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 of great importance. A case in point is solving the chemical master equation (CME) that models a system of biochemical reactions. This is a challenging problem that gives rise to an extremely large matrix due to the curse of dimensionality. Inexact Krylov subspace methods combined with 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. Numerical experiments demonstrating the theory are reported.

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