The Spectral Transformation Lanczos Algorithm for the Symmetric-Definite Generalized Eigenvalue Problem: A Comparative Analysis with Conditioning Insights

by

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ABSTRACT

This thesis investigates the application of the spectral transformation Lanczos algorithm (ST-Lanczos) to a generalized symmetric-definite eigenvalue problem involving real symmetric matrices A and B, with B being positive definite and possibly ill conditioned. The Lanczos algorithm is a well-known iterative algorithm for computing the eigenvalues of a symmetric matrix and it works well for finding the extreme points in the spectrum. By leveraging a shifted and inverted formulation of the problem, the ST-Lanczos algorithm relies on iterative projection to approximate extremal eigenvalues near a shift σ. While previous work has been done using direct methods, the goal of this thesis is to use an iterative approach, and analyze how the error bounds already proven for direct methods play out in an iterative context.

This study focuses primarily on benchmarking the ST-Lanczos method against established direct methods in the literature and addresses challenges in numerical stability, computational efficiency, and sensitivity of residuals to ill-conditioning.

INDEX WORDS: eigenvalues, eigenvectors, Lanczos algorithm, Ritz values, Krylov subspaces, spectral transformation, orthogonality

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DEDICATION

I dedicate this project to God.

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[1] **[1]:** With titles like Mr. and Mrs. you want to use "\" (backslash space) instead of just space so it doesn't look like the end of a sentence as it does here.

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CHAPTER 1
INTRODUCTION

1.1 Background

The problem of computing eigenvalues and eigenvectors of matrices in numerical linear algebra is a well-studied one. The computation of eigenvalues and eigenvectors plays a central role in scientific computing with applications in structural analysis, quantum mechanics, data science and control theory. However, eigenvalue problems(standard and generalized) involving dense and sparse matrices present significant computational challenges, especially as the size of the matrices increases. These problems are fundamental in many scientific and engineering disciplines where the underlying mathematical models are often expressed in terms of eigenvalue equations. Historically, methods for solving eigenvalue problems date back to the early 20th century with foundational contributions from David Hilbert, Erhard Schmidt, and John von Neumann, who laid the groundwork for understanding linear operators and their spectral properties.

With the advent of digital computing in the mid-20th century, numerical methods for eigenvalue problems began to flourish. Classical iterative methods, such as the power iteration and inverse iteration, were among the first to be employed due to their simplicity and effectiveness for small-scale problems. However, as computational requirements grew, particularly with the need to solve larger sparse systems, researchers turned to more sophisticated algorithms. The Lanczos method, introduced by Cornelius Lanczos in 1950, represented a significant advancement for efficiently solving eigenvalue problems for large symmetric ma-

trices. The method exploits the sparsity of matrices and reduces the dimensionality of the problem by constructing a tridiagonal matrix whose eigenvalues approximate those of the original matrix.

An important class of eigenvalue problems which is the main focus of this thesis, is the generalized eigenvalue problem (GEP). The GEP takes the form $A\mathbf{v} = \lambda B\mathbf{v}$ where A and B are square matrices, λ is a generalized eigenvalue, and $\mathbf{v} \neq \mathbf{0}$ is the corresponding generalized eigenvector. This class of problems arises naturally in a number of application areas, including structural dynamics, data analysis and has a long history in the research literature on numerical linear algebra.

1.2 Literature Review

Generalized eigenvalue problems involving symmetric and positive definite matrices are fundamental in numerical linear algebra with applications in structural dynamics, quantum mechanics, and control theory. Solving these kind of problems involve computing the eigenvalues λ and eigenvectors v that satisfies the equation. The choice of method depends on the properties of the matrix involved in the problem we are trying to solve (e.g, sparsity, symmetry) and computational constraints. In this section, we discuss some of the research that has been done on this topic.

[2][1] considered the case when B[2] is invertible, in which the problem is reduced to $B^{-1}A\mathbf{v} =$

[1] **[2]:** Use numbered citations by commenting out some of the astronomical citation style things in the LaTeX preamble. I suggest adding instead \bibliographystyle{siam}. You can diff to see the changes I made to the preamble. As you have here, don't start a sentence with a reference; numbered references are common in math, but they look weird at the start of a sentence.

[2] **[3]:** use math mode here

$\lambda\mathbf{v}$. However, explicity forming $B^{-1}A$ is numerically unstable if B is ill-conditioned. Since B a symmetric and positive definite B, one can compute a Cholesky factorization $B = LL^T$ which allows us to reduce the equation to a standard eigenvalue problem $L^{-1}AL^{-T}\mathbf{y} = \lambda\mathbf{y}$ where $\mathbf{y} = L^T\mathbf{v}$, which can then be solved by using the symmetric QR algorithm to compute a Schur decomposition.

The QZ algorithm ([3]) for the non-symmetric GEP, is an iterative method that generalized the QR algorithm, to handle singular or ill-conditioned B. It applies orthogonal transformations to simutaneously reduce A and B to upper triangular forms from which the eigenvalues are extracted. Although this method is robust and backward stable, it is computationally expensive, thereby limiting its use to small or medium sized matrices.

1.3 Mathematical Preliminaries

In this section, we shall introduce some notations and the key mathematical concepts underlying the eigenvalue problems that will be used throughout this study.

1.3.1 Notation

Throughout this study, we make use of the following notations:

$A \in \mathbb{R}^{m \times n}$: denotes a matrix

$[A]_{ij}$: denotes element (i, j) of A

$\mathbf{x} \in \mathbb{R}^m$: denotes a column vector

A^T : denotes the transpose of matrix A

$\| \cdot \|$: denotes a vector or matrix norm

$\otimes$: denotes the Kronecker product of two matrices

$A_{i:i',j:j'}$: denotes the $(i' - i + 1) \times (j' - j + 1)$ submatrix of A

$A^{(k)}$: denotes the matrix A at the kth step of an iteration

1.3.2 Floating Point Arithmetic

We define a *floating point* number system, $\mathbf{F}$ as a bounded subset of the real numbers $\mathbb{R}$, such that the elements of $\mathbf{F}$ are the number 0 together with all numbers of the form

$$x = \pm(m/\beta^t)\beta^e,$$

where m is an integer in the range $1 \leq m \leq \beta^t$ known as the significand, $\beta \geq 2$ is known as the *base* or *radix* (typically 2), e is an arbitrary integer known as the exponent and $t \geq 1$ is known as the precision.

To ensure that a nonzero element $x \in \mathrm{F}$ is unique, we can restrict the range of $\mathbf{F}$ to $\beta^{t-1} \leq m \leq \beta^t - 1$. The quantity $\pm(m/\beta^t)$ is then known as the *fraction* or *mantissa* of x. We define the number $u \coloneqq \frac{1}{2}\beta^{1-t}$ as the *unit roundoff* or *machine epsilon*. In a relative sense, the *unit roundoff* is as large as the gaps between floating point numbers get.

Let $fl : \mathbb{R} \to \mathbf{F}$ be a function that gives the closest floating point approximation to a real number, then the following theorem gives a property of the unit roundoff.

Theorem 1.3.1. *If $x \in \mathbb{R}$ is in the range of $\mathbf{F}$, then $\exists\ \epsilon$ with $|\epsilon| \leq u$ such that $fl(x) = x(1+\epsilon)$.*

One way we could think of this is that, the difference between a real number and its closest floating point approximation is always smaller than u in relative terms.

1.3.3 Conditioning and Stability

Given any mathematical problem $f : X \to Y$, the conditioning of that problem pertains to the perturbation behaviour of the problem, while stability of the problem pertains to the perturbation behaviour of an algorithm used in solving that problem on a computer. A *well-conditioned* problem is one with the property that small perturbations of the input lead to only small changes in the output. An *ill-conditioned* problem is one with the property that small perturbations in the input leads to a large change in the output.

For any mathematical problem, we can associate a number called the *condition number* to that problem that tells us how well-conditioned or ill-conditioned the problem is. For the purpose of this thesis, we shall only be considering the condition number of matrices. Since

matrices can be viewed as linear transformations from one vector space to another, it makes sense to define a condition number for matrices.

For a matrix $A \in \mathbb{R}^{m\times n}$, the condition number with respect to a given norm is defined as

$$\kappa(A) = \|A\| \cdot \|A\|^{-1}.$$

In simpler terms, the condition number quantifies how the relative error in the solution of a linear system $Ax = b$ can be amplified when there is a small perturbation in the input vector x If $\kappa(A)$ is small, A is said to be *well-conditioned*; if $\kappa(A)$ is large, then A is said to be *ill-conditioned*. It should be noted that the notion of being "small" or "large" depends on the application or problem we are solving. If $\|\cdot\| = \|\cdot\|_2$ (spectral norm or 2-norm), then $\|A\| = \sigma_1$ and $\|A^{-1}\| = 1/\sigma_m$, so that

$$\kappa(A) = \frac{\sigma_1}{\sigma_m}, \tag{1.1}$$

where σ_1 and σ_m are the largest and smallest singular values of A respectively.

1.3.4 The Generalized Eigenvalue Problem

Let $A, B \in \mathbb{R}^{m\times m}$, be any general square matrices. A *pencil* is an expression of the form $A - \lambda B$, with $\lambda \in \mathbb{R}$. The *generalized eigenvalues* of $A - \lambda B$ are the elements of the set $\Lambda(A, B)$ defined by

$$\Lambda(A, B) = \{z \in \mathbb{R} : \det(A - zB) = 0\}. \tag{1.2}$$

In other words, the generalized eigenvalues of A and B are the roots of the characteristic polynomial of the pencil $A - \lambda B$ given by

$$p_{A,B}(\lambda) = \det(A - \lambda B) = 0 \tag{1.3}$$

A pencil is said to be *regular* if there exists at least one value of $\lambda \in \mathbb{R}$ such that $\det(A - \lambda B) = 0$, otherwise it is called *singular*.

If $\lambda \in \Lambda(A, B)$ and $0 \neq \mathbf{v} \in \mathbb{R}^m$ satisfies

$$A\mathbf{v} = \lambda B\mathbf{v}, \tag{1.4}$$

then $\mathbf{v}$ is a generalized eigenvector of A and B corresponding to λ. The problem of finding non-trivial solutions to (1.4) is known as the *generalized eigenvalue problem*.

If B is non-singular, then the problem reduces to a standard eigenvalue problem

$$B^{-1}A\mathbf{v} = \lambda\mathbf{v} \tag{1.5}$$

In this case, the generalized eigenvalue problem has m eigenvalues if $\text{rank}(B) = m$. This suggests that the generalized eigenvalues of A and B are equal to the eigenvalues of $B^{-1}A$.

If B is singular or rank deficient, then the set of generalized eigenvalues $\Lambda(A, B)$ may be finite, empty or infinite. If the $\Lambda(A, B)$ is finite, the number of eigenvalues will be less than m. This is because the characteristic polynomial $\det(A - \lambda B)$ is of degree less than m, so that there is not a complete set of eigenvalues for the problem.

If A and B have a common null space, then every choice of λ will be a solution to (1.4). In this case, we say that the pencil $A - \lambda I$ is *singular*. Otherwise, we say that the pencil is

regular. For the purpose of this study, we shall assume that A and B do not have a common null space, that is

$$\mathcal{N}(A) \cap \mathcal{N}(B) = \{\mathbf{0}\} \tag{1.6}$$

When A and B are symmetric and B is positive definite, we shall call the problem symmetric-definite generalized eigenvalue problem, which will be the focus of this thesis.

1.3.5 Lanczos Algorithm

The Lanczos algorithm is an iterative method in numerical linear algebra used in finding the eigenvalues and eigenvectors of a *symmetric* matrix. It is particularly useful when dealing with large scale problems, where directly computing the eigenvalues and eigenvectors of the matrix would be computationally expensive of infeasible. It works by finding the "most useful" eigenvalues of the matrix — typically those at the extreme of the spectrum, and their eigenvectors. At it's core, the main goal of the algorithm is to approximate the extreme eigenvalues and eigenvectors of a large, sparse, symmetric matrix by transforming the matrix into a smaller tridiagonal matrix that preserves the extremal spectral properties of the original matrix. This reduction is achieved by iteratively constructing an orthonormal basis of the Krylov subspace associated with the matrix.

Given a symmetric matrix $A \in \mathbb{R}^{m \times m}$, and an initial vector $\mathbf{v_1}$, the Lanczos algorithm produces a sequence of vectors $\mathbf{q_1}, \mathbf{q_2}, \cdots, \mathbf{q_n}$ (where n is the number of iterations) that forms an orthonormal basis for the n-dimensional Krylov subspace

$$\mathcal{K}_n(A, \mathbf{v_1}) = \text{span}(\{\mathbf{v_1}, A\mathbf{v_1}, A^2\mathbf{v_1}, \ldots, A^{n-1}\mathbf{v_1}\}) \tag{1.7}$$

This orthonormal basis is used to form a tridiagonal matrix T_n whose eigenvalues approximate the eigenvalues of A.

1.3.6 Spectral Transformation

Spectral transformation in numerical linear algebra is a technique that is used to modify the spectrum of matrix in a controlled way. This is usually done to improve the convergence properties of an algorithm or to make certain matrix properties more accessible. In the context of eigenvalue problems, spectral transformation is often used in direct and iterative methods, where manipulating the matrix can help focus on certain eigenvalues or improve numerical stability.

The central idea behind spectral transformation is that by applying a rational or polynomial transformation to the matrix A, we can manipulate its eigenvalues to increase the magnitude of the eigenvalues we are interested in without changing their eigenvectors. There are various types of spectral transformation, but the one of particular interest in this thesis is the *shift-invert* transformation. The shift-invert transformation involves transforming the original problem into a shifted and inverted one which can then be solved using a direct or iterative solver. This method focuses on finding the eigenvalues near a specified shift σ. It is useful when one is interested in a few eigenvalues near a given point in the spectrum.

Consider the problem of computing the eigenvalues of a matrix $A \in \mathbb{R}^{m\times m}$. Assume that m is so large that computing all the eigenvalues of A is not computationally feasible but rather, we are interested in computing the eigenvalues in a certain region of the spectrum of A. We can pick a shift $\sigma \in \mathbb{R}$ that is not an eigenvalue of A. The shifted and inverted

matrix is then given by $(A - \sigma I)^{-1}$. The eigenvectors of $(A - \sigma I)^{-1}$ are the same as the eigenvectors of A, and the corresponding eigenvalues are $(\lambda_j - \sigma)^{-1}$, for each eigenvalue λ_j of A. This shifts the spectrum of A, making the eigenvalues near σ much more prominent in the transformed matrix.

For a generalized eigenvalue problem given in (1.4), if we introduce a shift $\sigma \in \mathbb{R}$ so that $A - \sigma B$ is non singular, the shifted and inverted formulation of the problem is given by

$$(A - \sigma B)^{-1} B\mathbf{v} = \theta \mathbf{v}, \tag{1.8}$$

where $\theta = 1/(\lambda - \sigma)$.

Suppose σ is close enough to a generalized eigenvalue $\lambda_J \in \Lambda(A, B)$ much more than the other generalized eigenvalues, then $(\lambda_J - \sigma)^{-1}$ may be much larger than $(\lambda_j - \sigma)^{-1}$ for all $j \neq J$. This transformation will map the eigenvalues in the neighborhood of σ to the extreme part of the new spectrum and, by using an iterative method like the Lanczos algorithm, it is likely that the algorithm will converge quickly to these extreme eigenvalues in the new spectrum. [3]

1.4 Problem Discussion

In this section, we provide a brief but formal statement of the problem we are trying to solve, the methodological approach we used in solving the problem, and discuss the challenges involved in solving these kind of problems.

[3] **[4]:** You still need to state a precise Lemma on the relation of the spectral transformation to the generalized eigenvalue problem. I would suggest you just restate the lemma from my paper.

The symmetric-definite dense generalized eigenvalue problem is formally given by:

$$A\mathbf{v} = \lambda B\mathbf{v}, \qquad \mathbf{v} \neq 0 \tag{1.9}$$

where A and B are $m \times m$ real symmetric matrices, B positive definite. Both A and B are dense matrices, meaning that a significant proportion of their entries are non-zero.

The goal is to compute the set of generalized eigenvalues $\Lambda(A, B)$ that satisfy this equation using the ST-Lanczos algorithm. We then proceed by formulating a shift-inverted form of the problem given by equation (1.8), thereby transforming it into a standard eigenvalue problem, which can then be solved using the Lanczos algorithm. In practice, we often compute a subset of these generalized eigenvalues corresponding to those in the vicinity of a given shift σ. To have a deep understanding of how well this method performs of these type of problems, we will setup a well-defined problem by generating synthetic matrices with known eigenvalue distribution, and we will implement the ST-Lanczos algorithm and see if we can achieve the same level of accuracy with direct methods. We will then investigate the relationship between matrix conditioning, the accuracy of computed eigenvalues and the sensitvity of the residuals to ill-conditioning.

1.5 Motivation of Study

This study is motivated by several key factors that underscore the importance of advancing our understanding and capabilities in solving these type of problems. Originally, the motivation for this study arises from the need to compare the efficiency, accuracy and stability of iterative and direct methods for solving eigenvalue problems. In particular, the proven error

bounds for the direct method in the paper by [4], shows that for a shift of moderate size, the relative residuals are small for generalized eigenvalues that are not much larger than the shift. It is natural to ask if the same can be said for an iterative method like the lanczos algorithm.

On another hand, the motivation is based on the goal of advancing the field of numerical linear algebra. The insights gained from analyzing the ST-Lanczos algorithm for dense generalized eigenvalue problems may inform the development of new algorithms or hybrid methods that combine the strengths of different methods. This could potentially lead to breakthroughs in the development of eigenvalue algorithms that are faster and more efficient that the current ones we have today.

CHAPTER 2
METHODOLOGY AND ALGORITHM DESCRIPTION

2.1 Spectral Transformation

In this chapter, we shall present a detailed description of the methodologies and implementation of algorithms used in this thesis to solve the generalized eigenvalue problem. We begin by describing the problem setup, followed by a discussion of the algorithms used, together with their implementation details. This chapter aims to provide a comprehensive understanding of how these algorithms are applied to derive the solutions to the problem at hand. We shall also give a description of the numerical experiments we setup to investigate the efficiency of these algorithms.

Consider the symmetric-definite generalized eigenvalue problem:

$$A\mathbf{v} = \lambda B\mathbf{v}, \qquad \mathbf{v} \neq 0 \tag{2.1}$$

where A and B are $m \times m$ real, sparse, symmetric and B is positive definite or positive semi-definite.

Problem (2.1) can be reformulated as

$$\beta A\mathbf{v} = \alpha B\mathbf{v}, \qquad \mathbf{v} \neq 0 \tag{2.2}$$

We have replaced λ with α/β for convenience so that the generalized eigenvalues will be of the form (α, β). If $\beta = 0$, then the generalized eigenvalues $\Lambda(A, B)$ will be infinite. The formulation using equation(2.2) is useful when describing the error bounds, as we shall later see. We shall alternate between (2.1) and (2.2) when convenient. We also observe that the

symmetric-definite generalized eigenvalue problem have real eigenvalues.

To compute the eigenvalues and eigenvectors that satisfy equation(2.1) with spectral transformation lanczos algorithm, our approach will be in two steps:

- Transform the generalized problem into a spectral transformed standard eigenvalue problem.
- Solve the spectral problem with Lanczos algorithm.

Let $\sigma \in \mathbb{R}$ be a desired shift such that $A - \sigma B$ is non-singular. The shifted problem takes the form:

$$(A - \sigma B)\mathbf{v} = (\lambda - \sigma)B\mathbf{v}. \tag{2.3}$$

We shall begin by computing decompositions for $A - \sigma B$ and B. If B is positive definite, we can compute a Cholesky decomposition $B = C_b C_b^T$ using SciPy `cholesky` method which calls LAPACK `xPOTRF`. However, if B is semi positive definite, this function call fails and we use the more robust pivoted Cholesky factorization `xPSTRF` by calling the inbuilt LAPACK bindings in SciPy.

There are various possible factorization options for $A - \sigma B$. One option is to use the pivoted LDL^T factorization used by [4] and [1] where D is a block diagonal matrix with 1×1 and 2×2 on the diagonal, and L is a lower triangular matrix. This factorization uses the Bunch-Kaufman pivoting scheme with "rook pivoting" which is stable. Although the standard LDL^T factorization (without "rook pivoting") is available in SciPy linear algebra module, there is no option to use the rook pivoting scheme except if one chooses to write a custom

LAPACK binding that makes use of `DSYTRF_ROOK`. While this can guarantee some stability for the problem we are trying to solve, it usually involves extra work in processing the 2×2 blocks to make D diagonal.

Another factorization is an eigenvalue decomposition of $A - \sigma B$. If we use a symmetric eigenvalue decomposition $A - \sigma B = WDW^T$, our numerical experiments reveals that this stabilizes the Ritz residuals and generalized form of the residuals together with the advantage that these residuals are insensitive to the conditioning of A and B. This can be done using inbuilt eigenvalue solvers in SciPy or any linear algebra library. This is the most promising factorization, however computing eigenvalue decompositions for large problems become computationally expensive and not feasible in reality.

Lastly, we can make use of an LU factorization for $A - \sigma B$. Unlike the previous factorizations, the stability for the Ritz residuals is not as great, as we observe that they depend on the conditioning of A and B. However, for the purpose of this thesis, we make use of the LU decomposition since it is computationally less expensive and easy to use and implement.

One major takeaway from our experiments with the various options of factorizing $A - \sigma B$ is that symmetry is clearly important for stability. We plan to give a mathematical justification for this in future work.

Continuing with the algorithm derivation, if we assume $\lambda \neq \infty$ and $\mathbf{v} \neq \mathbf{0}$. Since B is positive definite, [4], proved that we can compute a Cholesky factorization $B = C_b C_b^T$, and apply the shift-invert spectral transformation to transform equation(2.1) into its spectral

form as described in section (1.3.6) such that $\theta = 1/(\lambda - \sigma)$ is an eigenvalue of the problem :

$$C_b^T (A - \sigma B)^{-1} C_b \mathbf{u} = \theta \mathbf{u}, \qquad \mathbf{u} \neq \mathbf{0} \tag{2.4}$$

where $\mathbf{u} = C_b^T \mathbf{v} \neq \mathbf{0}$.

Conversely, assume that $\mathbf{u} \neq \mathbf{0}$ is an eigenvector of (2.4) and θ its corresponding eigenvalue, then the vector $\mathbf{v} = (A - \sigma B)^{-1} C_b \mathbf{u} \neq \mathbf{0}$ is an eigenvector for (2.2), with eigenvalue $(1 + \sigma\theta, \theta)$, provided $C_b \mathbf{u} \neq \mathbf{0}$.

Equation (2.4) gives us the spectral transformed version of the original generalized problem. Since the problem is now in a standard form, we can then apply the Lanczos algorithm to compute the desired eigenvalues within the neighborhood of σ, together with their corresponding eigenvectors. It should be noted that forming the spectral matrix in (2.4) is not desirable in a realistic problem since it does not preserve sparsity and will be very inefficient on most realistic problems. Given our recent results, one might suggest using a stable decomposition such as the LU factorization. However, as we will demonstrate, decompositions that preserve symmetry exhibit certain stability advantages in practice.

2.2 Lanczos decomposition

In this section, we revisit the Lanczos algorithm, and discuss how we apply it to the spectral transformed problem. As discussed in section (1.3.5), the Lanczos algorithm approximates the eigenvalues of the original problem by projecting it onto a Krylov subspace spanned by successive powers of the system matrix applied to an initial vector. The eigenvalues approximation arises from the tridiagonal matrix obtained through the Lanczos process,

which captures the essential spectral characteristics of the original matrix.

Given $A \in \mathbb{R}^{m\times m}$, with $A = A^T$, the pesudocode for the lanczos algorithm is described by Algorithm 1. After the completion of algorithm 1, the γ's and δ's are used to construct the

Algorithm 1 Lanczos Algorithm for a Symmetric Matrix

Require: $A = A^T$, number of iterations: n, tolerance: tol

function LANCZOS(A, n, tol)
  Choose an arbitrary vector $\mathbf{b}$ and set an initial vector $\mathbf{q_1} = \mathbf{b}/\|\mathbf{b}\|_2$
  Set $\delta_0 = 0$ and $\mathbf{q_0} = \mathbf{0}$
  for $j = 1, 2, \ldots, n$ **do**
    $\mathbf{v} = A\mathbf{q_j}$
    $\gamma_j = \mathbf{q_j}^T\mathbf{v}$
    $\mathbf{v} = \mathbf{v} - \delta_{j-1}\mathbf{q_{j-1}} - \gamma_j\mathbf{q_j}$
    Full reorthogonalization: $\mathbf{v} = \mathbf{v} - \sum_{i\leq j}(\mathbf{q_i}^T\mathbf{v})\mathbf{q_i}$
    $\delta_j = \|\mathbf{v}\|_2$
    if $\delta_j < tol$ **then**
      restart or **exit**
    end if
    $\mathbf{q_{j+1}} := \mathbf{v}/\delta_j$
  end for
end function

tridiagonal matrix $T_n \in \mathbb{R}^{n\times n}$ and the vectors $\mathbf{q_j}$'s are stacked together to form an orthogonal matrix $Q_n \in \mathbb{R}^{m\times n}$ given by:

$$T_n = \begin{pmatrix} \gamma_1 & \delta_1 & & & \\ \delta_1 & \gamma_2 & \delta_2 & & \\ & \delta_2 & \gamma_3 & \delta_3 & \\ & & \ddots & \ddots & \vdots \\ & & & \delta_{n-1} & \gamma_n \end{pmatrix}$$

$$Q_n = \left[\begin{array}{c|c|c|c} & & & \\ \mathbf{q_1} & \mathbf{q_2} & \cdots & \mathbf{q_n} \\ & & & \end{array}\right].$$

The decomposition is given by

$$AQ_n = Q_n T_n + \delta_n \mathbf{q_{n+1}} \mathbf{e_n}^T \tag{2.5}$$

In theory, the vectors q_j's should be orthonormal, but due to floating-point errors, there will be loss of orthogonalization, hence the need for line 8 in the Algorithm 1.

Let $\theta_i, i = 1, 2, \ldots n$(which can be computed by standard functions in using any eigenvalue solver) be the eigenvalues of T_n, and $\{\mathbf{y_i}\}_{i=1:n}$ be the associated eigenvectors. The $\{\theta_i\}$ are called the *Ritz values* and the vectors $\{Q_n \mathbf{y_i}\}_{i=1:n}$ are called the *Ritz vectors*. Hence, the eigenvalues of A are on both ends of the are well approximated by the Ritz values, with the Ritz vectors as their approximate corresponding eigenvectors of A.

Since the generalized eigenvalue problem we started with has been reduced to a standard one as shown in equation (2.3), Algorithm (1) can be applied to equation (2.3) with some slight modifications. The spectral form of Algorithm (1) is give by Algorithm (2). After applying the lanczos procedure to the spectral transformed problem (2.4), we then compute the converged Ritz pairs using a certain tolerance. The converged Ritz pairs are mapped to the generalized eigenvalues and eigenvectors where we can observe the behaviour of these residuals with respect to conditioning.

2.3 Problem Setup

To evaluate the performance and robustness of the spectral transformation lanczos algorithm, we setup a problem with predetermined eigenvalues, use the algorithm to compute the eigenvalues, and show that the residuals follow closely with the bounds predicted by di-

Algorithm 2 Spectral Lanczos Algorithm for (2.4)

Require: $A = A^T$, $B = B^T$, with B being positive definite or semidefinite
Require: number of iterations: n, size of matrix A or B: m, tolerance: tol
Require: $\sigma \in \mathbb{R}$: shift not close to a generalized eigenvalue

function SPECTRAL_LANCZOS(A, B, m, n, σ, tol)
  Choose an arbitrary vector $\mathbf{b}$ and set an initial vector $\mathbf{q_1} = \mathbf{b}/\|\mathbf{b}\|_2$
  Set $\beta_0 = 0$ and $\mathbf{q_0} = \mathbf{0}$
  Set $Q = \text{zeros}(m, n+1)$
  Precompute the LU factorization of $A - \sigma B$: $LU = (A - \sigma B)$
  Factor: $B = CC^T$
  for $j = 1, 2, \ldots, n$ **do**
    $Q[:, j] = \mathbf{q}_j$
    $\mathbf{u} = C\mathbf{q}_j$
    Solve: $(LU)\mathbf{v} = \mathbf{u}$ for $\mathbf{v}$
    $\mathbf{v} = C^T\mathbf{v}$
    if $j < n$ **then**
      $\alpha_j = \mathbf{q}_j^T\mathbf{v}$
      $\mathbf{v} = \mathbf{v} - \beta_{j-1}\mathbf{q}_{j-1} - \alpha_j\mathbf{q}_j$
      Full reorthogonalization: $\mathbf{v} = \mathbf{v} - \sum_{i \le j}(\mathbf{q}_i^T\mathbf{v})\mathbf{q}_i$
      $\beta_j = \|\mathbf{v}\|_2$
      if $\beta_j < tol$ **then**
        restart or **exit**
      end if
      $\mathbf{q}_{j+1} := \mathbf{v}/\beta_j$
    end if
  end for
  $Q = Q[:, : n]$
  $\mathbf{q} = Q[:, n]$
  return $(Q, T, \mathbf{q})$
end function

rect methods. While there are other options of using matrices from open source repositories like Matrix Market, we choose to use this approach so that we can control the size, condition number and other properties of the matrix so as to observe the effect of this properties on the algorithm.

Starting with a diagonal matrix $D \in \mathbb{R}^{m \times m}$ with known eigenvalues, we generate a

random matrix P of size $m \times m$ with standard normal distribution. Since the QR factorization is guaranteed to exist for any matrix, we take the QR factorization of P to obtain an orthogonal matrix Q, which is used to create a matrix C using orthogonal transformation. Hence $C = QDQ^T$ is unitarily similar to D.

Next, we initialize a random lower triangular matrix $L_0 \in \mathbb{R}^{m \times m}$ with a normal distribution. A symmetric positive definite $B \in \mathbb{R}^{m \times m}$ is formed by

$$B = L_0 L_0^T + \delta I_m, \qquad \delta > 0 \tag{2.6}$$

where I_m is an identity matrix of order m. Clearly, B is symmetric. The matrix $L_0 L_0^T$ is positive semi-definite since for any non-zero vector $\mathbf{x}$

$$\mathbf{x}^T (L_0 L_0^T)\mathbf{x} = (L_0^T \mathbf{x})^T (L_0^T \mathbf{x}) = \|L_0^T \mathbf{x}\|^2 \geq \mathbf{0}. \tag{2.7}$$

However, $L_0 L_0^T$ may not be strictly positive definite if L_0 is singular. The term δI_m ensures strict positve definiteness by adding δ to its diagonals, thereby shifting all eigenvalues by δ. If $\delta > 0$, then all eigenvalues of B will be strictly positive, ensuring B is positive definite. This guarantees that we can compute the Cholesky factorization of B without any numerical issues.

Another important thing to note is that, δ can be used to control the conditioning of B. We recall from section (1.3.3), that the condition number of B when B is symmetric, is defined as:

$$\kappa(B) = \frac{\lambda_{\max}(B)}{\lambda_{\min}(B)} \tag{2.8}$$

where $\lambda_{\max}(B)$ and $\lambda_{\min}(B)$ are the largest and smallest eigenvalues of B, respectively. In gen-

eral, B is usually ill-conditioned with a very large condition number so that if δ is large, the process of adding δI_m can regularize the condition number of B, making B well-conditioned, since that will equate to increasing $\lambda_{\min}(B)$. If δ is small, B can still be ill-conditioned but not in an astronomical way. Hence, δ is a hyperparameter we can use to control the condition of B. In this experiment, we choose $\delta = 10^{-2}$, which gives a condition number of $\kappa(B) = 5.39 \times 10^5$.

Since B is symmetric and positive definite, we can compute its Cholesky factorization $B = LL^T$ and construct A using a congruence transformation

$$A = LCL^T \tag{2.9}$$

So that the generalized eigenvalues $\Lambda(A, B)$ is equal to the eigenvalues of the diagonal matrix D. This can be summarized by the following lemma:

Lemma 2.3.1. *Let $A - \lambda B$ be a pencil, where A and B are symmetric, and B is strictly positive definite. Let D be a diagonal matrix and C be unitarily similar to D. Assuming (2.9) holds, then the generalized eigenvalues $\Lambda(A, B)$ is similar to D*

Proof. Given the generalized problem

$$A\mathbf{v} = \lambda B\mathbf{v}, \qquad \mathbf{v} \neq \mathbf{0} \tag{2.10}$$

Since B is positive definite, then clearly, it is invertible and the generalized eigenvalues $\Lambda(A, B)$ will be the eigenvalues of $B^{-1}A$.

Now

$$\begin{aligned} B^{-1}A &= (LL^T)^{-1}(LCL^T) \\ &= L^{-T}L^{-1}LQDQ^TL^T \\ &= (L^{-T}Q)D(Q^{-1}L^T) \\ &= (L^{-T}Q)D(L^{-T}Q)^{-1} \end{aligned}$$

Therefore $B^{-1}A$ is similar to D and hence $\Lambda(A, B)$ is similar to D. □

The pseudocode for generating A and B is described in Algorithm 3. With the problem

Algorithm 3 Setting up a GEP

Require: D: diagonal matrix with known eigenvalues, δ: regularization hyperparameter

function GENERATE_MATRIX(D, δ)
    Set $m =$ `size`(D)
    Q, _ = `qr`(random.randn(m, m))
    $C = QDQ^T$
    $L_0 =$ `tril`(`random.randn`(m, m))
    $B = (L_0L_0^T) + \delta I$
    $L =$ `cholesky`(B)
    $A = LCL^T$
    return (A, B)
end function

setup completed, and the algorithm described, in the next chapter, we shall discuss the results obtained in these experiments.

CHAPTER 3
EXPERIMENTAL RESULTS AND DISCUSSION

In this chapter, we will present a comprehensive analysis of the experimental results obtained from our implementation of the Spectral Transformation Lanczos algorithm for the symmetric definite generalized eigenvalue problem. We examine the algorithm performance on a test matrix, analyze the effects of ill-conditioning on convergence and accuracy, and compare the error bounds with what was predicted with direct methods.

3.1 Software and Computational Environment

The numerical experiments in this thesis are performed using the Python programming language together with the NumPy 2.0.2 and SciPy 1.13.1 libaries which makes function calls to optimized and efficient LAPACK and BLAS routines for linear algebra computations. These libraries ensure high-performance matrix operations and numerical stability. All computations are performed in **double precision** (64 bit floating point, `float64`) to maintain numerical accuracy and consistency.

For reproducibility, all code is written in Python 3.9.6 and executed within a controlled environment using `virtualenv`. All numerical results have been validated by comparing different levels of precision where applicable and verifying consistency with analytical results when available. Code for the experiments is managed using version control with Git to ensure reproducibility and can be found in https://github.com/AyobamiAdebesin/ayobami_thesis

3.2 Experimental Setup

To evaluate the ST-Lanczos algorithm, we employ Algorithm (3) to generate test matrices A and B with controlled eigenvalue distribution. For the purpose of this thesis, we will be testing with dense matrices The eigenvalues are divided into 3 distinct groups, each with a specified range (spread). For each of the three groups, a random set of eigenvalues was generated using a uniform distribution, ensuring that the eigenvalues are distributed evenly within their respective ranges.

- Group 1 contains 1500 eigenvalues in the range $(1, 199)$
- Group 2 contains 400 eigenvalues in the range $(200, 300)$
- Group 3 contains 100 eigenvalues in the range $(301, 400)$

The three sets of eigenvalues are then concatenated into a single array $D \in \mathbb{R}^{2000\times 2000}$, which is then used with a regularization hyperparameter $\delta = 10^{-2}$, to generate A and B of size 2000×2000. Our shift is choosen to be $\sigma = 201$. For this choice of δ, the condition number of A and B are as follows:

$$\kappa(A) = 1.23 \times 10^7, \qquad \kappa(B) = 5.39 \times 10^5$$

As discussed in section 2.3, A and B will be symmetric with B being positive definite. B is factored using the SciPy `cholesky` method which calls LAPACK `xPOTRF`. We chose to use this since B was designed to be strictly positive definite. We run Algorithm 2 for $n = 1200$

iterations for the spectral problem

$$C_b^T(A-\sigma B)^{-1}C_b\mathbf{u}=\theta\mathbf{u}, \qquad \mathbf{u}\neq\mathbf{0} \tag{3.1}$$

to compute the lanczos decomposition using various decompositions techniques for $A-\sigma B$ that was discussed in section 2.1. We explored these techniques and discuss the results in the following sections.

3.3 Metrics

To evaluate the efficiency of the ST-Lanczos algorithm, we define the following metrics

$$\text{Relative Decomposition Residual} = \frac{\|BQ_n - Q_nT_n - \mathbf{q}\mathbf{x}^T\|}{\|B\|}, \tag{3.2}$$

where $B = C_b^T(A-\sigma B)^{-1}C_b$.

$$\text{Generalized Relative Residual} = \frac{\|(\beta A-\alpha B)\mathbf{v}\|}{(|\beta|\|A\|+|\alpha|\|B\|)\|v\|} \tag{3.3}$$

[1]

$$\text{ST Relative Residual} = \frac{\|C_b^T(A-\sigma B)^{-1}C_b\mathbf{u}-|\theta|\mathbf{u}\|}{(C_b^T(A-\sigma B)^{-1}C_b+|\theta|)\|\mathbf{u}\|} \tag{3.4}$$

[1] **[5]:** I would write the numerator as $\|\beta A\mathbf{v}-\alpha B\mathbf{v}\|$ both here and in the code.

3.4 LU decomposition

The LU decomposition of $A - \sigma B$ is performed using the `linalg.lu_factor` function in SciPy, which employs partial pivoting. For $n = 1200$ iterations, the Krylov solution subspace has a dimension of 1200, and the ST Lanczos algorithm achieves a decomposition residual of the order of 10^{-10}, despite a full reorthogonalization. This reduction in accuracy is attributed to pivot-limited accuracy. Using a tolerance of 10^{-10} for the Ritz pair residuals computed by (3.4), approximately 75% of the Ritz pairs converge with an accuracy of the order 10^{-13} for Ritz values close to the shift. However, the generalized residuals for these converged Ritz pairs remain on the order of machine precision $u = 10^{-16}$. As shown in Fig 3.1, the residuals are small for eigenvalues near the shift and gradually tends to increase for larger eigenvalues, consistent with the error bounds proven by (Michael Stewart, 2024)[2] for a direct method. To examine the effect of conditioning, δ was increased to $\delta = 10^2$ so that $\kappa(A) = 4013$ and $\kappa(B) = 54.9$. For this *well-conditioned* problem, the Lanczos decomposition residual decreases to the order of 10^{-13}, indicating that the accuracy of the Lanczos decomposition is influenced by the problem's conditioning. Additionally, for the same tolerance, an improvement in the Ritz pair residuals was observed while the generalized residuals was not impacted by the problem's conditioning as shown in Fig 3.2. [3]

[4]

[2] **[6]:** Please use \cite like you did elsewhere.

[3] **[7]:** The range of values here isn't wide enough to see how much the order of magnitude of the generalized eigenvalues impacts the residual. With all eigenvalues between 150 and 400, they are all roughly the same order of magnitude. I'd go up to 10,000 and maybe down to 10^{-3}. The generalized eigenvalues for eigenvectors computed in the usual way should show residuals that increase away from the shift. The ones that are computed using the SVD should be better.

[4] **[8]:** Shouldn't there be three sets of residuals? Specifically: Generalized eigenvalues using the computed

Figure 3.1 Residuals plot for ill-conditioned problem

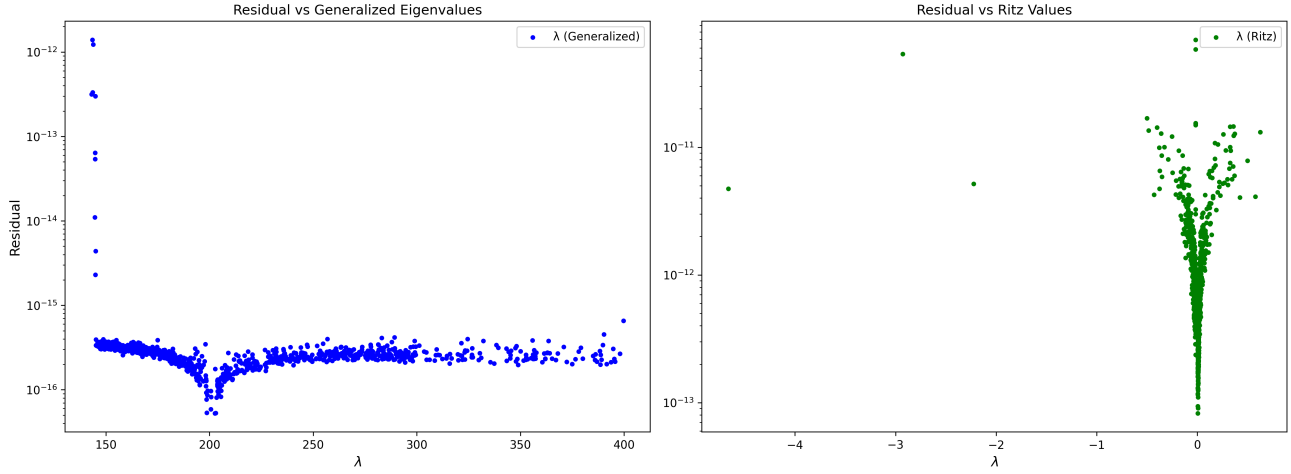
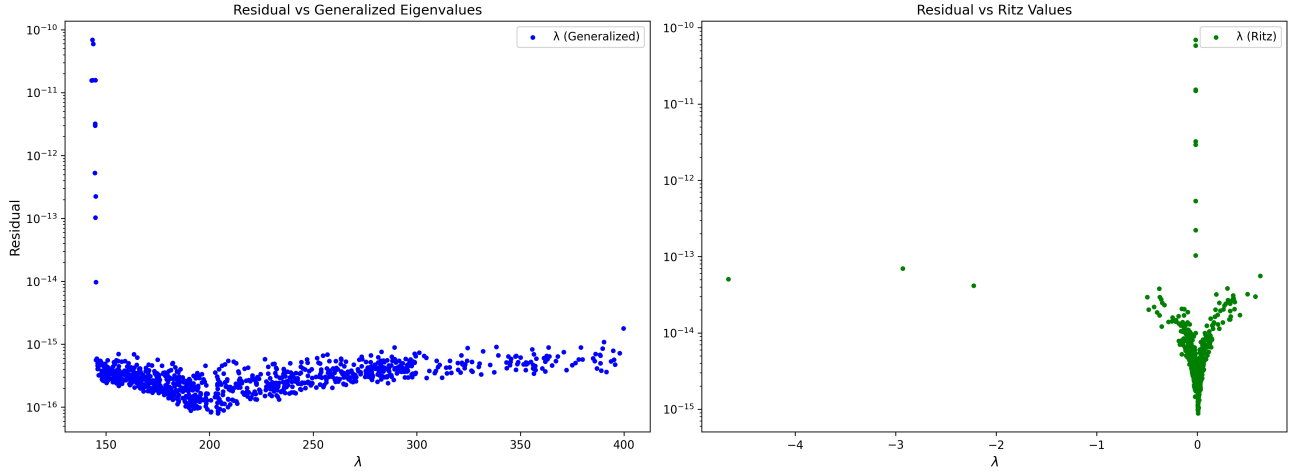


Figure 3.2 Residuals plot for well-conditioned problem



5

6

eigenvector, the Spectral transformed residuals, and the generalized eigenvalue residuals.

[5] **[9]:** You might also comment on the points that have much larger residuals; those correspond to not fully converged Ritz pairs.

[6] **[10]:** You haven't really done a comparison with the theorems in the paper. You still need to say what those theorems are and something about how they relate to the graphs. You need to state precise error bounds from the paper to do this.

3.5 Eigenvalue Decomposition

Another decomposition technique we employed is the symmetric eigenvalue decomposition of $A - \sigma B$ given by

$$A - \sigma B = WDW^T, \tag{3.5}$$

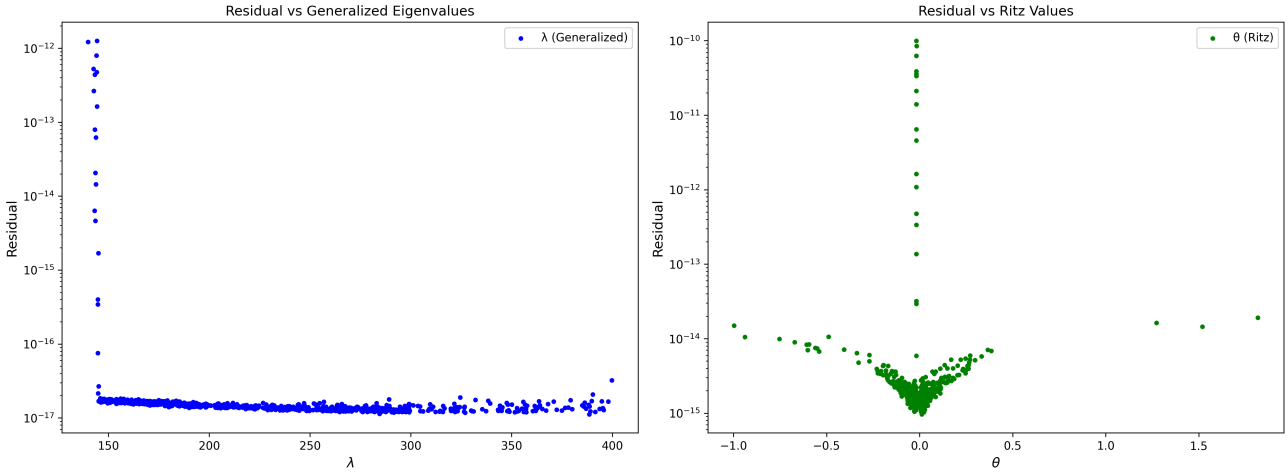
so that the spectral transformed problem is given by

$$C_b^T W^{-T} D^{-1} W^{-1} C_b \mathbf{u} = \theta \mathbf{u}, \qquad \mathbf{u} \neq \mathbf{0} \tag{3.6}$$

This decomposition, done using `linalg.eigh` function in SciPy, uses the LAPACK `dsyevd` routine for real symmetric matrices, which in turn uses divide-and-conquer algorithms for efficiency. The Lanczos decomposition residual was observed to be of the order 10^{-23}, indicating a highly accurate decomposition. The results of the residual analysis are presented in Fig 3.3 On the left plot, the residuals remain on the order of machine precision 10^{-17} for most eigenvalues. Similarly, on the right of the plot, the Ritz residuals are minimized near $\theta = 0$ with values on the order of machine precision and gradually increasing for larger Ritz values. To assess the effect of ill-conditioning, δ was reduced to $\delta = 10^{-5}$, so that $\kappa(A) = 8.2 \times 10^9$ and $\kappa(B) = 5.4 \times 10^8$. It was observed that this ill-conditioning did not affect the computed residuals with.

Overall, the extremely low decomposition residual confirms the robustness of using a decomposition that preserves symmetry, while the observed trends in residuals highlight the sensitivity of numerical accuracy to the spectrum of the problem.

Figure 3.3 Residuals plot for $A - \sigma B = W D W^T$



CHAPTER 4
CONCLUSION

This thesis has investigated the application and performance of the Spectral Transformation Lanczos algorithm for solving symmetric definite dense generalized eigenvalue problem. Through the numerical experiments, we validated our results with proven error bounds in direct methods, considered the implication of several methods, and the impact of certain properties of the matrix on the accuracy of the results. In this concluding chapter, we summarize our key findings, discuss the broader implications of this work, acknowledge limitations, and outline promising directions for future research.

4.1 Summary of Key Findings

The experiments in this thesis have uncovered some interesting results regarding the spectral transformation lanczos algorithm for generalized eigenvalue problems. First, we have established that the generalized residuals increases for eigenvalues farther away from the shift, if the shift is not too large in magnitude, validating the analytical error bounds proven for direct methods.

Secondly, our analysis of the eigenvalue sensitivity revealed the relationship between the conditioning of the matrices, and the accuracy of computed eigenvalues for various factorizations of the shifted matrix $A - \sigma B$. We observed that for any factorization involving symmetry(eigenvalue decomposition or LDL^T factorization), the ST-Lanczos is stable and the Ritz pairs converged to the order of unit round off u for the $n-$ lanczos steps. The

generalized eigenvalues also converged, achieving unit round off for all computed eigenvalues closer and farther away from the shift. This poses an interesting question: "Can we prove stability for any symmetric decomposition of $A - \sigma B$"?

Finally, for the LU decomposition of $A - \sigma B$, we observe that the lanczos procedure was stable but the behavior is largely dependent on the conditioning of A and B. However, our results indicated that, the generalized residuals were insensitive to the conditioning of the problem.

4.2 Importance and Implications

From a theoretical perspective, this work advances our knowledge of spectral transformation, matrix conditioning and eigenvalue sensitivity in the context of dense generalized eigenvalue problems. Our results showed that the conditional bounds for direct methods, holds true for iterative methods. This work goes a step further at highlighting an interesting property of spectral transformation methods that can determine stability for such methods, both in the direct and iterative context. This contributes to the broader field of numerical linear algebra by providing a more comprehensive framework for analyzing iterative eigenvalue solvers.

By characterizing the relationship between matrix factorizations and algorithm convergence, we have developed a better understanding of how spectral transformations affect the convergence of properties of Krylov subspace methods.

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[3] C. B. Moler and G. W. Stewart, *An algorithm for generalized matrix eigenvalue problems*, SIAM Journal on Numerical Analysis, 10 (1973), pp. 241–256.

[4] M. Stewart, *Spectral transformation for the dense symmetric semidefinite generalized eigenvalue problem*, 2024.