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Analysis of inexact Krylov subspace methods for approximating the matrix exponential

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Abstract

Krylov subspace methods have proved quite effective at approximating the action of a large sparse matrix exponential on a vector. Their numerical robustness and matrix-free nature have enabled them to make inroads into a variety of applications. A case in point is solving the chemical master equation (CME) in the context of modeling biochemical reactions in biological cells. This is a challenging problem that gives rise to an extremely large matrix due to the curse of dimensionality. Inexact Krylov subspace methods that build on truncation techniques have helped solve some CME models that were considered computationally out of reach as recently as a few years ago. However, as models grow, truncating them means using an even smaller fraction of their whole extent, thereby introducing more inexactness. But experimental evidence suggests an apparent success and the aim of this study is to give theoretical insights into the reasons why. Essentially, we show that the truncation can be put in the framework of inexact Krylov methods that relax matrix–vector products and compute them expediently by trading accuracy for speed. This allows us to analyze both the residual (or defect) and the error of the resulting approximations to the matrix exponential from the viewpoint of inexact Krylov methods.

Keywords: Matrix exponential; Inexact Krylov method; Chemical master equation

1. Introduction

Given a large sparse nonsymmetric matrix $\boldsymbol{A} \in \mathbb{R}^{n\times n}$ and vector $\boldsymbol{p}_0 \in \mathbb{R}^n$, letting $\boldsymbol{v} = \boldsymbol{p}_0$ and taking $m \ll n$ Arnoldi steps with a starting vector $\boldsymbol{v}_1 = \boldsymbol{v}/\|\boldsymbol{v}\|$, where $\|\cdot\|$ means the 2-norm, we obtain an orthonormal basis $\boldsymbol{V}_m = [\boldsymbol{v}_1, \ldots, \boldsymbol{v}_m] \in \mathbb{R}^{n\times m}$ of the Krylov subspace $\mathcal{K}_m(\boldsymbol{A}, \boldsymbol{v}) = \text{span}\{\boldsymbol{v}, \boldsymbol{A}\boldsymbol{v}, \ldots, \boldsymbol{A}^{m-1}\boldsymbol{v}\}$, and an upper Hessenberg matrix $\boldsymbol{H}_m \in \mathbb{R}^{m\times m}$ that satisfy

$$\boldsymbol{A}\boldsymbol{V}_m = \boldsymbol{V}_{m+1}\overline{\boldsymbol{H}}_m = \boldsymbol{V}_m\boldsymbol{H}_m + h_{m+1,m}\boldsymbol{v}_{m+1}\boldsymbol{e}_m^T, \tag{1a}$$

$$\boldsymbol{H}_m = \boldsymbol{V}_m^T\boldsymbol{A}\boldsymbol{V}_m, \tag{1b}$$

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where $\boldsymbol{e}_m = (0, \ldots, 0, 1)^T$, and $\overline{\boldsymbol{H}}_m \in \mathbb{R}^{(m+1)\times m}$ is $\boldsymbol{H}_m$ augmented with $h_{m+1,m}\boldsymbol{e}_m^T$ under its last row. The standard Krylov approximation to the matrix exponential takes the form

$$\exp(\tau \boldsymbol{A})\boldsymbol{v} \approx \boldsymbol{V}_m \exp(\tau \boldsymbol{H}_m)\beta \boldsymbol{e}_1, \quad \boldsymbol{e}_1 = (1, 0, \ldots, 0)^T, \ \beta = \|\boldsymbol{v}\|. \tag{2}$$

It is well-known that (1) is also the cornerstone for building very efficient Krylov subspace solution techniques for other problems such as eigenvalue problems or linear systems. In the latter, there has been recent interest in transitioning from exact to inexact (or relaxed) matrix–vector products in the Arnoldi process [3,4,15], either out of necessity or deliberately, trading accuracy for speed. It is customary to model these inexact products as

$$\boldsymbol{A}\boldsymbol{v}_k \approx (\boldsymbol{A} + \boldsymbol{E}_k)\boldsymbol{v}_k, \tag{3}$$

where $\boldsymbol{E}_k$ is some error matrix that varies at each invocation, and note that setting $\boldsymbol{E}_k = \boldsymbol{0}$ recovers the exact evaluation. To make the difference clear, we refer to the classical method as the exact Arnoldi and it is not meant to imply exact arithmetic. The foremost implication of such a relaxation is that the classical Arnoldi relationship (1) does not hold anymore, but Simoncini and Szyld [15] made the key observation that we end up with

$$(\boldsymbol{A} + \boldsymbol{\mathcal{E}}_m)\boldsymbol{V}_m = \boldsymbol{V}_m\boldsymbol{H}_m + h_{m+1,m}\boldsymbol{v}_{m+1}\boldsymbol{e}_m^T, \quad \boldsymbol{\mathcal{E}}_m = \sum_{k=1}^{m} \boldsymbol{E}_k\boldsymbol{v}_k\boldsymbol{v}_k^T, \tag{4}$$

which is similar to (1), except that $\boldsymbol{V}_m$, which still remains orthonormal, is now a basis of a Krylov subspace obtained by a perturbed $\boldsymbol{A}$. When we use the computed $\boldsymbol{V}_m$ and $\boldsymbol{H}_m$ from (4) in GMRES for instance, classical error bounds do not apply anymore. However, from theoretical and experimental evidence (such as [14]), the method can withstand cases where the norm of the perturbation $\boldsymbol{\mathcal{E}}_m$ grows quite large.

The analysis of Simoncini and Szyld [15] provided insights into inexact GMRES for solving a linear system $\boldsymbol{A}\boldsymbol{x} = \boldsymbol{b}$, but it has so far remained unclear how inexactness affects the Krylov approximation (2). Since we now have (4) instead of (1), we also lose classical error bounds on the matrix exponential (e.g., Gallopoulos and Saad [5], Saad [11], Hochbruck and Lubich [9]). Thus our study fills a gap in the literature by looking at the error in the inexact Krylov counterpart of (2). We additionally offer another related way of assessing the accuracy by investigating the defect or residual [2] from the fact that (2) arises when solving a system of linear ODEs of the form

$$\begin{cases} \boldsymbol{p}'(t) = \boldsymbol{A}\boldsymbol{p}, & t \in [0,\ t_f] \\ \boldsymbol{p}(0) = \boldsymbol{p}_0, & \text{initial condition.} \end{cases} \tag{5}$$

It is worth recalling that, in the exact case, the effectiveness of approximating $\exp(\boldsymbol{A})\boldsymbol{v}$ by projecting it onto $\mathcal{K}_m(\boldsymbol{A}, \boldsymbol{v})$ hinges on the fact that all polynomials of $\boldsymbol{A}$ of degree $\leq m-1$ can be calculated exactly through $\boldsymbol{H}_m$, or more precisely,

$$q_{m-1}(\boldsymbol{A})\boldsymbol{v} = \boldsymbol{V}_m q_{m-1}(\boldsymbol{H}_m)\beta \boldsymbol{e}_1,$$

where q_{m-1} is any polynomial of degree $\leq m-1$. By the same reasoning as in the exact case (e.g., Saad [11, Lemma 3.1]), it can be shown from (4) that, for the same polynomial q_{m-1},

$$q_{m-1}(\boldsymbol{A} + \boldsymbol{\mathcal{E}}_m)\boldsymbol{v} = \boldsymbol{V}_m q_{m-1}(\boldsymbol{H}_m)\beta \boldsymbol{e}_1.$$

The significance of all this is that the inexact Krylov subspace method for $\mathcal{K}_m(\boldsymbol{A}, \boldsymbol{v})$ with the relaxation matrices $\boldsymbol{E}_k$, $k = 1, \ldots, m$, can be seen as the exact Krylov subspace method for $\mathcal{K}_m(\tilde{\boldsymbol{A}}, \boldsymbol{v})$ with

$$\tilde{\boldsymbol{A}} = \boldsymbol{A} + \boldsymbol{\mathcal{E}}_m = \boldsymbol{A} + \sum_{k=1}^{m} \boldsymbol{E}_k\boldsymbol{v}_k\boldsymbol{v}_k^T,$$

which is another simple way to understand the method.

The rest of the paper is organized as follows: Section 2 gives some background on modeling biochemical reactions and on the finite state projection (FSP) algorithm for solving the underlying chemical master equation (CME), which was the challenging application that initially motivated the research presented here. Section 3 analyzes the residual (or defect) of the inexact Krylov method both when the ODE problem is homogeneous or nonhomogeneous, with two different approaches considered for the latter. Section 4 analyzes the error and includes a special treatment that