrum,[1] convergence of Krylov subspace methods can be slow. In this case the performance can often be dramatically improved with rational Krylov subspace methods [22,12], in particular by switching to the shift-and-invert (SAI) Krylov subspace $\mathcal{K}((I + \gamma A)^{-1}, w)$ [23,24], where $\gamma > 0$ is a parameter related to T. The price for the faster convergence is that in these methods a system with the matrix $I + \gamma A$ has to be solved at each Krylov step.

Another useful property of the Krylov subspace methods is that they can be applied to solve (1) iteratively. More specifically, assume we have an approximation $y_k(t) \approx y(t)$ for which the residual $r_k(t)$, defined by (4), is known (here we intentionally changed the subindex from m to k). Then a better approximation can be obtained by the following iteration:

$$\text{(a) find an approximate solution } \xi_k(t) \text{ of } \begin{cases} \xi'(t) = -A\xi(t) + r_k(t), \\ \xi(0) = 0, \end{cases} \tag{6}$$

$$\text{(b) update } y_{k+1}(t) = y_k(t) + \xi_k(t). \tag{7}$$

Clearly, if the correction problem (6) is solved exactly then the iteration converges to the exact solution $y(t)$ after one step. One possible option is to solve (6) by a Krylov subspace method: at each iteration k, a number m of Krylov iterations are applied to solve (6) approximately. In fact this can be seen as an efficient restarting procedure for the Krylov subspace methods [15,17]. See also related work on Krylov subspace methods and restarting [25–28,12].

[1] Following [20, p. 36], by a matrix with a stiff spectrum we understand a matrix A such that implicit time integrators perform much better for $y' = -Ay$ than explicit ones. For a more formal definition of stiffness see [21].

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