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An Efficient Algorithm to Construct an Orthonormal Basis for the Extended Krylov Subspace

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Abstract. Subspace projection methods based on the Krylov subspace using powers of a matrix A have often been standard for solving large matrix computations in many areas of application. Recently, projection methods based on the extended Krylov subspace using powers of A and A^{-1} have attracted attention, particularly for functions of a matrix times a vector and matrix equations. In this article, we propose an efficient algorithm for constructing an orthonormal basis for the extended Krylov subspace. Numerical experiments indicate that this algorithm has less computational cost and approximately the same accuracy as the traditional algorithm.

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Key words: Extended Krylov subspace, Krylov subspace, subspace projection methods, orthonormal basis, linear systems.

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1. Introduction

In this article, we investigate relevant subspaces and algorithms for constructing orthonormal bases used in subspace projection methods. These methods are commonly used in large matrix computations associated with linear systems $A\boldsymbol{x} = \boldsymbol{b}$, eigenvalue problems $A\boldsymbol{x} = \lambda\boldsymbol{x}$, functions of a matrix times a vector $f(A)\boldsymbol{b}$ and matrix equations $AX+XB+C=O$. Subspace projection methods reduce large dimensional matrix computations into smaller dimensional matrix computations, in a wide variety of large scale simulations from several areas of application.

Subspace projection methods involve constructing a given type of subspace, and then computing approximate solutions using the constructed subspace. The efficiency of a subspace projection method is largely dependent on the subspace used. There are two conditions to achieve high performance: 1) the solution of the target problem must be well

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approximated on a small dimensional subspace; and 2) the efficient construction of an orthonormal basis should be possible.

One of the most successful subspaces used in subspace projection methods where $A \in \mathbb{C}^{n\times n}, \boldsymbol{b} \in \mathbb{C}^n$ is the Krylov subspace, which involves powers of the matrix A as follows:

$$\mathbf{K}_m(A,\boldsymbol{b}) := \mathrm{span}\{\boldsymbol{b}, A\boldsymbol{b}, \cdots, A^{m-1}\boldsymbol{b}\}. \tag{1.1}$$

State-of-the-art algorithms for solving linear systems and eigenvalue problems are largely based on the Krylov subspace (1.1), which has also been actively studied for the more complicated matrix computations arising with functions of a matrix times a vector and matrix equations — e.g. see. Refs. [7, 12, 13].

Druskin & Knizhnerman [2] proposed an alternative to the Krylov subspace — viz. the extended Krylov subspace, involving not only powers of A but also of A^{-1} and defined by

$$\mathbf{EK}_m(A,\boldsymbol{b}) := \mathrm{span}\{\boldsymbol{b}, A^{-1}\boldsymbol{b}, A\boldsymbol{b}, A^{-2}\boldsymbol{b}, \cdots, A^{m-1}\boldsymbol{b}, A^{-m}\boldsymbol{b}\}, \tag{1.2}$$

where A is assumed to be nonsingular. This extended Krylov subspace has since received much attention in computations for functions of a matrix times a vector and matrix equations, because it can generally approximate solutions with higher accuracy than the Krylov subspace [5,6,8,15,16]. The extended Krylov subspace generally shows good convergence behaviour. However, multiple linear systems must be solved in order to construct its orthonormal basis, and this is the most time consuming step. Here we analyse characteristics of the linear systems that arise in the construction of the basis, and then propose a novel and more efficient algorithm for constructing an orthonormal basis of the extended Krylov subspace. The efficiency of our proposed algorithm is also evaluated in a series of numerical experiments. Throughout this article, $\mathbf{V}$ and $\mathbf{W}$ are subspaces and $\mathbf{V}+\mathbf{W}$ is their sum — i.e. $\mathbf{V}+\mathbf{W} := \{\boldsymbol{v}+\boldsymbol{w} | \boldsymbol{v} \in \mathbf{V}, \boldsymbol{w} \in \mathbf{W}\}$. The MATLAB colon notation is used, where for example $A(:,i)$ denotes the i-th column of a matrix A.

In Section 2, we briefly introduce the extended Krylov subspace and basic algorithm concepts used in constructing its orthonormal basis. In Section 3, we propose an efficient algorithm for constructing the basis of the extended Krylov subspace via an analysis of the characteristics of the arising linear systems. In Section 4, we evaluate the efficiency of our proposed algorithm in a series of numerical experiments. Our conclusions are summarized in Section 5.

2. The Extended Krylov Subspace and its Orthonormal Basis

As shown in Algorithm 2.1 below, subspace projection methods for large matrix computations consist of two steps: 1) constructing a subspace; and 2) computing an approximate solution. It is notable that the dimension of the subspace $\widetilde{k} := \dim \mathbf{L}_k$ is not always equivalent to the number of iterations k.

When the target problem has a vector solution (as is the case for linear systems, eigenvalue problems, and functions of a matrix times a vector), the approximate solutions