



A restarted Induced Dimension Reduction method to approximate eigenpairs of large unsymmetric matrices

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ABSTRACT

This work presents a new algorithm to compute eigenpairs of large unsymmetric matrices. Using the Induced Dimension Reduction method (IDR(s)), which was originally proposed for solving systems of linear equations, we obtain a Hessenberg decomposition, from which we approximate the eigenvalues and eigenvectors of a matrix. This decomposition has two main advantages. First, IDR(s) is a short-recurrence method, which is attractive for large scale computations. Second, the IDR(s) polynomial used to create this Hessenberg decomposition is also used as a filter to discard the unwanted eigenvalues. Additionally, we incorporate the implicitly restarting technique proposed by D.C. Sorensen, in order to approximate specific portions of the spectrum and improve the convergence.

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1. Introduction

A variety of applications involve the solution of the eigenvalue problem. This problem consists in finding a subset of pairs $(\lambda, \mathbf{x})$ of a matrix $A \in \mathbb{C}^{n \times n}$, such that:

$$A\mathbf{x} = \lambda\mathbf{x}, \quad (1)$$

where $\lambda \in \mathbb{C}$ is called eigenvalue, and the nonzero vector $\mathbf{x} \in \mathbb{C}^n$ is its corresponding eigenvector. When the matrix A is large and unsymmetric, solving the eigenvalue problem becomes computationally challenging.

Methods to approximate a subset of eigenpairs of large unsymmetric matrices are usually based on the construction of a standard Hessenberg decomposition associated with the matrix A , i.e.

$$AU_m = U_mB_m + \mathbf{u}_{m+1}\mathbf{e}_m^T, \quad (2)$$

where $U_m \in \mathbb{C}^{n \times m}$, B_m is a Hessenberg matrix of order m , $\mathbf{u}_{m+1} \in \mathbb{C}^n$, and $\mathbf{e}_m$ is the m th canonical vector, with m being typically much smaller than n . Under certain conditions, the eigenvalues of the matrix B_m approximate a subset of eigenvalues of A .

The Induced Dimension Reduction (IDR(s)) was introduced in 2008 for solving systems of linear equations [1]. IDR(s) is a short-recurrence method which has obtained attention for its rapid convergence and computational efficiency. IDR(s) as a method to compute eigenvalues was first studied by M. H. Gutknecht and J.-P. M. Zemke in [2]. The work that we present here is a continuation of [3]. We describe how to obtain an underlying Hessenberg decomposition of the form (2) from IDR(s), and

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we combine it with the implicitly restarting technique introduced by D.C. Sorensen [4] for Arnoldi in order to approximate the eigenpairs of interest. Additionally, we suggest a parameter selection for our proposed method which defines a filter polynomial for the spectrum.

This document is structured as follows. In Section 2, we present an overview of the Hessenberg decompositions, which are the basis for large scale eigenvalues/eigenvectors approximation. Section 3 explains how to compute a Hessenberg decomposition based on the IDR method. Two techniques to refine the information obtained from the IDR-Hessenberg factorization are discussed in Section 4. In Section 5, we present numerical experiments to illustrate the behavior of the method proposed.

We use the following notation: capital letters denote matrices, and the transpose of a matrix A is represented by A^T . Column vectors are represented by bold-face, lower case letters. Greek lower case letters represent complex scalars. I_n is the identity matrix of order n , and wherever the context is clear the subindex n is eliminated. Subspaces are denoted by uppercase calligraphic letters.

2. Background on Hessenberg decompositions

In Eq. (2), the columns of the matrix U_m represent a basis for the Krylov subspace,

$$\mathcal{K}_m(A, \mathbf{x}) = \{\mathbf{x}, A\mathbf{x}, A^2\mathbf{x}, \dots, A^{m-1}\mathbf{x}\}. \quad (3)$$

The upper Hessenberg matrix B_m is the projection of the matrix A over $\mathcal{K}_m(A, \mathbf{x})$. Projections onto Krylov subspaces are the basis for several methods to solve system of linear equations and eigenpairs approximation (see for example [5,6]). To compute eigenvalues of large, unsymmetric, and sparse matrices, the most common options between the Krylov methods are Bi-Lanczos [7] and the Arnoldi method [8]. Each of them creates a different Hessenberg decomposition associated with the matrix A . Bi-Lanczos method uses a short-recurrence formulas to create two Hessenberg tridiagonal decompositions of the form

$$AV_m = V_m T_m + \mathbf{f} \mathbf{e}_m^T$$

and

$$A^T W_m = W_m T_m^T + \mathbf{s} \mathbf{e}_m^T,$$

where $\mathbf{e}_m$ is the m th canonical vector, $\mathbf{f}$ and $\mathbf{s} \in \mathbb{C}^n$, $T_m \in \mathbb{C}^{m \times m}$ is a tridiagonal matrix, the matrix $V_m \in \mathbb{C}^{n \times m}$ is a basis for $\mathcal{K}_m(A, \mathbf{v}_1)$, $W_m \in \mathbb{C}^{n \times m}$ is a basis for $\mathcal{K}_m(A^T, \mathbf{w}_1)$ and the matrices V_m and W_m are bi-orthogonal ($W_m^T V_m = I_m$). However, despite being an efficient short-recurrence method, Bi-Lanczos is numerically unstable (see [9]).

Arnoldi method, on the other hand, builds a Hessenberg decomposition

$$AV_m = V_m H_m + \mathbf{f} \mathbf{e}_m^T,$$

where $\mathbf{f} \in \mathbb{C}^n$ and V_m is a matrix with orthogonal columns and represents a basis for $\mathcal{K}_m(A, \mathbf{v}_1)$. This method is widely used to approximate a subset of the eigenpairs of A ; nevertheless, its computational and memory cost increases per iteration. An option to overcome this issue is to restart the process (see [10]). Other Hessenberg decompositions to approximate eigenpairs based on Newton and Chebyshev polynomials can be found in [11–14].

The IDR(s) is a Krylov method proposed for solving systems of linear equations. It is based on the following theorem.

Theorem 1. Let A be any matrix in $\mathbb{C}^{n \times n}$, let $P = [\mathbf{p}_1, \mathbf{p}_2, \mathbf{p}_3, \dots, \mathbf{p}_s]$ be an $n \times s$ matrix, and let $\{\mu_j\}$ be a sequence in $\mathbb{C}$. With $\mathcal{G}_0 \equiv \mathbb{C}^n$, define

$$\mathcal{G}_{j+1} \equiv (A - \mu_{j+1}I)(\mathcal{G}_j \cap P^\perp) \quad j = 0, 1, 2, \dots,$$

where $P^\perp$ represents the orthogonal complement of P . If $P^\perp$ does not contain an eigenvector of A , then, for all $j = 0, 1, 2, \dots$, the following hold:

1. $\mathcal{G}_{j+1} \subset \mathcal{G}_j$, and
2. $\text{dimension}(\mathcal{G}_{j+1}) < \text{dimension}(\mathcal{G}_j)$ unless $\mathcal{G}_j = \{\mathbf{0}\}$.

Proof. See [15,1]. $\square$

In order to solve a system of linear equations, IDR(s) forces the residual vector $\mathbf{r}_k = \mathbf{b} - A\mathbf{x}_k$ to be in the nested and shrinking spaces $\mathcal{G}_j$, and then extracts the approximate solution $\mathbf{x}_k$. In the original implementations of IDR(s), the authors do not create explicitly any Hessenberg decomposition [1,16]. M. H. Gutknecht and J.-P. M. Zemke in [17] deduce a generalized Hessenberg decomposition from the IDR(s) method

$$AW_m U_m = W_m \hat{H}_m + \mathbf{w} \mathbf{e}_m^T, \quad (4)$$

from which only the eigenvalues values of A are approximated by the solution of the eigenvalue pencil $(\hat{H}_m, U_m)$. Here the matrices U_m and $\hat{H}_m$ are in $\mathbb{C}^{m \times m}$, with U_m upper triangular and, H_m is a Hessenberg matrix. The matrix W_m is not explicitly built.

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