Lanczos Algorithm and Conjugate Gradient

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A thesis submitted in partial fulfillment of the

requirements for the degree of

Master of Science

University of Washington

2022

Committee:

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Program Authorized to Offer Degree:

Applied Mathematics

University of Washington

Abstract

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We review results from the literature on the conjugate gradient algorithm for solving symmetric positive definite linear systems and the related Lanczos algorithm. We derive the conjugate gradient algorithm from the more general conjugate direction method, using projectors. We establish error bounds using exact arithmetic theory and also discuss what can happen when floating-point arithmetic is used. We present numerical experiments to illustrate this behavior.

Contents

Acknowledgement

Firstly, I need to express my upmost gratitude to Professor Greenbaum for taking the time to review the several drafts of this thesis and for her help with my research throughout the year. Next, I am very grateful to the NARC reading group and participants and my Committee members, Professor Tom Trogdon for attending a trial run of the presentation for the content of this thesis. Finally, a big thanks to my old undergraduate classmate who is also a friend of mine who helped with fixing the typos on the later drafts.

1 Notations

1. $\mathrm{ran}(A) := \{Ax : \forall x \ \in \mathbb{R}^n\}, A \in \mathbb{R}^{m\times n}$, the range of a matrix.

2. $(A)_{i,j}$: The element in ith row and jth column of the matrix A.

3. $(A)_{i:i',j:j'}$: The submatrix whose top left corner is the (i, j) element in matrix A, and whose' right bottom corner is the (i', j') element in the matrix A. The notation is similar to MATLAB's rules for indexing.

4. $\forall\ 0 \le j \le k$: under certain context it indicates the range for an index: $j = 0, 1, \cdots, k-1, k$

5. Boldface $\mathbf{0}$ denotes the zero vector or matrix, depending on the context it can be either a zero row/column vector, or a zero matrix.

6. The $\hat{}$ decorator is reserved for denoting the unit vector of some non zero vector. For example $\hat{x} := x/\|x\|, x \neq \mathbf{0}$.

7. $p_k(A|w)$ denotes the matrix polynomial $\sum_{j=0}^{k} w_j A^j$.

8. $(\xi_i)_{i=1}^k$ are used to denote the ith standard basis vector. Its size depends on the context, sometimes it is denoted without ambguity for example: $\xi_i^{(k)}$ would denote the ith standard basis vector for $\mathbb{R}^k$.

2 Introduction

The conjugate gradient method is an iterative method used for solving symmetric positive definite linear systems. It dates back to the period when computers were programmed using punched cards. It didn't receive much attention at the start but was revised and reappeared as a method for solving large sparse linear systems decades later, becoming the best option for positive definite linear systems that are sparse and large and, by extension, for optimizing strongly convex functions as well. In this thesis, we discuss the conjugate gradient method without pre-conditioning by deriving it and analyzing it along with the Lanczos algorithm, a closely related algorithm for solving symmetric eigenproblems. Finally, we use their connections to analyze their behaviors under floating-point arithmetic. The thesis will require some background in numerical linear algebra for the best understanding.

In the first section, we introduce projectors and subspace projection methods. We then specialize to Krylov subspaces and demonstrate that the conjugate gradient method can be thought of as producing an oblique projection onto a Krylov subspace. We also derive the Lanczos algorithm as the symmetric version of the more general Arnoldi algorithm. In the second section, we establish the well-known relationship between these two algorithms and we derive bounds on the convergence rate of the conjugate gradient algorithm. In the third section, we use numerical experiments to better understand the algorithm behaviors under floating-point arithmetic, and we discuss possible ways to mitigate the effects of floating-point arithmetic, as well as what to expect if these effects are not mitigated.

3 Foundations

In this section, we go over the foundations of the conjugate gradient and the Lanczos algorithms. We introduce the important ideas at the beginning, and then we proceed to derive the conjugate gradient algorithm from the method of conjugate directions. We then derive the Lanczos algorithm as a symmetric case of the Arnoldi iteration.

3.1 The Basics

In this subsection, we go over some basic concepts and mathematical entities that are important to Subspace Projection methods in general.

3.1.1 Krylov Subspace

Definition 1 (Krylov Subspace)**.**

$$\mathcal{K}_k(A|b) = \text{span}(b, Ab, A^2b, \cdots A^{k-1}b)$$

Observe that every element in the subspace is the product of a matrix polynomial with the vector b; we write it as $p_{k-1}(A|w)b$, where p_{k-1} is a $(k-1)^{st}$ degree polynomial and w is a vector denoting the coefficients.

Definition 2 (The Grade of Krylov Subspace)**.** The grade of the Krylov subspace for matrix A and vector b is $k-1$ where k is the smallest k such that the vectors in $\mathcal{K}_k(A|b)$ are linearly dependent. This will be denoted as $\text{grade}(A|b)$. Alternatively, it is also the degree of the minimal polynomial $p(A)$ such that $p(A)b = \mathbf{0}$. Using the invariant property of the Krylov Subspace we could claim that: $\text{grade}(A|b) = \max_k \dim(\mathcal{K}_k(A|b))$.

The terminology "grade of a Krylov subspace" is used in Y. Saad's book[13] on page 158. Once the grade is reached, the Krylov subspace becomes an invariant subspace for the matrix A. For a proof, see Krylov Subspace Grade Invariant Theorem (B.1) in the appendix.

Proposition 3.1 (When the Grade is Reached)**.** Assuming that matrix A is diagonalizable whose eigendecomposition is $A = V\Lambda V^{-1}$, then grade$(A|u)$ is the number of unique λ_i such that $(V^{-1}u)_i$ is non-zero.

Proof. Let $\mathcal{K}_{k+1}(A|u)$ be linearly dependent, then there is a nonzero vector w such that:

$$\mathbf{0} = \sum_{j=0}^{k} w_j A^j u \tag{3.1.1}$$

$$\mathbf{0} = V \sum_{j=0}^{k} w_j \Lambda^j V^{-1} u \tag{3.1.2}$$

$$\forall i \quad 0 = \left(\sum_{j=0}^{k} w_j \lambda_i^j \right) (V^{-1}u)_i \tag{3.1.3}$$

It follows that $\sum_{j=0}^{k} w_j \lambda_i^j = 0$ whenever $(V^{-1}u)_i \neq 0$. If there are more than k indices i, corresponding to distinct eigenvalues λ_i, for which $(V^{-1}u)_i \neq 0$, then the only vector w for which the above equations will be satisfied is $w = \mathbf{0}$. This is because the $k+1$ by $k+1$ matrix whose $(i, j+1)$ entry is λ_i^j is a Vandermonde matrix and hence is nonsingular. However, if there are k such indices i, then there will be a nonzero vector w that satisfies the above k equations in the $k+1$ unknowns, $w_0, \ldots, w_k$. If there are fewer than k nonzero entries of $(V^{-1}u)_i$ corresponding to distinct eigenvalues λ_i, then, by the same arguments, the grade will be less than k. □

3.1.2 Projectors

Definition 3. A matrix P is a projector when $P^2 = P$, we call this property idempotent.

There are two types of projectors, oblique and orthogonal projectors. A projector is an orthogonal projector when it's Hermitian and oblique when it's not Hermitian.

Proposition 3.2 (Projector Complementary)**.** The projector $I - P$ projects onto the null space of P and vice versa.

$$\mathrm{ran}(P) = \mathrm{null}(I - P) \tag{3.1.4}$$

$$\mathrm{ran}(I - P) = \mathrm{null}(P) \tag{3.1.5}$$

The proof is immediate from the definition. For more coverage of facts, refer to Trefethen's Book on Numerical Linear Algebra page 41.[17].

3.2 Subspace Projection Methods

Let $\mathcal{K}, \mathcal{L}$ be two subspaces of $\mathbb{R}^n$. We will choose approximate solutions to our linear system $Ax = b$ from $\mathcal{K}$, and we will orthogonalize the residual $b - A\tilde{x}$ against $\mathcal{L}$. This is a description of this framework:

$$\text{choose } \tilde{x} \in x_0 + \mathcal{K} \text{ s.t: } b - A\tilde{x} \perp \mathcal{L}. \tag{3.2.1}$$

Let the columns of $V \in \mathbb{R}^{n\times m}$ be a basis for $\mathcal{K}$ and let the columns of $W \in \mathbb{R}^{n\times m}$ be a basis for $\mathcal{L}$. Then

$$\tilde{x} = x_0 + Vy \tag{3.2.2}$$

$$\text{choose } x \text{ s.t: } b - A\tilde{x} \perp \mathrm{ran}(W) \tag{3.2.3}$$

$$\implies W^T(b - Ax_0 - AVy) = \mathbf{0} \tag{3.2.4}$$

$$W^T r_0 - W^T AVy = \mathbf{0} \tag{3.2.5}$$

$$W^T AVy = W^T r_0 \tag{3.2.6}$$

Thus we can determine the approximate solution $\tilde{x}$ by solving the linear system $W^T AVy = W^T r_0$ for y (assuming that the matrix $W^T AV$ is nonsingular) and then setting $\tilde{x} = x_0 + Vy$. The new residual is $\tilde{r} = b - A\tilde{x} = b - Ax_0 - AVy = r_0 - AV(W^T AV)^{-1}W^T r_0$, and the matrix $AV(W^T AV)^{-1}W^T$ is a projection since

$$[AV(W^T AV)^{-1}W^T][AV(W^T AV)^{-1}W^T] = AV(W^T AV)^{-1}W^T \tag{3.2.7}$$

Alternatively, for some symmetric positive definite matrix B, one might choose $\tilde{x} = x_0 + Vy$ to minimize the B-norm of the residual $\|r_0 - AVy\|_B = \langle r_0 - AVy, B(r_0 - AVy)\rangle^{1/2}$. Setting the gradient of this function to zero leads to the normal equations:

$$V^T A^T BAVy = V^T A^T Br_0 \tag{3.2.8}$$

If A itself is symmetric and positive definite, then we can take $B = A^{-1}$ and minimize the A^{-1}-norm of the residual or, equivalently, the A-norm of the error $\langle A^{-1}b - \tilde{x}, A(A^{-1}b - \tilde{x})\rangle$. The formula for y then becomes

$$V^T AVy = V^T r_0 \tag{3.2.9}$$

This is what the conjugate gradient algorithm does, taking the columns of V to be an orthonormal basis of the Krylov space $\mathcal{K} = \mathcal{K}(A|b)$. Note that this also involves a projection but the two spaces $\mathcal{K}$ and $\mathcal{L}$ and their bases V and W described above, are the same. Now

$$\tilde{r} = b - A\tilde{x} \tag{3.2.10}$$

$$= b - Ax_0 - AVy \tag{3.2.11}$$

$$= r_0 - AV(V^T AV)^{-1}V^T r_0 \tag{3.2.12}$$

and the matrix $AV(V^T AV)^{-1}V^T$ satisfies

$$[AV(V^T AV)^{-1}V^T][AV(V^T AV)^{-1}V^T] = AV(V^T AV)^{-1}V^T \tag{3.2.13}$$

The A-norm of the error often represents energy in a mechanical system and so it is often referred to as the energy norm.

3.3 Deriving Conjugate Gradient from Conjugate Directions

At the time this is being written, it's been 70 years since the conjugate gradient algorithm was proposed by Hestenes and Stiefel back in 1952[8]. Upon their first discussion of the algorithm, numerous perspectives were explored. Three of the most important ideas are using Conjugate Directions, minimizing the energy norm of the error of the linear system and coming up with an update of the conjugate vectors using the residual vector at the current iteration. Here, we use the exact same idea, but we diverge from Hestenes and Stiefel's approach in favor of using the oblique projector and the subspace orthogonality conditions to derive it. At the end, we point out the relations between conjugate gradient and Krylov Subspace. Usually under classroom settings or textbooks, the relations of conjugate gradient, Lanczos Iterations and Krylov Subspaces are discussed together to explain some of the more important properties of the algorithm so that we can move on and talk about other things. However, in this section we derive it in a way similar to the approach used in course notes by Shewchuk [15].

3.3.1 CG Objective and Framework

We introduce the algorithm as an attempt to minimize the energy norm of the error for a system of linear equations $Ax = b$, and we make the assumptions:

1) The matrix A is symmetric positive definite.

2) There is a matrix $P_k = [p_0\ p_1\ \cdots p_{k-1}]$ whose columns form a basis for the space over which we are minimizing.

Let's consider the following objective of minimizing the energy norm of the error over a subspace.

$$\min_{w\in\mathbb{R}^k} \|A^{-1}b - (x_0 + P_k w)\|_A^2 \iff P_k^T r_0 = P_k^T A P_k w \tag{3.3.1}$$

Refer back to equation (3.2.9) for how to obtain the above condition. Using the matrix from equation (3.2.2), where $W = V = P_k$, we reformulate the norm minimization conditions as:

$$\text{choose: } x \in x_0 + \text{ran}(P_k) \text{ s.t: } b - Ax \perp \text{ran}(P_k) \tag{3.3.2}$$

Take note that the link between a norm minimization and an equivalent subspace orthogonality condition isn't guaranteed to happen for other subspace projection methods. For example, the FOM and Bi-Lanczos Methods are orthogonalization methods that don't directly link to a norm minimization objective [14].

To solve for w, we wish to make $P_k^T AP_k$ to be a diagonal matrix, which is an easy-to-solve matrix, which implies that P_k is a *matrix whose columns are A-Orthogonal vectors*, also referred as *conjugate vectors*.

$$P_k^T AP_k = D_k \text{ where: } (D_k)_{i,i} = \langle p_{i-1}, Ap_{i-1}\rangle \tag{3.3.3}$$

$$P_k^T r_0 = P_k^T AP_k w = D_k w \tag{3.3.4}$$

$$w = D_k^{-1} P_k^T r_0 \tag{3.3.5}$$

Now we have the following expressions for x_k and r_k:

$$\begin{cases} x_k = x_0 + P_k D_k^{-1} P_k^T r_0 \\ r_k = r_0 - AP_k D_k^{-1} P_k^T r_0 \end{cases} \tag{3.3.6}$$

Let this algorithm be the prototype.

3.3.2 Using the Projector

Observe that $AP_k D_k^{-1} P_k$ is a projector, and so is $P_k D_k^{-1} P_k^T A$. We can check by:

$$AP_k D_k^{-1} P_k^T (AP_k D_k^{-1} P_k^T) = AP_k D_k^{-1} \underbrace{(P_k^T AP_k)}_{D_k} D_k^{-1} P_k^T = AP_k D_k^{-1} P_k^T \tag{3.3.7}$$

$$P_k D_k^{-1} \underbrace{P_k^T A(P_k}_{D_k} D_k^{-1} P_k^T A) = P_k D_k^{-1} D_k D_k^{-1} P_k^T A = P_k D_k^{-1} P_k^T A \tag{3.3.8}$$

They are not Hermitian, therefore they are oblique projectors. For convenience, we denote $\overline{P}_k = P_k D_k^{-1} P_k^T$; So we can simply denotes them by $A\overline{P}_k, \overline{P}_k A$. Observe that:

$$\operatorname{ran}(I - A\overline{P}_k) \perp \operatorname{ran}(P_k) \tag{3.3.9}$$

$$\operatorname{ran}(I - \overline{P}_k A) \perp \operatorname{ran}(AP_k) \tag{3.3.10}$$

because:

$$\begin{aligned}
P_k^T(I - A\overline{P}_k) &= P_k^T - P_k^T A\overline{P}_k && (3.3.11)\\
&= P_k^T - D_k D_k^{-1} P_k^T = \mathbf{0} && (3.3.12)\\
(AP_k)^T(I - \overline{P}_k A) &= P_k^T A - P_k^T A\overline{P}_k A && (3.3.13)\\
&= P_k^T A - P_k^T A P_k D_k^{-1} P_k^T A && (3.3.14)\\
&= P_k^T A - P_k^T A = \mathbf{0} && (3.3.15)
\end{aligned}$$

Proposition 3.3 (Generating A-Orthogonal Vectors)**.** Given any set of linearly independent vectors, for example $\{u_i\}_{i=0}^{n-1}$, one can generate a set of A-Orthogonal vectors from it. More specifically:

$$p_k = (I - \overline{P}_k A)u_k \implies p_k \perp \operatorname{ran}(AP_k) \tag{3.3.16}$$

Proof. It's direct from the properties of the projectors. □

3.3.3 Method of Conjugate Directions

So far, we have this particular scheme of solving the optimization problem, coupled with the way to compute the solution x_k at each step, and the residual r_k at each step. However, it would be great if we could update x_k, r_k, and p_k using results from previous iterations.

Definition 4 (Conjugate Direction Method)**.**

$$\begin{cases} \overline{P}_k = P_k D_k^{-1} P_k^T \\ x_k = x_0 + \overline{P}_k r_0 \\ r_k = (I - A\overline{P}_k) r_0 \\ P_k^T A P_k = D_k \\ p_k = (I - \overline{P}_k A) u_k \quad \{u_i\}_{i=0}^{n-1} \text{linearly independent vectors} \end{cases} \tag{3.3.17}$$

With the assistance of a set of basis vectors that span the whole space, this algorithm can achieve the objective.

Remark 3.3.1. This conjugate direction method (CDM) method is nothing new, in the original paper from Hestenes and Stiefel back in 1952[8], they commented on the method of Conjugate Direction, for each choice of basis $\{u_i\}_{i=0}^{n-1}$ there is a unique algorithm. If one were to choose the basis to be the set of standard basis vectors, then the resulting algorithm would be the equivalent of Gaussian Elimination.

Remark 3.3.2 (Geometric Intuition of CDM)**.** What is happening geometrically is that the A-Orthogonal vectors are orthogonal when described under the eigenspace. Intuitively, one should think of a high-dimensional sphere that sits along some orthogonal basis, and the transformation of A is stretching and rotating sphere, along with the orthogonal axis, resulting in a new ellipsoid in a different orientation; when the transformation is applied, the orthogonal coordinate inside the sphere got stretched along with it, and now these axes had become A-orthogonal vectors. Tracing along the direction of these vectors will ensure minimum redundancy of search directions.

3.3.4 Properties of CDM

Here we set up several useful lemma and propositions that can derive the short recurrences of A-Orthogonal vectors

Proposition 3.4 (CDM Property 1)**.**

$$p_{k+j}^T r_k = p_{k+j}^T r_0 \quad \forall\, 0 \leq j \leq n-k \tag{3.3.18}$$

Proof.

$$p_{k+j}^T r_k = p_{k+j}^T (I - A\overline{P}_k) r_0 \tag{3.3.19}$$

$$= (p_{k+j}^T - p_{k+j}^T A\overline{P}_k) r_0 \tag{3.3.20}$$

$$= p_{k+j}^T r_0 \tag{3.3.21}$$

□

Proposition 3.5 (CDM Recurrence)**.**

$$r_k - r_{k-1} = r_0 - A\overline{P}_k r_0 - (r_0 - A\overline{P}_{k-1} r_0) \tag{3.3.22}$$

$$= -A\overline{P}_k r_0 + A\overline{P}_{k-1} r_0 \tag{3.3.23}$$

$$= -Ap_{k-1} \frac{\langle p_{k-1}, r_0 \rangle}{\langle p_{k-1}, Ap_{k-1} \rangle} \tag{3.3.24}$$

$$\implies x_k - x_{k-1} = p_{k-1} \frac{\langle p_{k-1}, r_0 \rangle}{\langle p_{k-1}, Ap_{k-1} \rangle} \tag{3.3.25}$$

$$\text{def: } a_{k-1} := \frac{\langle p_{k-1}, r_0 \rangle}{\langle p_{k-1}, Ap_{k-1} \rangle} = \frac{\langle p_{k-1}, r_{k-1} \rangle}{\langle p_{k-1}, Ap_{k-1} \rangle} \tag{3.3.26}$$

On (3.3.26) we used CDM Property 1. The value of a_{k-1} is defined above,, we have two equivalent representations for a_{k-1}. This recurrence remains true for the future regardless of the set $\{u\}_{i=0}^{n-1}$ that generates these conjugate vectors.

3.3.5 Conjugate Gradient

Now, consider the case where the set of basis vectors: $\{u_i\}_{i=0}^{n-1}$ are the residual vectors generated from the CDM itself. This generates the CG method.

Lemma 3.3.1.

$$\langle p_{k+j}, Ap_k \rangle = \langle r_k, Ap_{k+j} \rangle = \langle p_{k+j}, Ar_k \rangle \quad \forall\, 0 \leq j \leq n-k \tag{3.3.27}$$

Proof.

$$p_{k+j}^T A p_k = p_{k+j}^T A r_k - p_{k+j}^T A \overline{P}_k A r_k \quad \forall\, 0 \le j \le n-k \tag{3.3.28}$$

$$= p_{k+j}^T A r_k \tag{3.3.29}$$

$$\langle p_{k+j}, Ap_k \rangle = \langle r_k, Ap_{k+j} \rangle = \langle p_{k+j}, Ar_k \rangle \tag{3.3.30}$$

On the first line we invoked the CDM algorithm's definition back in (3.3.27), replacing u_k with r_k, hence $p_k = (I - \overline{P}_k A) r_k$, which is then substituted into line (3.3.28). □

Lemma 3.3.2.

$$\langle r_k, p_k \rangle = \langle r_k, r_k \rangle \tag{3.3.31}$$

Proof.

$$\langle r_k, p_k \rangle = \langle r_k, r_k \rangle - \langle r_k, \overline{P}_k A r_k \rangle = \langle r_k, r_k \rangle \tag{3.3.32}$$

First equality used $p_k = (I - \overline{P}_k A) r_k$, second equality used the fact that r_k is orthogonal to P_k. □

Proposition 3.6 (CG Generates Orthogonal Residuals)**.**

$$\langle r_k, r_j \rangle = 0 \quad \forall\, 0 \le j \le k-1 \tag{3.3.33}$$

Let this above claim be inductively true then consider:

Proof.

$$r_{k+1} = r_k - a_k A p_k \tag{3.3.34}$$

$$\implies \langle r_{k+1}, r_k \rangle = \langle r_k, r_k \rangle - a_k \langle r_k, Ap_k \rangle \tag{3.3.35}$$

$$= \langle r_k, r_k \rangle - \frac{\langle r_k, r_k \rangle}{\langle p_k, Ap_k \rangle} \langle r_k, Ap_k \rangle \tag{3.3.36}$$

$$= 0 \tag{3.3.37}$$

The first line is from the recurrence of CDM residuals, and then next we make use of a_k from (CDM Recurrence (3.5)) together with Lemma 3.3.1. Next we consider:

$$p_j = (I - \overline{P}_j A) r_j \quad \forall\, 0 \le j \le k-1 \tag{3.3.38}$$

$$\implies r_j = p_j + \overline{P}_j A r_j \tag{3.3.39}$$

$$r_k = (I - A\overline{P}_k) r_0 \tag{3.3.40}$$

$$r_k \perp \mathrm{ran}(P_k) \implies \langle r_k, r_j \rangle = \langle r_k, p_j + \overline{P}_j A r_j \rangle = 0 \tag{3.3.41}$$

The second line (3.3.39) is a result of the first line (3.3.38) rearranged. Here we again make use of the projector $I - A\overline{P}_k$. The last line (3.3.53) is using the second line 3.3.39. The base case of the argument is simple, because $p_0 = r_0$, and by the property of the projector, $\langle r_1, r_0 \rangle = 0$. The theorem is now proven. □

Proposition 3.7 (CG Recurrences)**.**

$$p_k = r_k + b_{k-1} p_{k-1} \quad b_{k-1} = \frac{\|r_k\|_2^2}{\|r_{k-1}\|_2^2} \tag{3.3.42}$$

Proof. The proof is direct, starting with the definition of CDM, which is given as:

$$p_k = (I - \overline{P}_k A) r_k \tag{3.3.43}$$

$$r_k - \overline{P}_k A r_k = r_k - P_k D_k^{-1} P_k^T A r_k \tag{3.3.44}$$

$$= r_k - P_k D_k^{-1} (AP_k)^T r_k \tag{3.3.45}$$

Observe:

$$(AP_k)^T r_k = \begin{bmatrix} \langle p_0, Ar_k \rangle \\ \langle p_1, Ar_k \rangle \\ \vdots \\ \langle p_{k-1}, Ar_k \rangle \end{bmatrix} \tag{3.3.46}$$

Next, we can make use of lemma 3.3.1 to get rid of Ar_k:

$$\langle p_j, Ar_k \rangle \quad \forall\, 0 \le j \le k-2 \tag{3.3.47}$$

$$\langle p_j, Ar_k \rangle = \langle r_k, Ap_j \rangle \tag{3.3.48}$$

$$= \langle r_k, a_j^{-1}(r_j - r_{j+1}) \rangle \tag{3.3.49}$$

$$= a_j^{-1}\langle r_k, (r_j - r_{j+1}) \rangle = 0 \tag{3.3.50}$$

The second line is also using the property that the matrix A is symmetric, the third line is using the recurrence of the residual established for CDM (CDM Recurrences (Proposition 3.5)), and the last line is true for all $0 \le j \le k-2$ by the orthogonality of the residual proved in CG Generates Orthogonal Residuals (Proposition 3.6). Therefore we have:

$$(AP_k)^T r_k = \begin{bmatrix} \langle p_0, Ar_k \rangle \\ \langle p_1, Ar_k \rangle \\ \vdots \\ \langle p_{k-1}, Ar_k \rangle \end{bmatrix} = a_{k-1}^{-1}\langle r_k, (r_{k-1} - r_k) \rangle \xi_k \tag{3.3.51}$$

Take note that the vector ξ_k is the k th standard basis vector in $\mathbb{R}^k$, keep in mind that $r_k \perp r_{k-1}$ as well. Using these facts we can simplify the expression for p_k into:

$$p_k = r_k - P_k D_k^{-1}(AP_k)^T r_k \tag{3.3.52}$$

$$= r_k - P_k D_k^{-1} a_{k-1}^{-1}(\langle r_k, (r_{k-1} - r_k) \rangle)\xi_k \tag{3.3.53}$$

$$= r_k - \frac{a_{k-1}^{-1}\langle -r_k, r_k \rangle}{\langle p_{k-1}, Ap_{k-1} \rangle} p_k \tag{3.3.54}$$

$$= r_k + \frac{a_{k-1}^{-1}\langle r_k, r_k \rangle}{\langle p_{k-1}, Ap_{k-1} \rangle} p_k \tag{3.3.55}$$

$$= r_k + \left(\frac{\langle r_{k-1}, r_{k-1} \rangle}{\langle p_{k-1}, Ap_{k-1} \rangle} \right)^{-1} \frac{\langle r_k, r_k \rangle}{\langle p_{k-1}, Ap_{k-1} \rangle} p_k \tag{3.3.56}$$

$$= r_k + \frac{\langle r_k, r_k \rangle}{\langle r_{k-1}, r_{k-1} \rangle} p_k \tag{3.3.57}$$

We make use of the definition for a_{k-1} for the CDM algorithm (proposition 3.5 together with lemma 3.3.2). At this point, we have proven the short CG recurrences for p_k. $\square$

Up until this point we have developed the standard form of the conjugate gradient algorithm proposed by Hestenes & Stiefel[8]. We started with the minimization objective and the properties of P_k, then we defined a recurrence for the residual (and simultaneously the solution x_k), and the A-Orthogonal vectors using a set of basis vectors to assist in the generation process. Next, we chose the basis vectors to be the set of residual vectors generated from the algorithm itself; after some proofs, we uncovered the exact same parameters found in most of the definitions of the CG algorithm:

Definition 5 (CG)**.**

$$p^{(0)} = b - Ax^{(0)} \tag{3.3.58}$$

$$\text{For } i = 0, 1, \cdots \tag{3.3.59}$$

$$\begin{aligned} a_i &= \frac{\|r^{(i)}\|^2}{\langle p^{(i)}, Ap^{(i)}\rangle} \\ x^{(i+1)} &= x^{(i)} + a_i p^{(i)} \\ r^{(i+1)} &= r^{(i)} - a_i A p^{(i)} \\ b_i &= \frac{\|r^{(i+1)}\|_2^2}{\|r^{(i)}\|_2^2} \\ p^{(i+1)} &= r^{(i+1)} + b_i p^{(i)} \end{aligned} \tag{3.3.60}$$

All the iteration numbers listed as superscripts inside parentheses. Which is equivalent to what we have proven for the CG.

3.3.6 CG and Krylov Subspace

The conjugate Gradient Algorithm is actually a CDM. It's a special case of the CDM method where the first direction of descend is the gradient at the initial guess (the residual). Next, we want to show how CG is related to the Krylov Subspace, which only happens with CG and not the CDM.

Proposition 3.8.

$$p_k \in \mathcal{K}_{k+1}(A|r_0) \tag{3.3.61}$$

$$r_k \in \mathcal{K}_{k+1}(A|r_0) \tag{3.3.62}$$

Proof. The base case is trivial and it's directly true from the definition of CG: $r_0 \in \mathcal{K}_1(A|r_0), p_0 = r_0 \in \mathcal{K}_1(A|r_0)$. Next, we inductively assume that $r_k \in \mathcal{K}_{k+1}(A|r_0), p_k \in \mathcal{K}_{k+1}(A|r_0)$, then we consider:

$$\begin{aligned}
r_{k+1} &= r_k - a_k A p_k && (3.3.63)\\
&\in r_k + A\mathcal{K}_{k+1}(A|r_0) && (3.3.64)\\
&\in r_k + \mathcal{K}_{k+2}(A|r_0) && (3.3.65)\\
r_k &\in \mathcal{K}_{k+1}(A|r_0) \subseteq \mathcal{K}_{k+2}(A|r_0) && (3.3.66)\\
\implies r_{k+1} &\in \mathcal{K}_{k+2}(A|r_0) && (3.3.67)
\end{aligned}$$

At the same time the update of p_k would assert the property that:

$$\begin{aligned}
p_{k+1} &= r_{k+1} + b_k p_k && (3.3.68)\\
&\in r_{k+1} + \mathcal{K}_{k+1}(A|r_0) && (3.3.69)\\
&\in \mathcal{K}_{k+2}(A|r_0) && (3.3.70)
\end{aligned}$$

This is true because r_{k+1} is already a member of the expanded subspace $\mathcal{K}_{k+2}(A|r_0)$. And from this formulation of the algorithm, we can update the Petrov Galerkin's Conditions to be:

Theorem 1 (CG and Krylov Subspace)**.**

$$\text{choose: } x_k \in x_0 + \mathcal{K}_k(A|r_0) \text{ s.t: } r_k \perp \mathcal{K}_k(A|r_0) \tag{3.3.71}$$

Take note that, $\text{ran}(P_k) = \mathcal{K}_k(A|r_0)$ because the index starts with zero for the Conjugate Vectors. □

3.4 Arnoldi Iterations and Lanczos

In this section, we introduce another important algorithm: The Lanczos Algorithm. Instead of deriving the tridiagonal matrix produced by the Lanczos algorithm in the usual way, we will derive it from the Arnoldi algorithm, which, like the Lanczos algorithm produces an orthonormal basis for a Krylov space, but now with a nonsymmetric matrix.

3.4.1 The Arnoldi Iterations

We first define the Arnoldi Algorithm, and then we proceed to derive it using the idea of an orthogonal projector. Next, we discuss a special case of the Arnoldi Iteration: the Lanczos Algorithm, which is just Arnoldi applied to a symmetric matrix. And such an algorithm will inherit the properties of the Arnoldi Iterations.

We initialize the orthogonal projector with the vector q_1, which is $q_1 q_1^H$. Next, we apply the linear operator A on the current range of the projector: Aq_1. Then we orthogonalize it against q_1: $(I - q_1 q_1^H)Aq_1$. Let $h_{11}q_1$ be the orthogonal projection of Aq_1 onto q_1; i.e., $h_{11} = q_1^H A q_1$. Then we normalize the new vector $q_2 = (I - q_1 q_1^H)Aq_1 / \|(I - q_1 q_1^H)Aq_1\|_2$, and set $h_{21} = \|(I - q_1 q_1^H)Aq_1\|_2$. This completes the first column of H, and we do this recursively.

$$Q_j = [q_1, \ldots, q_j] \tag{3.4.1}$$

$$q_{j+1} = \frac{(I - Q_j Q_j^H)Aq_j}{\|(I - Q_j Q_j^H)Aq_j\|_2} \tag{3.4.2}$$

$$h_{1:j,j} = Q_j Q_j^H A q_j \tag{3.4.3}$$

$$h_{j+1,j} = \|(I - Q_j Q_j^H)Aq_j\|_2. \tag{3.4.4}$$

Q_k is going to be orthogonal because we are using orthogonal projectors. As a consequence, we can express the recurrence in matrix form:

$$AQ_k = Q_{k+1}\tilde{H}_k \tag{3.4.5}$$

$$Q_k^H AQ_k =: H_k, \tag{3.4.6}$$

where $\tilde{H}_k$ is a $k+1$ by k matrix and H_k is the k by k principal submatrix of $\tilde{H}_k$. Please observe that, if A is symmetric, then $Q_k^H AQ_k$ is also symmetric, which makes H_k symmetric, implying that H_k is a symmetric tridiagonal matrix. This is the matrix produced by the Lanczos algorithm.

3.4.2 Arnoldi Produces Orthogonal Basis for Krylov Subspace

One important observation the reader should make is that, during each iteration, the columns of Q_k span the Krylov space $\mathcal{K}_k(A|q_1)$.

Proposition 3.9.

$$\operatorname{ran}(Q_k) = \mathcal{K}_k(A|q_1) \tag{3.4.7}$$

Proof. Clearly $\mathcal{K}_1(A|q_1)$ is just q_1, and assuming that $\operatorname{ran}(Q_{k-1}) = K_{k-1}(A|q_1)$ and that the Arnoldi iteration does not terminate at step k, the new vector Aq_{k-1} is in $\mathcal{K}_k(A|q_1)$ and is not in $\mathcal{K}_{k-1}(A|q_1)$. Thus, the vector q_k obtained after orthogonalizing Aq_{k-1} against $\mathcal{K}_{k-1}(A|q_1)$ is nonzero and so the columns of Q_k form an orthonormal basis for $\mathcal{K}_k(A|q_1)$. $\square$

Remark 3.4.1 (Arnoldi Produces Minimal Monic Polynomial)**.** The characteristic polynomial of H_k, minimizes $\|p(A|w)q_1\|_2$ among all monic polynomials with degree k. For more information, Trefethen has a coverage on the topic in his works [17] on page 259. The minimization property in Arnoldi translates to Lanczos Iterations as well.

3.4.3 The Lanczos Iterations

Definition 6 (Lanczos Iterations)**.**

$$\text{Given arbitrary: } q_1 \text{ s.t: } \|q_1\| = 1 \tag{3.4.8}$$

$$\text{set: } \beta_0 = 0 \tag{3.4.9}$$

$$\text{For } j = 1, 2, \cdots \tag{3.4.10}$$

$$\begin{aligned} &\tilde{q}_{j+1} := Aq_j - \beta_{j-1} q_{j-1} \\ &\alpha_j := \langle q_j, \tilde{q}_{j+1} \rangle \\ &\tilde{q}_{j+1} \leftarrow \tilde{q}_{j+1} - \alpha_j q_j \\ &\beta_j = \|\tilde{q}_{j+1}\| \\ &q_{j+1} := \tilde{q}_{j+1} / \beta_j \end{aligned} \tag{3.4.11}$$

Here, let it be the case that H_k is a symmetric tridiagonal matrix with α_i on the diagonal, β_i on the sub and super diagonal; the Lanczos is Arnoldi, but we make use of the symmetric properties to orthogonalize Aq_j against q_{j-1} using β_{j-1}, and in this case, each iteration only consists of one vector inner product.Other variants of the Lanczos Iterations exist. See appendix item 7 for one such variant.

The algorithm generates the following two matrices: Q_k, which is orthogonal and has columns that span $\mathcal{K}_k(A|q_1)$, and a symmetric tridiagonal matrix T_k:

$$Q_k = \begin{bmatrix} q_1 & q_2 & \cdots & q_k \end{bmatrix} \tag{3.4.12}$$

$$T_k = \begin{bmatrix} \alpha_1 & \beta_1 & & \\ \beta_1 & \ddots & \ddots & \\ & \ddots & \ddots & \beta_{k-1} \\ & & \beta_{k-1} & \alpha_k \end{bmatrix} \tag{3.4.13}$$

Similar to the recurrence from the Arnoldi algorithm, the Lanczos algorithm also create a recurrence between Aq_k and Q_k and q_{k+1}, but the recurrence is shorter so that it simply makes use of the previous two vectors. In addition, the tridiagonal matrix that is produced has no repeated eigenvalues, which is a useful fact and for a proof, see appendix item B.5.

Theorem 2 (Lanczos Recurrences)**.**

$$AQ_k = Q_kT_k + \beta_k q_{k+1}\xi_k^T = Q_{k+1}\tilde{T}_k \tag{3.4.14}$$

$$\implies Aq_j = \beta_{j-1}q_{j-1} + \alpha_j q_j + \beta_j q_{j+1} \quad \forall\, 2 \le j \le k \tag{3.4.15}$$

$$\implies Aq_1 = \alpha_1 q_1 + \beta_1 q_2 \tag{3.4.16}$$

Proposition 3.10 (Lanczos Termination Conditions)**.** The Lanczos Iteration produces a symmetric tridiagonal matrix that has no zero element on its super and sub-diagonal, and if β_k is zero, then the algorithm must terminate, and k would equal to grade$(A|q_1)$, the grade of the Krylov Subspace.

Proof. The β_k in the Lanczos is equivalent to $h_{k+1,k}$. if $h_{k+1,1} = 0$ for the Arnoldi's Iteration, then the Krylov Subspace $\mathcal{K}_k(A|q_1)$ became an invariant subspace under A, and in that sense, the algorithm has to terminate because $q_{k+1} = \mathbf{0}$. □

Remark 3.4.2 (Minimal Polynomial from Lanczos Iterations)**.** The characteristic polynomial of T_k has a special minimization property. Here recall remark 3.4.1, we make use of the minimization property of the characteristic polynomial of the Hessenberg matrix from the Arnoldi Iterations. Under Lanczos iterations the matrix H_k becomes the tridiagonal T_k. Since matrix A is symmetric, we consider its eigendecomposition in the form: $A = V\Lambda V^T$, we let $\bar{p}_k(x)$ denote the characteristic polynomial of matrix T_k, then using the 2-norm minimization properties we have:

$$\min_{p_k \in \mathcal{P}_k:\text{monic}} \|p_k(A)q_1\|_2 \tag{3.4.17}$$

$$= \|\overline{p}_k(A)q_1\|_2 \tag{3.4.18}$$

$$= \|V\bar{p}_k(\Lambda)V^T q_1\|_2 \tag{3.4.19}$$

$$= \|\bar{p}_k(\Lambda)V^T q_1\|_2 \tag{3.4.20}$$

$$= \sqrt{\sum_{i=1}^{n} p_{k2}(\lambda_i)^2 (V^T q_1)_1^2} \tag{3.4.21}$$

The last line is saying the characteristic polynomial for T_k from the Lanczos iterations is minimizing a weighted squared sum at the eigenvalues of the matrix A. This provides us with the intuitions that as the Lanczos iterations proceed, the roots of the characteristic polynomial of T_k will get closer to the eigenvalues of matrix A.

Another fact about the characteristic polynomial of T_k is that the Lanczos vector q_k represents an orthogonal polynomial in $\mathcal{K}_k(A|q_1)$ under a discrete weighted measure over the eigenvalues of A, [1] and such a polynomial is a rescaled version of the characterstic polynomial of T_{k-1}. (see proposition B.2 in the appendix for a proof), which means that the characteristic polynomial of T_k is orthogonal under a discrete weighted measure at the eigenvalues of A.

4 Analysis of Conjugate Gradient and Lanczos Iterations

In this section, we state the termination conditions for the Lanczos iterations and the CG algorithm we developed using the property of Krylov Subspace.

[1]The discrete measure is defined via inner product $\langle f, g\rangle_{V^T q_1} = \sum_{i=1}^{n} f(\lambda_i)g(\lambda_i)(V^T q_1)_i^2$.

4.1 Conjugate Gradient and Matrix Polynomial

One important result of the optimization objective listed theorem 1 is the connection with the matrix polynomial of A and the relative energy norm of error. More specifically:

Proposition 4.1 (CG Relative Energy Error)**.**

$$x_k \in \mathcal{K}(A|r_0)w + x_0 \tag{4.1.1}$$

$$\frac{\|e_k\|_A^2}{\|e_0\|_A^2} = \min_{w\in\mathbb{R}^k} \|(1 + Ap_{k-1}(A|w))A^{1/2}e_0\|_2^2 \leq \min_{p_k\in\mathcal{P}^k:p_k(0)=1} \max_{x\in[\lambda_{\min},\lambda_{\max}]} |p_k(x)| \tag{4.1.2}$$

Here we use the notation $e_k = A^{-1}b - x_k$ to denote the error vector and $\mathcal{P}_k$ to denotes polynomial with a maximum degree of k.

Proof.

$$\|e_k\|_A^2 = \min_{x_k\in x_0+\mathcal{K}_k(A|r_0)} \|x^+ - x_k\|_A^2 \tag{4.1.3}$$

$$x_k \in x_0 + \mathcal{K}_k(A|r_0) \implies e_k = e_0 + p_{k-1}(A|w)r_0 \tag{4.1.4}$$

$$\implies = \min_{w\in\mathbb{R}^k} \|e_0 + p_{k-1}(A|w)r_0\|_A^2 \tag{4.1.5}$$

$$= \min_{w\in\mathbb{R}^k} \|e_0 + Ap_{k-1}(A|w)e_0\|_A^2 \tag{4.1.6}$$

$$= \min_{w\in\mathbb{R}^k} \|A^{1/2}(I + Ap_{k-1}(A|w))e_0\|_2^2 \tag{4.1.7}$$

$$\leq \min_{w\in\mathbb{R}^k} \|I + Ap_{k-1}(A|w)\|_2^2\|e_0\|_A^2 \tag{4.1.8}$$

$$= \min_{w\in\mathbb{R}^k} \left(\max_{i=1,\ldots,n} |1 + \lambda_i p_{k-1}(\lambda_i|w)|^2\right) \|e_0\|_A^2 \tag{4.1.9}$$

$$\leq \min_{w\in\mathbb{R}^k} \left(\max_{x\in[\lambda_{\min},\lambda_{\max}]} |1 + \lambda_i p_{k-1}(\lambda_i|w)|^2\right) \|e_0\|_A^2 \tag{4.1.10}$$

$$= \min_{p_k\in\mathcal{P}^k:p_k(0)=1} \max_{x\in[\lambda_{\min},\lambda_{\max}]} |p_k(x)|^2\|e\|_A^2 \tag{4.1.11}$$

$$\implies \frac{\|e_k\|_A}{\|e_0\|_A} \leq \min_{p_k\in\mathcal{P}^k:p_k(0)=1} \max_{x\in[\lambda_{\min},\lambda_{\max}]} |p_k(x)| \tag{4.1.12}$$

(4.1.3) is the Error Energy norm minimization objective of CG, we proceed with writing up the affine subspace where x_k is from: $x_0 + \mathcal{K}_k(A|r_0)$ at (4.1.4), putting Krylov subspace in terms of a matrix polynomial multiplied by r_0 and then use $A^{-1}b$ to subtract both sides to get the expression for e_k. From the (4.15) line to the (4.16), we use the fact that $r_0 = Ae_0$, allowing us to extract out a factor A.

Next, from (4.1.6) to (5.1.7), we use the fact that every symmetric definite matrix A has the factorization of $A^{1/2}A^{1/2}$ where $A^{1/2}$ is also a symmetric definite matrix. After that we moved the $A^{1/2}$ to e_0 to get $\|e_0\|_A^2$ from (4.1.7) to (4.1.8), the matrix polynomial part is left with the 2-norm. From (4.1.8) to (4.1.9) we use the eigen decomposition of A: $Q\Lambda Q^T = A$ where Q is an Unitary Matrix and diagonals of Λ are the eigenvalues of A:

$$\|I + Ap_{k-1}(A|w)\|_2^2 = \|Q(I + \Lambda p_{k-1}(\Lambda|w))Q^T\|_2^2 \tag{4.1.13}$$

$$= \|I + \Lambda p_{k-1}(\Lambda|w)\|_2^2 \tag{4.1.14}$$

$$= \max_{i=1,\cdots,n} |1 + \lambda_i p_{k-1}(\lambda_i|w)|^2 \tag{4.1.15}$$

Where, the 2-norm of a diagonal matrix Λ is just its biggest diagonal element. And then we relax the conditions for λ_i by reducing it to be some element in the interval between the minimum and the maximum of the eigenvalues for the matrix A (from (4.1.9) to (4.1.10)). $\square$

The above results will be useful for proving the convergence of CG.

Remark 4.1.1. The matrix A is SPD, therefore $\|Ax\| \leq \|A\|\|x\|$ is tight, so (4.1.10) is tight in the sense that for any iteration k, we can choose an initial vector e_0 such that the equality is achieved. (4.1.12) can still be tight if we have the freedom to choose the eigenvalues of the matrix A. However, the bound is rarely tight if the initial error vector e_0 and the matrix A is fixed.

4.1.1 Termination Conditions of CG

Proposition 4.2 (Termination of CG)**.** For all initial guesses, the maximum iterations underwent by the CG algorithm is the number of unique eigenvalues for the matrix A.

This result is direct from (4.1.9), the CG algorithm terminates when a polynomial that interpolates all the unique eigenvalues is found. This bound is true for all initial guesses, and sometimes for some given e_0, the terminations can come with fewer iterations.

4.2 Convergence Rate of CG under Exact Arithmetic

In this section discuss an analysis for convergence rate of the algorithm, following a similar work in Greenbaum chapter 3[6]. The core idea is to use a Chebyshev Polynomial to establish a bound on the interval containing the eigenvalues of A. We will see that the distribution of the eigenvalues of A affects for the speed of convergence of CG.

4.2.1 Uniformly Distributed Eigenvalues

Theorem 3 (CG Convergence Rate)**.** The relative error squared measured over the energy norm is bounded by:

$$\frac{\|e_k\|_A}{\|e_k\|_A} \le 2\left(\frac{\sqrt{\kappa}-1}{\sqrt{\kappa}+1}\right)^k \tag{4.2.1}$$

Where k is the number of iterations of CG, κ is the condition number for A, and $e_k = A^{-1}b - x_k$, the upper bound is general and it's able to bound the convergence given $\lambda_{\min}, \lambda_{\max}$ for A. The bound is loose when eigenvalues of matrix A is not quite uniform on the interval, and the bound would be tighter given that $k << n$ and the eigenvalues of A are evenly spread out on the spectrum.

The analysis uses Chebyshev as an interpolating polynomial for the spectrum of A, and we make use of the inf norm minimization property of the Chebyshev polynomial.

Here, we order all the eigenvalues of matrix A so that λ_1, λ_n denotes the minimum and the maximum eigenvalues for A.

Proof. We start by adapting the Chebyshev Polynomial to the convex hull of the spectrum for matrix A.

$$T_k(x) = \arg\min_{p\in\mathcal{P}_k} \max_{x\in[-1,1]} |p(x)| \tag{4.2.2}$$

$$p_k(x) := \frac{T_k(\varphi(x))}{T_k(\varphi(0))} \quad \text{where: } \varphi(x) := \frac{2x - \lambda_1 - \lambda_n}{\lambda_n - \lambda_1} \tag{4.2.3}$$

$$\implies p_k(x) = \arg \min_{\substack{p\in\mathcal{P}_k \\ \text{s.t: } p(0)=1}} \max_{x\in[\lambda_1,\lambda_n]} |p(x)| \tag{4.2.4}$$

At this point, we have defined a new polynomial p_k that minimizes the inf norm over the convex hull of the eigenvalues. Note that here we use T_k for the type T Chebyshev polynomial of degree k and it's not the tridiagonal symmetric matrix from Lanczos iterations. Next, we use the property that the range of the Chebyshev is bounded within the interval $[-1, 1]$ to obtain inequality:

$$\forall x \in [\lambda_1, \lambda_n] : \left|\frac{T_k(\varphi(x))}{T_k(\varphi(0))}\right| \leq \left|\frac{1}{T_k(\varphi(0))}\right| \tag{4.2.5}$$

Next, our objective is to find any upper bound for the quantities on the RHS in relation to the condition number for matrix A and the degree of the Chebyshev polynomial. Firstly observe that $\varphi(0) < -1, \varphi(0) \notin [\lambda_1, \lambda_n]$, because all eigenvalues are larger than zero, therefore it's out of the range of the Chebyshev polynomial and we need to find the actual value of it by considering alternative form of Chebyshev T for values outside of the $[-1, 1]$:

$$T_k(x) = \cosh(k \text{ arccosh}(z)) \quad \forall z \geq 1 \tag{4.2.6}$$

$$\implies T_k(\cosh(\zeta)) = \cosh(k\zeta) \quad z := \cosh(\zeta) \tag{4.2.7}$$

We need to match the form of the expression $T_k(\varphi(0))$ with the expression of the form $T_k(\cosh(\zeta))$ given the freedom of varying ζ. To do that we consider a substitution of

$\zeta = \ln(y)$, so that we only need to match $\varphi(0)$ with the form $(y+y^{-1})/2$, which is just a quadratic equation.

$$\varphi(0) = \cosh(\zeta) = \cosh(\ln(y)) \quad \ln(y) := \zeta \tag{4.2.8}$$

$$\text{recall: } \cosh(x) = (\exp(-x) + \exp(x))/2 \tag{4.2.9}$$

$$\implies \cosh(\ln(y)) = (y + y^{-1})/2 \tag{4.2.10}$$

$$\varphi(0) = (y + y^{-1})/2 \tag{4.2.11}$$

Recall the definition of $\varphi(x)$ and then simplifies:

$$\begin{aligned}
\varphi(0) &= \frac{-\lambda_n - \lambda_1}{\lambda_n - \lambda_1} \\
&= \frac{-\lambda_n/\lambda_1 - 1}{\lambda_n/\lambda_1 - 1} \\
&= -\frac{\lambda_n/\lambda_1 + 1}{\lambda_n/\lambda_1 - 1} \\
\implies \varphi(0) &= -\frac{\kappa + 1}{\kappa - 1}
\end{aligned}$$

Our objective is now simple. We know what $\varphi(0)$ is, we want it to form match with $\cosh(\ln(y))$, and hence we simply solve for y:

$$-\frac{\kappa+1}{\kappa-1} = \frac{1}{2}(y + y^{-1}) \tag{4.2.12}$$

$$y = \frac{\sqrt{\kappa} \pm 1}{\sqrt{\kappa} \mp 1} \tag{4.2.13}$$

It's a quadratic and we solved it. The above $\pm, \mp$ are correlated, meaning that they are of opposite sign, which gives us two roots for the quadratic expression. Now, given the hyperbolic form for $\varphi(0)$, we can substitute and get the value of $T_k(\varphi(0))$ in terms of y and then κ:

$$\varphi(0) = \frac{1}{2}(y + y^{-1}) \tag{4.2.14}$$

$$\implies T_k(\varphi(0)) = T_k(\cosh(\ln(y))) \tag{4.2.15}$$

$$= \cosh(k \ln(y)) \tag{4.2.16}$$

$$= (y^k + y^{-k})/2 \tag{4.2.17}$$

Then, substituting the value of y, and invert the quantity we have:

$$\frac{1}{T_k(\varphi(0))} = 2(y^k + y^{-k})^{-1} \tag{4.2.18}$$

$$= 2\left(\left(\frac{\sqrt{\kappa} \pm 1}{\sqrt{\kappa} \mp 1}\right)^k + \left(\frac{\sqrt{\kappa} \mp 1}{\sqrt{\kappa} \pm 1}\right)^{-k}\right)^{-1} \tag{4.2.19}$$

$$= 2\left(\underbrace{\left(\frac{\sqrt{\kappa} + 1}{\sqrt{\kappa} - 1}\right)^k}_{>1} + \underbrace{\left(\frac{\sqrt{\kappa} - 1}{\sqrt{\kappa} + 1}\right)^{-k}}_{<1}\right)^{-1} \tag{4.2.20}$$

$$\leq 2\left(\frac{\sqrt{\kappa} - 1}{\sqrt{\kappa} + 1}\right)^k \tag{4.2.21}$$

Which completes the proof. Recall from the previous discussion for the squared of the relative error, we have:

$$\frac{\|e_k\|_A}{\|e_0\|_A} \leq \min_{p_k : p_k(0)=1} \max_{x \in [\lambda_1, \lambda_n]} |p_k(x)| \leq 2\left(\frac{\sqrt{\kappa} - 1}{\sqrt{\kappa} + 1}\right)^k \tag{4.2.22}$$

□

4.2.2 One Outlier Eigenvalue

Using the derived theorem 3, we can extend it to other types of distributions of eigenvalues. Imagine an extreme case where some matrices have one group of eigenvalues that are close together and one single eigenvalue that is far away from the cluster. In that case, we can use Chebyshev differently by focusing its minimizing power across the clustered eigenvalues and use a simple polynomial to interpolate the outlier eigenvalue.

Consider the following proposition:

Proposition 4.3 (Big Outlier CG Convergence Rate)**.** If, there exists a λ_n that is much later than all previous $n-1$ eigenvalues for the matrix A, then a tighter convergence bound that being only parameterized by the range of clustered eigenvalues can be obtained and it is:

$$\frac{\|e^{(k)}\|_A}{\|e^{(0)}\|_A} \le 2\left(\frac{\sqrt{\kappa_{n-1}}-1}{\sqrt{\kappa_{n-1}+1}}\right)^{k-1} \qquad \kappa_{n-1} = \frac{\lambda_{n-1}}{\lambda_1} \tag{4.2.23}$$

Reader, please observe that the outlier eigenvalue λ_n plays a smaller role in determining the convergence rate of the algorithm compared to the previous bound.

Proof. Here, we wish to show that a more focused use of the Chebyshev will introduce a better convergence rate for the conjugate gradient. We define the notation for the adapted k-th degree Chebyshev Polynomial over an closed interval: $[a, b]$ as:

$$\hat{T}^{(k)}_{[a,b]}(x) := T_k\left(\frac{2x-b-a}{b-a}\right) \tag{4.2.24}$$

Next, we consider the following polynomial:

$$p_k(x) := \frac{\hat{T}^{(k-1)}_{[\lambda_1,\lambda_{n-1}]}(x)}{T^{(k-1)}_{[\lambda_1,\lambda_{n-1}]}(0)}\left(\frac{\lambda_n - x}{x}\right) \tag{4.2.25}$$

Where, we use an $k-1$ degree polynomial for the clustered eigenvalues, and then we multiply that by a linear function $(\lambda_n - z)/\lambda_n$ which is zero at right boundary λ_n and it's less than one at the left boundary λ_1. Next, observe the following facts about the above polynomials:

$$\frac{\lambda_n - x}{\lambda_n} \in [0, 1] \quad \forall z \in [\lambda_1, \lambda_n] \tag{4.2.26}$$

$$|p_k(x)| \le \left|\frac{\hat{T}^{(k-1)}_{[\lambda_1,\lambda_{n-1}]}(x)}{\hat{T}^{(k-1)}_{[\lambda_1,\lambda_{n-1}]}(0)}\frac{\lambda_n - x}{\lambda_n}\right| \le \frac{1}{\left|\hat{T}^{(k-1)}_{[\lambda_1,\lambda_{n-1}]}(0)\right|} \tag{4.2.27}$$

As a result, we can apply (4.2.17) we proven for the uniform case, giving us:

$$T^{(k-1)}_{[\lambda_1,\lambda_{n-1}]}(0) = \left|T_{k-1}\left(\frac{-\lambda_{n-1}-\lambda_1}{\lambda_{n-1}-\lambda_1}\right)\right| \tag{4.2.28}$$

$$= \frac{1}{2}(y^{k-1}+y^{-(k-1)}) \tag{4.2.29}$$

$$\text{where: } y = \frac{\sqrt{\kappa_{n-1}}+1}{\sqrt{\kappa_{n-1}}-1}, \kappa_{n-1} = \frac{\lambda_{n-1}}{\lambda_1} \tag{4.2.30}$$

Substituting the value for y we obtain the bound:

$$\frac{\|e_k\|_A}{\|e_0\|_A} \leq 2\left(\frac{\sqrt{\kappa_{n-1}}-1}{\sqrt{\kappa_{n-1}}+1}\right)^{k-1} \tag{4.2.31}$$

□

Another case that is worth considering is when there is one eigenvalue that is smaller than all the other eigenvalues which are clustered at a way larger value than it, by which I mean the value of λ_1 is much smaller than all other eigenvalues and the other eigenvalues are clustered close together in an interval uniformly.

Proposition 4.4 (Small Outlier CG Convergence Rate)**.** The convergence rate is:

$$\frac{\|e_k\|_A}{\|e_0\|_A} \leq 2\left(\frac{\lambda_n-\lambda_1}{\lambda_1}\right)\left(\frac{\sqrt{\kappa_0}-1}{\sqrt{\kappa_0}+1}\right)^{k-1} \tag{4.2.32}$$

Where κ_0 is λ_n/λ_2.

Proof.

$$w(z) := \frac{\lambda_1 - z}{\lambda_1} \tag{4.2.33}$$

$$p_k(z) := w(z)\left(\frac{\hat{T}^{(k-1)}_{[\lambda_2,\lambda_n]}(z)}{\hat{T}^{(k-1)}_{[\lambda_2,\lambda_n]}(z)}\right) \tag{4.2.34}$$

$$\implies \max_{x\in[\lambda_2,\lambda_n]} |w(x)| = \frac{\lambda_n-\lambda_1}{\lambda_1} \tag{4.2.35}$$

In this case, the maximal value of the linear function w is achieved via $x = \lambda_1$, and the absolute value swapped the sign of the function. Therefore, we have:

$$|p_k(x)| = \left| w(x) \frac{\hat{T}^{(k-1)}_{[\lambda_2, \lambda_n]}(x)}{\hat{T}^{(k-1)}_{[\lambda_2, \lambda_n]}(0)} \right| \tag{4.2.36}$$

$$\leq \left| \frac{w(x)}{\hat{T}^{(k-1)}_{[\lambda_2, \lambda_n]}(0)} \right| \tag{4.2.37}$$

$$\leq \left| \left(\frac{\lambda_n - \lambda_1}{\lambda_1} \right) \hat{T}^{(k-1)}_{[\lambda_2, \lambda_n]}(0) \right| \tag{4.2.38}$$

$$\implies \leq \left(\frac{\lambda_n - \lambda_1}{\lambda_1} \right) 2 \left(\frac{\sqrt{\kappa_0} - 1}{\sqrt{\kappa_0} + 1} \right)^{k-1} \tag{4.2.39}$$

We applied the Chebyshev bound proved in the previous part(theorem 3). And $\kappa_0 = \lambda_n / \lambda_2$, and that is the maximal bound for the absolute value of the polynomial.

Take notice that it's not immediately clear which type of outlier eigenvalue makes the convergence better or worse, but in this case, the weight $w(x)$ introduces a term that grows inversely proportional to λ_1. $\square$

4.3 From Conjugate Gradient to Lanczos

We had been brewing the fact that the Iterative Lanczos algorithm and the conjugate gradient algorithm are related. From the previous discussion we can observe that:

1.) Both Lanczos and CG terminate when the grade of Krylov subspace is reached. For Lanczos it's $\mathcal{K}_k(A|q_1)$ and for CG it's $\mathcal{K}_k(A|r_0)$.

2.) Both Lanczos and CG generate orthogonal vectors, for Lanczos they are the q_i vector and for CG they are the r_i vectors.

In particular, these 2 properties are hinting at an equivalence between the residual vectors r_j from CG and the orthogonal vectors q_j from Lanczos. However, notice that the iterative Lanczos is for general symmetric matrices while CG is only for positive definite matrices, therefore We go in both directions to show the connections between these two iterative algorithms. Here, we refer Lanczos vectors as the sequence of q_j generated by the Lanczos iterations.

For this subsection, we state how to represent the parameters from the Lanczos algorithm: α_k, β_k, q_k using a_j, b_j, r_j from the conjugate gradient algorithm. We establish it by deriving the Lanczos algorithm using the conjugate gradient.

Proposition 4.5. The residual and the Lanczos vectors have the following relations:

$$q_1 = \hat{r}_0 \tag{4.3.1}$$

$$q_2 = -\hat{r}_1 \tag{4.3.2}$$

$$\vdots \tag{4.3.3}$$

$$q_j = (-1)^{j+1}\hat{r}_{j+1} \tag{4.3.4}$$

Here, $\hat{r}_j := r_j/\|r_j\|$ and we can fill in the Lanczos tridiagonal matrix using the CG parameters.

$$\begin{cases} \alpha_{j+1} = \frac{1}{a_j} + \frac{b_{j-1}}{a_{j-1}} & \forall 1 \le j \le k-1 \\ \beta_j = \frac{\sqrt{b_{j-1}}}{a_{j-1}} & \forall 2 \le j \le k-2 \\ \alpha_1 = a_0^{-1} & \\ \beta_1 = \frac{\sqrt{b_0}}{\alpha_0} & \end{cases} \tag{4.3.5}$$

Where α_j for $1 \le j \le n-1$ are the diagonal of the tridiagonal matrix T_k generated by Lanczos, and β_j for $2 \le j \le k-2$ are the lower and upper subdiagonals of the matrix T_k.

Proof. The proof is long and it's presented in appendex item: B.8 □

CG is a special case of applying the Lanczos Iterations with $q_1 = r_0$ to a positive definite matrix. However there are still questions left.

1.) How are the solutions x_k generated by CG related to the parameters of Lanczos iterations?

2.) How are the A-Orthogonal vectors p_k from CG related to Lanczos?

Remark 4.3.1 (A Better Terminations Conditions for CG)**.** The derivation hinted at a better termination condition for the CG algorithm. Because CG is equivalent to the Lanczos iterations initialized with $q_1 = r_0$, and we can directly apply from proposition 3.4.2 to get the precise number of iterations of CG under exact arithmetic given r_0, improving the result we got from proposition 4.2.

4.4 From Lanczos to Conjugate Gradient

CG is a special case of Lanczos iterations that solves T_k using LU without pivoting.

4.4.1 Matching the Residual and Conjugate Vectors

In this section, we represent the solution x_k, p_k from CG using the Lanczos vectors and entries inside the symmetric tridiagonal matrix generated by Lanczos iterations. In the remark we highlight some of the insights lead to solvers for symmetric indefinite systems.

Proposition 4.6 (Lanczos Vectors and Residuals)**.** The Q_k is the orthogonal matrix generated by Lanczos Iteration. To match the Krylov Subspace generated by the Lanczos iterations and CG, we initialize $q_1 = \hat{r}_0$, then the following relationship between Lanczos and CG occurs between their parameters:

$$\begin{cases} y_k = T_k^{-1}\beta\xi_1 \\ x_k = x_0 + Q_k y_k \\ r_k = -\beta_k \xi_k^T y_k q_{k+1} \end{cases} \tag{4.4.1}$$

The quantities α_i, β_i are the diagonal and the sub/super diagonal of the matrix T_k from the iterative Lanczos but β without the subscript denotes $\|r_0\|$. r_k is the residual from the conjugate gradient algorithm, and Q_k is the orthogonal matrix generated from the Lanczos algorithm. For notations, we use ξ_i to denote the ith canonical basis vector.

Proof. Recall Lanczos recurrence:

$$AQ_k = Q_{k+1}\begin{bmatrix} T_k \\ \beta_k \xi_k^T \end{bmatrix} \tag{4.4.2}$$

Recall that the conjugate gradient algorithm takes the guesses from the affine space of $x_0 + \mathcal{K}_k(A|r_0)$, from section CG and Krylov Subspace 3.3.6 we know that: $p_k \in \mathcal{K}_{k+1}(A|r_0)$, the matrix P_k, Q_k spans the same subspace. Consider changing $\overline{P}_k r_0$ into $Q_k y_k$, solving for y_k:

$$x_{k+1} = x_0 + Q_k y_k \tag{4.4.3}$$

$$r_{k+1} = r_0 - AQ_k y_k \tag{4.4.4}$$

$$Q_k^T r_{k+1} = Q_k^T r_0 - Q_k^T AQ_k y_k \tag{4.4.5}$$

$$\implies 0 = \beta\xi_1 - T_k y_k \tag{4.4.6}$$

$$y_k = T_k^{-1}\beta\xi_1 \tag{4.4.7}$$

Now to get the residual we simply consider:

$$r_{k+1} = r_0 - AQ_k y_k \tag{4.4.8}$$

$$= r_0 - AQ_k T_k^{-1}\beta\xi_1 \tag{4.4.9}$$

$$\implies = \beta q_1 - AQ_k T_k^{-1}\beta\xi_1 \tag{4.4.10}$$

$$= \beta q_1 - Q_{k+1}\begin{bmatrix} T_k \\ \beta_k \xi_k^T \end{bmatrix} T_k^{-1}\beta\xi_1 \tag{4.4.11}$$

$$= \beta q_1 - (Q_k T_k + \beta_k q_{k+1}\xi_k^T) T_k^{-1}\beta\xi_1 \tag{4.4.12}$$

$$= \beta q_1 - (Q_k \beta\xi_1 + \beta_k q_{k+1}\xi_{k+1} T_k^{-1}\beta\xi_1) \tag{4.4.13}$$

$$= -\beta_k q_{k+1}\xi_k^T T_k^{-1}\beta\xi_1 \tag{4.4.14}$$

On the third line (4.4.10) we recall the fact that $q_1 = \hat{r}_0$ which initialized the Krylov subspace for the Lanczos iteration. At the 4th line (4.4.11), we make use of the Lanczos vector recurrences and we simply substituted it.

By observing the fact that $\xi_k^T T_k^{-1}\xi_1$ the $(k,1)$ element of the matrix T_k^{-1} which is a scalar, we can conclude that the residual from CG and the Lanczos vector are scalar multiple of each other, therefore, r_k from the CG must be orthogonal as well. $\square$

Proposition 4.7 (Lanczos Vectors and Conjugate Vectors)**.** The P_k matrix as derived in the CG algorithm can be:

$$P_k = Q_k U_k^{-1} \tag{4.4.15}$$

Where $T_k = L_k U_k$, representing the LU decomposition of the tridiagonal matrix T_k from the Lanczos Iterations. Because of the tridiagonal nature of the matrix T_k, L_k will be a unit bi-diagonal matrix and U_k will be an upper bi-diagonal matrix.

Proof. Verify the fact that P_k as defined above is A-Orhogonal:

$$P_k^T A P_k \tag{4.4.16}$$
$$= (Q_k U_k^{-1})^T A Q_k U_k^{-1} \tag{4.4.17}$$
$$= (U_k^{-1})^T Q_k^T A Q_k U_k^{-1} \tag{4.4.18}$$
$$= (U_k^{-1})^T T_k U_k^{-1} \tag{4.4.19}$$
$$= (U^{-1})_k^T L_k \tag{4.4.20}$$

Reader please observe that U_k is upper triangular, therefore, it's inverse it's also upper triangular, therefore, U_k^{-T} is lower triangular, and because L_k is also lower triangular, their product is a lower triangular matrix, and therefore, the resulting matrix above is lower triangular, however, given that $P_k^T A P_k$ is symmetric, therefore, $U_k^{-T} L_k$ will have to be symmetric as well, and a matrix that is lower triangular and symmetric has to be diagonal. Therefore, the columns of P_k are conjugate vectors.

Next we show that the x_k is a specific combinations of columns of P_k and it's related to elements in matrix U_k:

$$
\begin{aligned}
x_k &= x_0 + Q_k y_k && (4.4.21)\\
&= x_0 + Q_k T_k^{-1}\beta\xi_1 && (4.4.22)\\
&= x_0 + Q_k U_k^{-1} L_k^{-1}\beta\xi_1 && (4.4.23)\\
&= x_0 + P_k L_k^{-1}\beta\xi_1 && (4.4.24)
\end{aligned}
$$

□

4.4.2 Matching the a_k, b_k in CG

Similar to how we can generate the tridiagonal matrix for the Lanczos iterations with $q_1 = \hat{r}_0$, we can also generate the parameters a_k, b_k in the CG algorithm using parameters from the Lanczos iterations. To achieve it, one can simply build up the recurrences for the y_k vectors using the elements from the L_k, U_k matrix which comes from LU decomposition of the T_k matrix. This will come at the expense of losing some degree of accuracy because it's equivalent to doing the LU decomposition of T_k without pivoting, but it comes at the advantage computing $\xi_k^T T_k^{-1}\xi_1$ with as little efforts as possible. Let's take a look.

For discussion in this section, we briefly switch the indexing and let it start counting from one instead of zero.

$$
P_k = \begin{bmatrix} p_1 & p_2 & \cdots & p_k \end{bmatrix} \quad Q_k = \begin{bmatrix} q_1 & q_2 & \cdots & q_k \end{bmatrix} \tag{4.4.25}
$$

Next, when T_k is invertible, we consider the LU decomposition of the symmetric tridiagonal matrix (See remark for more discussion about the conditions for invertibility of the matrix):

$$T_k = L_k U_k = \begin{bmatrix} 1 & & & \\ l_1 & 1 & & \\ & \ddots & \ddots & \\ & & l_{k-1} & 1 \end{bmatrix} \begin{bmatrix} u_1 & \beta_1 & & \\ & u_2 & \beta_2 & \\ & & \ddots & \beta_{k-1} \\ & & & u_k \end{bmatrix} \tag{4.4.26}$$

The upper diagonal of U_k is indeed the same as the upper diagonal of the symmetric tridiagonal matrix T_k. And recall the expression for x_k from the previous section, we have:

$$x_k = x_0 + P_k L_k^{-1} \beta \xi_1 \tag{4.4.27}$$

$$x_k - x_{k-1} = P_k L_k^{-1} \beta \xi_1 - P_{k-1} L_{k-1}^{-1} \beta \xi_1 \tag{4.4.28}$$

$$= P_k \beta (L_k^{-1})_{:,1} - P_{k-1} \beta (L_{k-1}^{-1})_{:,1} \tag{4.4.29}$$

$$= \beta (L_k^{-1})_{k,1} p_k \tag{4.4.30}$$

$$\implies x_k = x_{k-1} + \beta (L_k^{-1})_{k,1} p_k \tag{4.4.31}$$

On the third line (4.4.29), we factor out the last column for the matrix P_k. Next, we wish to derive the recurrence between p_{k+1} and p_k. Which is:

$$P_k = Q_k U_k^{-1} \tag{4.4.32}$$

$$P_k U_k = Q_k \tag{4.4.33}$$

$$\implies \beta_{k-1} p_{k-1} + u_k p_k = q_k \tag{4.4.34}$$

$$u_k p_k = q_k - \beta_{k-1} p_{k-1} \tag{4.4.35}$$

$$p_k = u_k^{-1} (q_k - \beta_{k-1} p_{k-1}) \tag{4.4.36}$$

In fact, a short recurrence can be built for u_k^{-1} and $(L_k^{-1})_{k,1}$, we stated it below:

$$\begin{cases} u_{k+1} & = \alpha_{k+1} - \beta_k^2/u_k \\ l_k & = \beta_k/u_k \\ (L_{k+1}^{-1})_{k+1,1} & = -l_k(L_k^{-1})_{k,1} \end{cases} \tag{4.4.37}$$

The derivation for above recurrence is more relevant to the LU decomposition of a Tridiagonal matrix, which is a digression and we put the proof in appendix item B.9.

Remark 4.4.1. Using the Lanczos iterations, we derived the conjugate gradient without using the fact that A is symmetric positive definite, this fact hinted at potential new algorithms that can solve symmetric indefinite systems directly.

The Lanczos algorithm for linear systems (we refer to the method derived in the above section) is a special case of FOM [14] when the matrix A is symmetric. The above algorithm is just FOM with a short term recurrence for its parameters, and it's based on convenience of solving a symmetric tridiagonal matrix. It's implied from the above derivation that under exact arithmetic, CG can be applied to a symmetric indefinite system, if we have the luck where T_j is non-singular for all $j \le k$. Recall that when we derived the CG algorithm, we convert it into solving the system: $P_k^T r_0 = P_k^T A P_k w$, and when the matrix A is indefinite, we can still solve the system by attaining the saddle point for the indefinite error norm.

However there are two problems for solving symmetric indefinite using CG. The first problem is the bad numerical accuracy of using the recurrence to perform LU decomposition on T_K without pivoting. Another problem is T_k can be singular during some iterations of the Lanczos algorithm. For example, T_j will become singular if A is a symmetric tridiagonal matrix with zeros as its diagonals and all ones on its subdiagonals. The good part is that T_j never will not become singular for more than 2 consecutive iteration[4]. These problems can be overcome by considering something other than LU without pivoting. In fact, the work by C. C. Paige and M. A. Saunders extends the idea and derives algorithms that can solve a symmetric indefinite system without using the norm equation [9].

5 Effects of Floating-Point Arithmetic

In this section, we exam the behaviors of the Lanczos iterations and CG algorithms under floating-point arithmetic using numerical experiments and some analysis. We wish to get deeper insights about the behaviors of Lanczos and conjugate gradient under floating-point arithmetic.

5.1 Partial Orthogonalization and Full Orthogonalization

The floating-point round of errors in the CG algorithm accumulates and manifests as loss of orthogonality and loss of conjugacy for the vectors r_k, p_k. Other stable algorithm such as Modified Gram Schmidt orthgonalize the current vector against all previous vectors to assert orthogonality of the basis vector, CG on the other hand, relies only on the short recurrences of r_k, p_k. One way to mitigate the effect is to use the CDM algorithm's projector to re-orthogonalize the conjugate vectors and then reorthogonalized residual vectors against all previous residuals vectors. Such idea is not new and it's stated in the original paper by Hestenes and Stiefel back in 1952[8]; in this section we present the more computationally expensive idea in the paper by Hestenes and Stiefel, but using what we derived in the first section.

Recall the proof for proposition 3.7. Next, we inductively consider the case where the newest residual vector is involving some round-off error $\overline{r}_{k+1}$ and it breaks the orthogonality conditions $\overline{r}_{k+1} \perp r_j \; \forall \; 0 \leq j \leq k$:

$$(AP_k)^T \overline{r}_k = \begin{bmatrix} \langle p_0, A\overline{r}_k \rangle \\ \langle p_1, A\overline{r}_k \rangle \\ \vdots \\ \langle p_{k-1}, A\overline{r}_k \rangle \end{bmatrix} \tag{5.1.1}$$

$$= a_{k-1}^{-1} \langle r_k, (r_{k-1} - r_k) \rangle \xi_k + \sum_{j=0}^{k-1} \langle p_j, A\overline{r}_k \rangle \xi_j \tag{5.1.2}$$

$$p_k := \overline{r}_k + b_k p_k - \frac{\langle \overline{r}_k, r_{k-1} \rangle}{\langle r_{k-1}, r_{k-1} \rangle} p_k - \sum_{j=0}^{k-1} \frac{\langle p_j, A\overline{r}_k \rangle}{\langle p_k, Ap_k \rangle} p_j \tag{5.1.3}$$

$$r_k := \overline{r}_k - \sum_{j=0}^{k-1} \langle \hat{r}_j, \overline{r}_k \rangle \hat{r}_j \tag{5.1.4}$$

Here, we generate the conjugate vectors p_k correctly by faithfully expanding the term $(AP_k)^T \overline{r}_k$, and then we update the residual $\overline{r}_k$ into r_k by orthogonalizing it against all previous residual vectors. Such procedure requires expensive storage of previous vectors p_k. One can use alternative formulas to A-orthogonalize p_k and re-orthogonalize r_k. In addition, we have the options for partially orthogonalizing the r_k, p_k vectors for less memory usage.

5.2 Relative Errors of CG Under Floating-Point Arithmetic

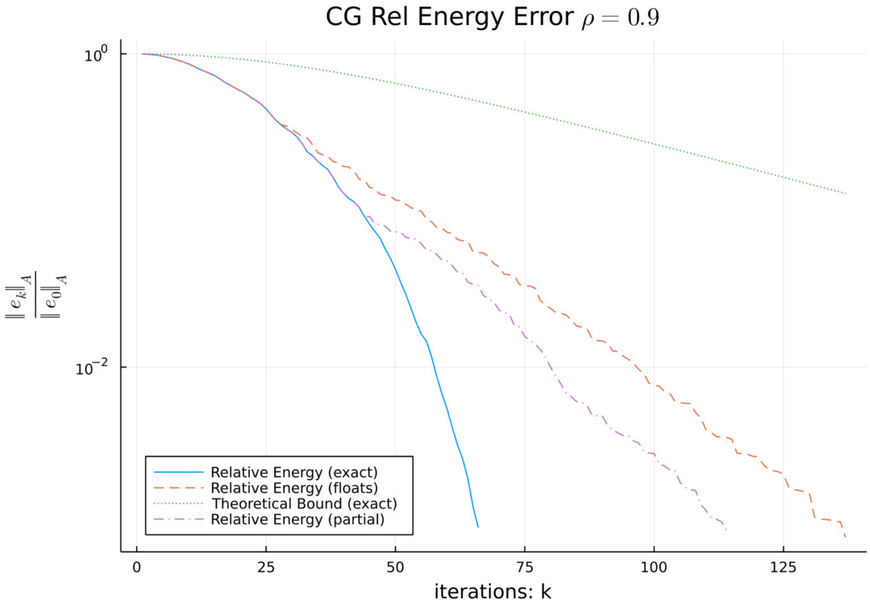
We investigate the relative energy norm of the error for fully re-orthogonalized CG, partially re-orthogonalized CG, and CG without re-orthogonalization numerically.

5.2.1 Experiments

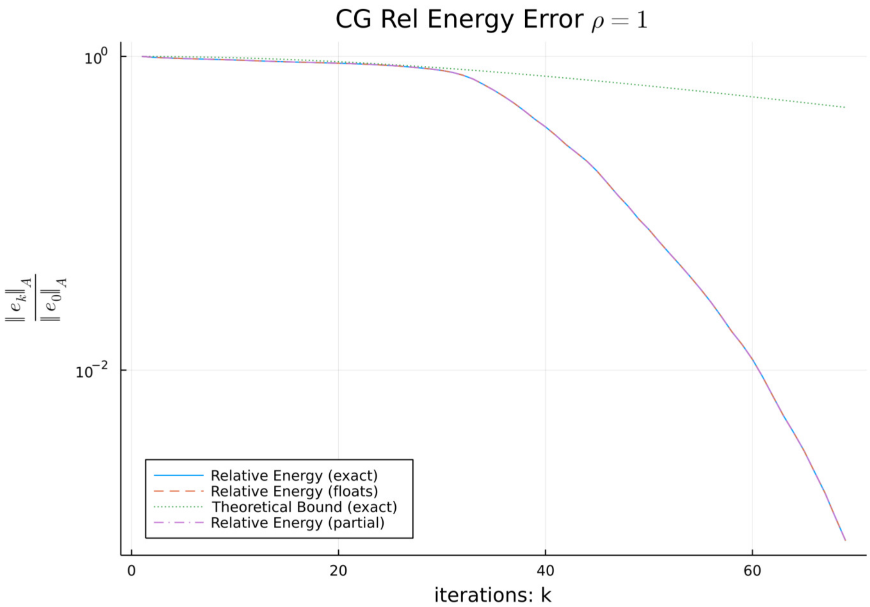
Here we use full re-orthogonalization to emulate the effects of exact arithmetic. the step required for convergence is less than or equal to the number of unique eigenvalues for the symmetric definite matrix, this is established in part termination of CG 4.2 of the discussion. However, in practice, this is not always the case. Similar experiments are conducted in Greenbaum's book chapter[6] 4. In this section, we replicate the same set of experiments using modern Julia to showcase the extra steps required for the CG algorithm to converge. For testing the convergence of the algorithm, we use float16 (16 digits binary digits), $\lambda_{\min} = 1e - 4, \lambda_{\max} = 1$ to exaggerate the convergence a bit, and the RHS vector b is all ones and $x_0 = b + \epsilon$ (ϵ is some tiny random vector as noise). The spectrum of the matrix we are using is taken to be the same from Greenbaum's book [6] page 62.

$$\lambda_{\min} + \left(\frac{j}{N-1}\right)(\lambda_{\max} - \lambda_{\min})\rho^{N-j+1} \quad \forall\, 1 \leq j \leq N-1,\ 0 \leq \rho \leq 1 \tag{5.2.1}$$

If the value of ρ is close to zero, then the eigenvalues are clustered around the origin, if it's close to 1, then the eigenvalues are tend to be more evenly distributed around the interval $[\lambda_{\min}, \lambda_{\max}]$.



(a) $\rho = 0.9$



(b) $\rho = 1$

Figure 5.2.1: The relative energy norm error for different methods. Blue solid line: The exact conjugate gradient convergence. Purple dot dashed: The conjugate gradient that is partially orthogonalized with previous 8 residual and conjugate vectors. orange dashed: the Original conjugate gradient. Green dot: The tighter theoretical upper bound derived by Chebyshev (4.2.20). The matrix is 256×256

The Chebyshev bound is no longer a tight bound because the distribution of the eigenvalues is not perfectly uniform for $\rho = 0.9$. The partially orthogonalized methods diverge from the exact error after more steps of iterations compared to the relative error without any orthogonalizations. These are seen in (fig 5.2.1a). In contrast, on the right with $\rho = 1$, then the eigenvalues are uniformly distributed, the relative energy errors of all 3 methods aligns and overlapped into one curve in (fig 5.2.1b) at the expense of slower convergence for the few iterations at the beginning.

Remark 5.2.1. The convergence is disappointing under floating-point arithmetic and the promised efficiency of the algorithm is not there anymore even if the matrix is not necessarily ill-conditioned. Just from (fig 5.2.1) it seems like outlier eigenvalues provide fast convergence under full orthogonalization, but not for floating point.

However, please observe from (fig 5.2.1b) that, all these 3 methods are identical, and the Chebyshev bound is relatively tight at the first few iterations of the algorithm, which is related to the discussion later and linked to the fact that the characteristic polynomial of T_k has roots closer to the spectrum of A where eigenvalues are sparse before converging to region of the spectrum where eigenvalues are denser.

5.3 Paige's Convergence rate of CG under Floating Points

In this section we present the backwards analysis of the CG convergence rate in a more thorough manner and examine its consequences. When floating-point arithmetic is used, the eigenvalues of the tridiagonal matrices might introduce ghost eigenvectors for the Lanczos Iterations, and using the equivalence of the Lanczos iterations and CG, we can capture a posteriori bound on how much the error is exactly during the iterations of CG.

5.3.1 Bounding the Relative Residuals

Recall from proposition Proposition 4.6 that the residuals of the CG can be expressed in terms of the Lanczos vectors. However, the Lanczos iterations under floating-point doesn't produce perfectly orthogonal Lanczos Vectors (The lost of orthogonality is experimented and visualized in the next section), $\tilde{Q}_k$ is not quite orthogonal, meaning that $\tilde{Q}_k^H A\tilde{Q}_k \neq T_k$ where T_k is the tridiagonal matrix from the Lanczos iterations. However the Lanczos iterations will still solve for y_k using the expression $y_k = \beta T_k^{-1}\xi_1$, the algorithm still T_k produces a perfectly tridiagonal matrix T_k. At first glance, tiny round-off errors in the Lanczos vectors are very problematic.

Surprisingly, the recurrence formula for Lanczos still holds to some extent, in addition we can leverage the fact that y_k is solved exactly and assume: $y_k = \beta T^{-1}\xi_1$ is at least, exact. Then it left us with fewer types of floating-point errors to keep track of. Next, we proceed to look for the residual of the CG algorithm by stating that the Lanczos recurrences[2]:

$$AQ_k = Q_{k+1}\begin{bmatrix} T_k \\ \beta_k \xi_k^T \end{bmatrix} + F_k \tag{5.3.1}$$

Reader, please reflect on the fact that the Q_k which is not orthogonal, and we are fixing the recurrences with F_k, a matrix representing the floating error to correct it so that the equality holds true. $\|F_k\|$ is small and it's on the magnitude of $\mathcal{O}(\epsilon\|A\|)$.

$$r_k = r_0 - AQ_k y_k \tag{5.3.2}$$

$$r_k = r_0 - \left(Q_{k+1}\begin{bmatrix} T_k \\ \beta_k \xi_k^T \end{bmatrix} + F_k\right) y_k \tag{5.3.3}$$

$$r_k = \underbrace{\left(r_0 - Q_{k+1}\begin{bmatrix} T_k \\ \beta_k \xi_k^T \end{bmatrix} y_k\right)}_{=-\beta_k \xi_k^T y_k q_{k+1}} + F_k \beta T_k^{-1}\xi_1 \tag{5.3.4}$$

$$\implies \frac{\|r_{k+1}\|}{\|r_0\|} \le \beta_k \|\xi_k^T T_k^{-1}\xi_1 q_{k+1}\| + \|F_k T_k^{-1}\xi_1\| \tag{5.3.5}$$

$$\frac{\|r_{k+1}\|}{\|r_0\|} \le \beta_k |\xi_k^T T_k^{-1}\xi_1| + \|F_k\|\|T_k^{-1}\xi_1\| \tag{5.3.6}$$

We make use of Proposition 4.6 and obtain a similar expression because it didn't make use of the fact that Q_k is orthogonal. This time, we take F_k into account. The residual is now bounded by the sum of scalar $\xi_k^T T_k^{-1}\xi_1$ and the floating-point error matrix F_k produced by the Lanczos iterations.

Remark 5.3.1 (When Finite Arithmetic Lanczos is Exact)**.** We can bound the first term that made up the upper bound for the residual of CG using previous convergence results of CG under exact arithmetic; recall CG convergence rate (theorem 3). It can

[2]statement 2.11 from C. C. Paige's 1980 paper.[10]. The result is surprising in the sense that Q_k is not orthogonal in finite precision doesn't affect the recurrence by much.

be applied here for the first term in (5.3.6): $\beta_k|\xi_k^T T_k^{-1}\xi_1|$.

This is true because if we were to perform an CG on the T_{k+1} produced by the finite precision algorithm with the initial Lanczos vector q_1 being $\xi_1^{(n)}$, then its residual $\overline{r}_k$ of equivalent CG would be exact and it's given as $-\beta_k T_k^{-1}\xi_k q_{k+1}$, but with $q_{k+1} = \xi_{k+1}^{(n)}$, the $k+1$ th standard basis vector in $\mathbb{R}^n$, and $T_k = (T_{k+1})_{1:k,1:k}$. And to our excitement, we already have the exact arithmetic bound for $\overline{r}_{k+1}$ proven in theorem 3.

5.3.2 Paige's Theorem and Floating-point Convergence of CG

We now introduce a new theorem proposed by Paige in chapter 4 of Greenbaum's book[6], originally appeared in 3.48 of C.C Paige's Thesis[10]. It gives a bound to the CG with floating-point errors by bounding the condition number of T_k from the Lanczos iterations. It's stated as follows:

Theorem 4 (Paige's Theorem)**.** The eigenvalues $\theta_i^{(j)}, i = 1, \cdots, j$ of the tridiagonal matrix T_j satisfies:

$$\lambda_1 - j^{5/2}\epsilon_2\|A\| \le \theta_i^{(j)} \le \lambda_n + j^{5/2}\epsilon_2\|A\| \tag{5.3.7}$$

$$\epsilon_2 := \sqrt{2}\max\{6\epsilon_0, \epsilon_1\} \tag{5.3.8}$$

Along with this theorem, the following quantities from Paige are also defined:

$$\epsilon_0 \equiv 2(n+4)\epsilon \tag{5.3.9}$$

$$\epsilon_1 \equiv 2(7 + m\|\,|A|\,\|/\|A\|)\epsilon \tag{5.3.10}$$

$$\epsilon_0 < \frac{1}{12} \quad k(3\epsilon_0 + \epsilon_1) < 1 \tag{5.3.11}$$

$$\|F_k\| \le \sqrt{k}(\epsilon_1)\|A\| \tag{5.3.12}$$

$$\|q_j^T q_j - 1\| \le 2\epsilon_0 \tag{5.3.13}$$

$$\beta_j \le \|A\|(1 + (2n+6)\epsilon + j(3\epsilon_0 + \epsilon_1)) \tag{5.3.14}$$

The quantity k is the current iterations number of the Lanczos Iterations, $j \le k$. m is the maximum number of non-zero elements in the matrix A, n is the size of matrix

A and ϵ is the machine precision. Using Paige's theorem, we can bound the condition number for the matrix T_{k+1} produced by the finite precision Lanczos, which is given by:

$$\tilde{\kappa} = \frac{\lambda_n + (k+1)^{5/2}\epsilon_2\|A\|}{\lambda_1 - (k+1)^{5/2}\epsilon_2\|A\|} \tag{5.3.15}$$

Using (remark 5.3.1), we can make the following proposition

Proposition 5.1.

$$|\beta_k \xi_k^T T_k^{-1} \xi_1| \le 2\sqrt{\tilde{\kappa}} \left(\frac{\sqrt{\tilde{\kappa}} - 1}{\sqrt{\tilde{\kappa}} + 1}\right)^k \tag{5.3.16}$$

$\tilde{\kappa}$ is the upper bound of the condition number of the T_k matrix (from (5.3.15)). Please observe that the about quantity is one of the terms for the upper bound on the relative residual of CG presented back in (5.3.6).

Proof. Using the lemma A.1.1 in appendix, we can derive the relations between the 2-norm of the relative residuals and the energy norm of the relative error:

$$\frac{\|Ae_k\|}{\|Ae_0\|} \le \kappa(T_k)\frac{\|e_k\|_A}{\|e_0\|_A} \le 2\sqrt{\kappa(T_k)} \left(\frac{\sqrt{\tilde{\kappa}} - 1}{\sqrt{\tilde{\kappa}} + 1}\right)^k \tag{5.3.17}$$

$$\frac{\|r_k\|}{\|r_0\|} = |\beta_k \xi_k^T T_k^{-1} \xi_1| \quad \text{by (remark 5.3.1)} \tag{5.3.18}$$

$$\implies |\beta_k \xi_k^T T_k^{-1} \xi_1| \le 2\sqrt{\tilde{\kappa}} \left(\frac{\sqrt{\tilde{\kappa}} - 1}{\sqrt{\tilde{\kappa}} + 1}\right)^k \tag{5.3.19}$$

The third inequality is simply from CG Convergence Rate (theorem 3) when we assume that the eigenvalues are uniformly spaced in the convex hull of the spectrum of A. The first fraction is actually the relative error of the 2-norm of the residual because $Ae_k = r_k$ by definition. Substituting the quantity $\kappa(T_k)$, the condition number of the matrix T_k, which we figured out using Paige's theorem and denoted it as $\tilde{\kappa}$. □

Finally, if we assume that T_k^{-1} is invertible, which requires that the conditions for all the quantities: ϵ_0, ϵ_1 holds true, and $\lambda_1 - (k+1)^{5/2}\epsilon_2\|A\| > 0$. Finally, we make can bound the relative residual of the CG algorithm by considering:

$$\frac{\|r_{k+1}\|}{\|r_0\|} \le \beta_k \|\xi_k^T T_k^{-1} \xi_1 q_{k+1}\| + \|F_k T_k^{-1} \xi_1\| \tag{5.3.20}$$

$$\le \beta_k |\xi_k^T T_k^{-1} \xi_1| \|q_{k+1}\| + \|F_k\| \|T_k^{-1} \xi_1\| \tag{5.3.21}$$

$$\le 2\|q_{k+1}\| \sqrt{\tilde{\kappa}} \left(\frac{\sqrt{\tilde{\kappa}} - 1}{\sqrt{\tilde{\kappa}} + 1} \right)^k + \sqrt{k}(\epsilon_1) \|A\| \|T_k^{-1}\| \tag{5.3.22}$$

Now, observe that $|q_j^T q_j - 1| \le 2\epsilon_0$ from (5.3.13), which implies that $\|q_{k+2}\|^2 \le (1+3\epsilon_0)$ which is $\|q_{k+1}\| \le \sqrt{1+2\epsilon_0}$. In pursuit of mathematical beauty, we look for alternative expression for the quantity $\|A\|\|T_k^{-1}\|$ giving us:

$$\|A\| \|T_k^{-1}\| = \frac{\lambda_n}{\lambda_1 - k^{5/2} \epsilon_2 \|A\|} \le \tilde{\kappa} \tag{5.3.23}$$

$$\implies \frac{\|r_{k+1}\|}{\|r_0\|} \le 2\sqrt{1+2\epsilon_0} \sqrt{\tilde{\kappa}} \left(\frac{\sqrt{\tilde{\kappa}} - 1}{\sqrt{\tilde{\kappa}} + 1} \right)^k + \sqrt{k}(\epsilon_1) \tilde{\kappa} \tag{5.3.24}$$

This is the upper bound on the convergence rate for the conjugate gradient Method under floating-point arithmetic.

Remark 5.3.2. This upper bound showed that if the T_{k+1} generated by floating point CG is nonsingular, $\beta_k \ne 0$, then the CG method will still have a chance to converge in the future iterations. Simplyput, it doesn't matter if the round-off error accumulated, conjugate gradient will converge as long as the matrix is not too ill-conditioned, or A being too pathological to worth with.

Finally, I want to point out the fact that Paige's theorem (theorem 4) is derived using forward error analysis on the Lanczos Iterations, which is the absolute worst case. For most cases in modern computing platforms, the summation process of vector dot products has much higher floating-accuracy compare to older computing platforms due to the use of parallelism, or floating-point specific summation instructions, which reduces the relative sizes for the summands, hence reducing the total round-off error accumulations. The bound of convergence rate we derive can be a huge over estimation.

5.4 Ghost Eigenvalues and Losing Orthogonality

The name ghost eigenvalues refers to the phenomena where the Lanczos Algorithm seems to produce tridiagonal matrix T_k whose eigenvalues are clustered extremely close to a simple eigenvalues of the matrix A, when in fact, those extremely close eigenvalues are a single eigenvalue of the original matrix A's spectrum.

The name "ghost eigenvalues" was spotted from lecture 36 of Trefethen's Book[17], the exact origin of the term is not important. This phenomena is more pronounce to eigenvalues in the exterior of A's spectrum. We know for a fact that the tridiagonal matrix produced via Lanczos can't have any repeated eigenvalues (appendix item B.5). What happens in this case is the floating point error propagating through the Lanczos Iterations causing lost of orthogonality of Q_k and eventually produce ghost eigenvalues.

5.4.1 Ghost Eigenvalues Experiments

Here, we conducted numerical experiments and carefully reproduce the phenomena for a diagonal matrix A with diagonals given by the formula:

$$\lambda_i = \left(-1 + \frac{2(i-1)}{(n-1)}\right)^3 \quad 1 \le i \le n \tag{5.4.1}$$

where $A \in \mathbb{R}^{n\times n}$. This matrix is particularly good for reproducing the phenomena. For this experiment, we set $n = 64$ and we use Float64.

We run the Lanczos iterations with q_1 being the vector of all ones, we marked the smallest and largest 10 eigenvalues during the iterations and plotted their trajectories from iteration 20 to 64. The results can be seen in (figure 5.4.1 left). On figure 5.4.1 right, we made the plot for what would happen if the Lanczos iterations are free of numerical round-off error. We didn't use exact arithmetic, instead, we simply re-orthogonalized all the Lanczos vector q_k using all previously obtained Lanczos vectors to emulate the effect, which is just an Arnoldi iteration. Please bear in mind that there are eigenvalues in the middle interior part of the spectrum, they are just not plotted in the figure.

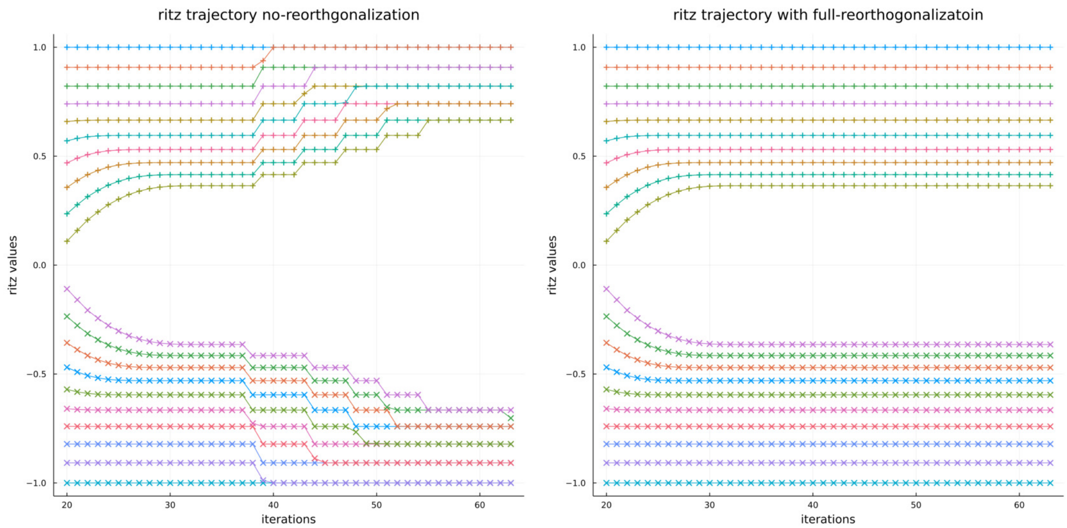


Figure 5.4.1: The highest and lowest 10 eigenvalues of the matrix T_k during the Lanczos Iterations are being tracked by their relative order. During each iteration, the first, the second, the third, ... etc eigenvalues of T_k are linked together by a line in a different color. Left is Lanczos with numerical round-off error, right is Lanczos iterations that fully re-orthogonalize q_k for each iteration which emulates the behaviors under exact arithmetic.

Recall from the Cauchy Interlace Theorem (theorem 6), the eigenvalues of the tridiagonal matrix T_{k+1} has to be in between each eigenvalues of T_k except for the first and the last eigenvalue of T_{k+1}. This implies that, the $\theta_i^{(k)}$, the i th eigenvalues during the k th iteration will move monotonically upwards or downwards during the Lanczos iterations. The ghost eigenvalues on the figure appear when some of the interior eigenvalues suddenly switch to another eigenvalue's trajectory that is on the exterior of the spectrum. It appears as though the matrix T_k has repeated eigenvalues which we know is not true due to (appendix item B.5), they are just very close.

However, judging the eigenvalues of the matrix T_k alone will not distinguish between two very close eigenvalues correspond to two different eigenvalues of A or it's due to the floating-point round-off error. It also will not tell whether the Lanczos vectors are losing orthogonality, even if the eigenvalue trajectories seem to suggest it. The lost of orthogonality must happen for the Lanczos vector while at the same time, we observed extremely close eigenvalues of T_k clustring around eigenvalues of A to confirm the fact that they are indeed ghost eigenvalues.

We can't tell it because if I keep the matrix T_k we used to produce fig 5.4.1 generated from a Lanczos iterations and use it as A with $q_1 - \xi_1$, then it will reproduce exactly the same graph as in left of fig 5.4.1 when we plot out the trajectories of the eigenvalues of T_k, but the Q_k in this case is the $k \times k$ identity matrix and it's exact (Using the exact same idea appeared in remark 5.3.1). Now consider performing another Lanczos iterations $A := T_k$ it but with the initial vector ξ_1, then we will exactly reproduce A itself because it's tridiagonal. But in this case, the eigenvalues of T_k are exact after termination of Lanczos iteration. In this case, all eigenvalues are actually presented in the original matrix A, which is just T_k, itself.

In fact, the ghost eigenvalues here are produced by floating-point errors because firstly we know what the actual eigenvalues of A is, we made A. To make sense of it better intuitively, we observe from the experiments that the loss of orthogonality of Q_k happens together with ghost eigenvalues on the spectrum of T_k. If the Q_k matrix is perfectly orthogonal, then there are no ghost eigenvalues, regardless of what the trajectories of the eigenvalues of T_k look like. In fact, a corresponding plot of $Q_k^H Q_k$ are plotted in (fig 5.4.1 left) for demonstrating the loss of orthogonality for the same diagonal matrix A proposed earlier. We plotted the heat map of the matrix $Q_k^H Q_k$ directly as well.

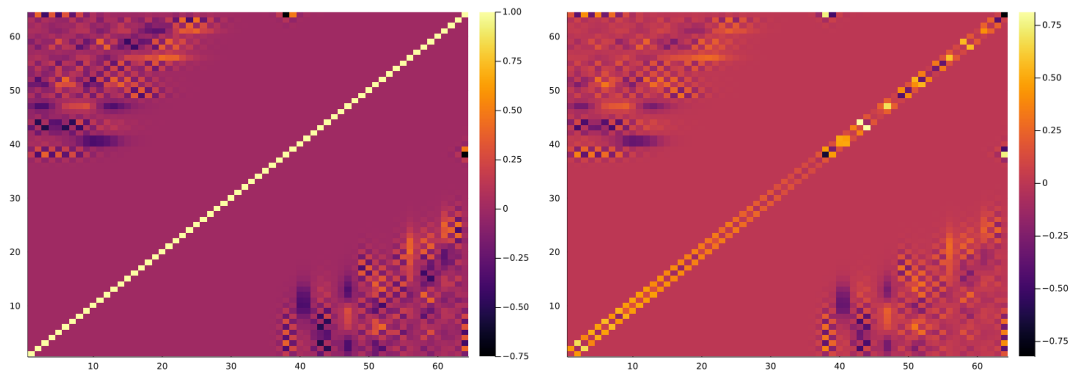


Figure 5.4.2: left: The heatmap of the plot of the absolute values of the matrix $Q_k^T Q_k$. right: The plot of $Q_k^T A Q_k$ from floating-point Lanczos iterations

In addition to the lost orthogonality of the matrix Q_k, we also visualized the actual tridiagonal matrix reproduced by $Q_k A Q_k$ which is plotted in (fig 5.4.1 right). Observe that most of the off tridiagonal entries are non-zero and relatively huge, which doesn't worry us too much because A itself has a large condition number. What is concerning is the blob of non-zero entries on the top left and the bottom right of the plot. And this is a significant loss of orthogonality created by floating-point arithmetic.

Remark 5.4.1. As a final remark for these numerical experiments, I suggest an intuitive way of understanding them. Which will be useful when we actually wish to analyze it rigorously. Simply put, the Lanczos Iterations might "forget" about the eigenvalues when it converged (usually manifested as the stable trajectories of eigenvalues on the exterior of the spectrum for the matrix T_k in (fig 5.4.1)), and when it happens, the Lanczos vectors produced by the algorithm has lost its orthogonality correspondingly, which then causes the interior eigenvalues of T_k to shift, creating ghost eigenvalues that doesn't exist in the spectrum of A.

Secondly, there is another phenomenon of Ritz values during the iterations of Lanczos iterations called misconvergence. It describes the process which a Ritz value is stuck between two eigenvalues of A, stagnated for few iterations and then suddenly shifts away, which is extremely similar to the shifting we observed in figure 5.4.1. It happens when 2 eigenvalues of matrix A is extremely close to each other. It should not be confused with ghost eigenvalues because they are two distinct phenomena where misconvergence can happen under exact arithmetic. For more description of such phenomena, refer to the first chapter from the book by M. G. Cox and S. Hammarling [1].

5.4.2 Lanczos Vectors Losing Orthogonality on converged Ritz vectors

To gain a better understanding, let's define the notion of Ritz values and Ritz vectors. For our discussion, the Ritz value $\theta_i^{(k)}$ are the ith eigenvalues of the matrix T_k from the and the Ritz vectors are $Q_k s_i^{(k)}$ where $s_i^{(k)}$ is the ith eigenvector for the matrix T_k. Recall from remark 3.4.2, the characteristic polynomial of T_k is the monic polynomial that minimizes the 2-norm error for the vector $p_k(A)q_1$ among all monic of the same degree; therefore intuitively, the Ritz values and Ritz vectors approximates eigenvalues and eigenvectors of matrix A due to the approximating characteristic polynomial. Let's suppose that $s_i^{(k)}$ for T_k is a good approximation for λ_j, let's consider the Lanczos iterations recurrences:

$$AQ_k = Q_k T_k + q_{k+1}\beta_k \xi_k^T \tag{5.4.2}$$

$$AQ_k s_i^{(k)} = \theta_j^{(k)} Q_k s_i^{(k)} + q_{k+1}\beta_k \xi_k^T v \tag{5.4.3}$$

$$AQ_k s_i^{(k)} = \theta_j^{(k)} Q_k s_i^{(k)} + \beta_k q_{k+1}(s_i^{(k)})_k \tag{5.4.4}$$

$$AQ_k s_i^{(k)} - \theta_j^{(k)} Q_k s_i^{(k)} = \beta_k q_{k+1}(s_i^{(k)})_k \tag{5.4.5}$$

Upon brief examinations, convergence of the Ritz value $\theta_i^{(k)}$ depends on β_k and $(s_i^{(k)})_k$, intuitively as the Krylov subspace expands, it contains more and more space for the the eigenvectors of A, and the Ritz vector will have more "room" to get closer to the eigenvector of A, by the approximation property of Lanczos. Assuming good convergence of $s_i^{(k)}$ convergences so that the value of $\beta_k, (s_i^{(k)})_k$ are both small (it's true regardless of orthogonality of Q_k), then we consider the projection of most recent Lanczos vector q_k onto the Ritz vector $Q_k s_i^{(k)}$, which is $q_k^T Q_k s_i^{(k)} = (s_i^{(k)})_k$. We expect the projection onto the Ritz vector to be small if the Ritz vector is converging to an eigenvector of A.

However, under floating-point arithmetic, once the Ritz vector $s_i^{(k)}$ is converging to an eigenvalue of A, then the projection of the latest Lanczos vector onto the Ritz vector begins to grow. On the plot showed in figure 5.4.2, we projected the log absolute value of $q_k^T Q_k s_i^{(k)}$ for $i = 1, 2, 3$ for all $k = 20, \cdots, 64$, and we used the same setup from the last section where we demonstrated ghost eigenvalues. For comparison, figure 5.4.2 showed us what happens in exact arithmetic. One very important observation to make from figure 5.4.2 is that the peak of the blue curve, projection onto the largest Ritz value happens around iteration 3.8, and around that exact same iteration in figure 5.4.1 is when the second-largest eigenvalue of T_k decides to shift over to the blue curve. Bear in mind that this is in a log plot, and without the log it looks like a sharp spike.

While floating arithmetic may sometimes cause the most recent Lanczos vector to lose orthogonality against converged Ritz vectors, the converse is not true. The phenomena itself doesn't imply the fact that floating point error is present and it's causing lost of orthogonality of Lanczos iterations, much similar to what had been discussed about ghost eigenvalues. To illustrate, an experiment is conducted in this way:

1. T_n is generated from the diagonal matrix A from finite precision Lanczos iterations. The same setup from ghost eigenvalues 5.4.1.

2. Lanczos is then performed on T_k initialized with $q_1 = \xi_i$.

3. The projection the most recent lanczos vector q_k is projected onto $Q_k s_i^{(k)}$ for $1 \le i \le 3$. Notice that Q_k is gonna be the $k \times k$ identity matrix. ‘’

The results of the projection are showed in fig 5.4.2. Please observe that projection onto the second Ritz vector $Q_k s_2^{(k)}$ seems to decrease and them jumped up again. This happens around the same iterations when the second largest eigenvalue of T_k shift to the trajectory of the largest eigenvalue in fig 5.4.1 left. However, this time the matrix Q_k is perfect orthogonal. Therefore, small ritz projections of the most recent Lanczos vector doesn't mean that the Ritz value has converged for all future iterations. If q_k is losing orthogonality against some Ritz vectors after it has converged, it doesn't mean that Q_k is losing orthogonality.

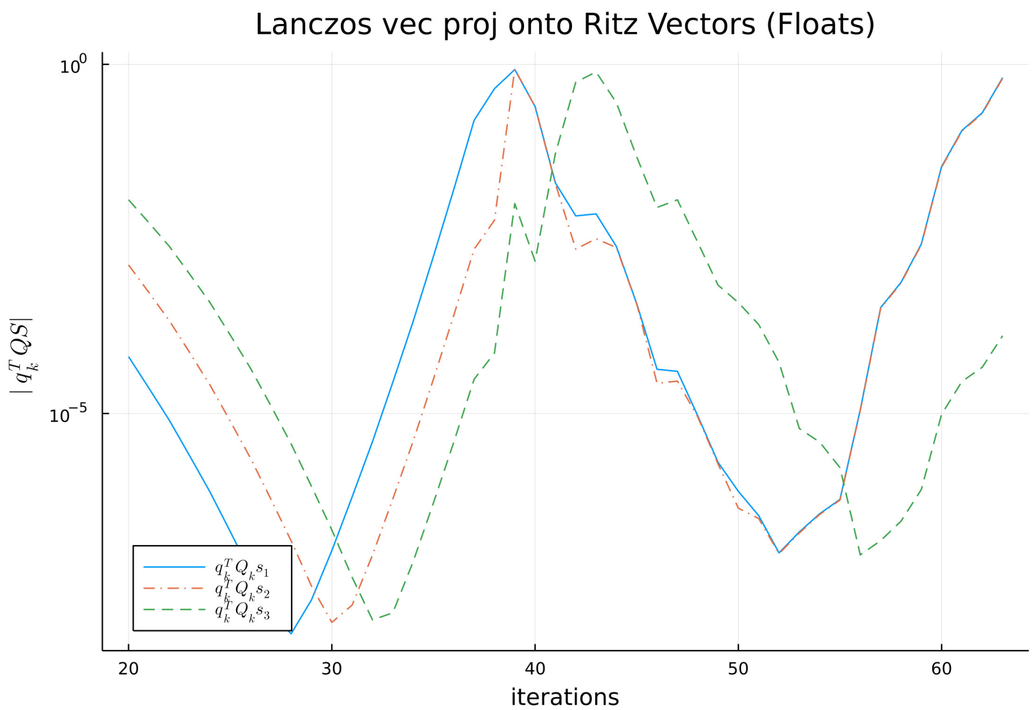


Figure 5.4.3: Projection of floating-point Lanczos vector q_k onto 3 of the largest Ritz vectors: $Q_k s_i^{(k)}$, for $i = k, k-1, k-2$

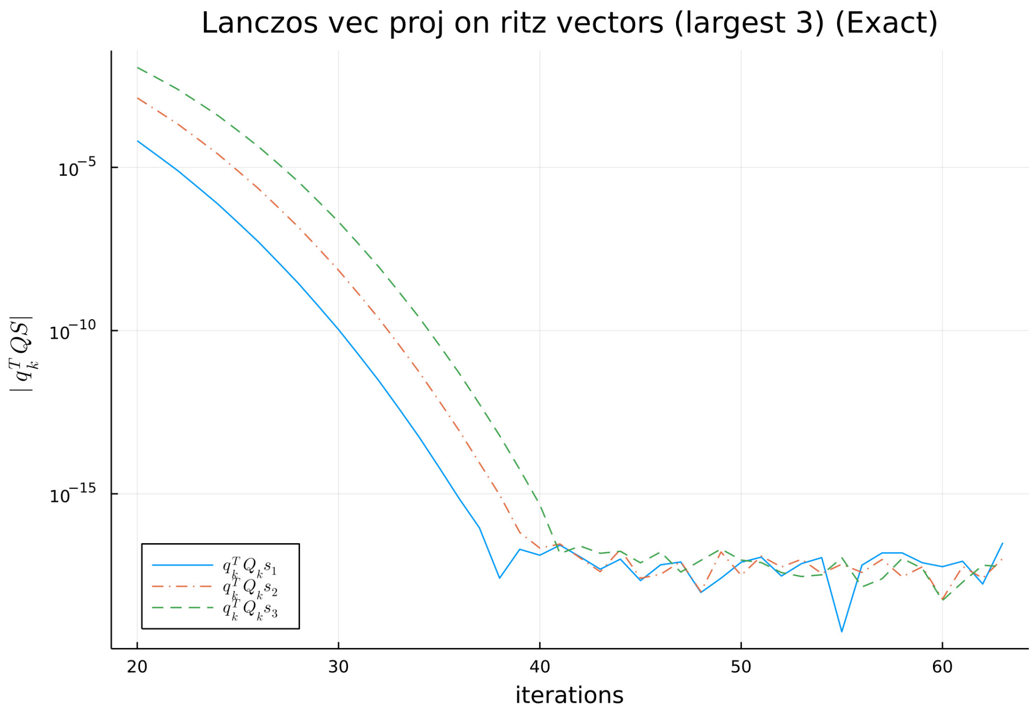


Figure 5.4.4: projection of the exact Lanczos vector q_k onto 3 of the largest Ritz vectors: $Q_k s_i^{(k)}$, for $i = k, k-1, k-2$

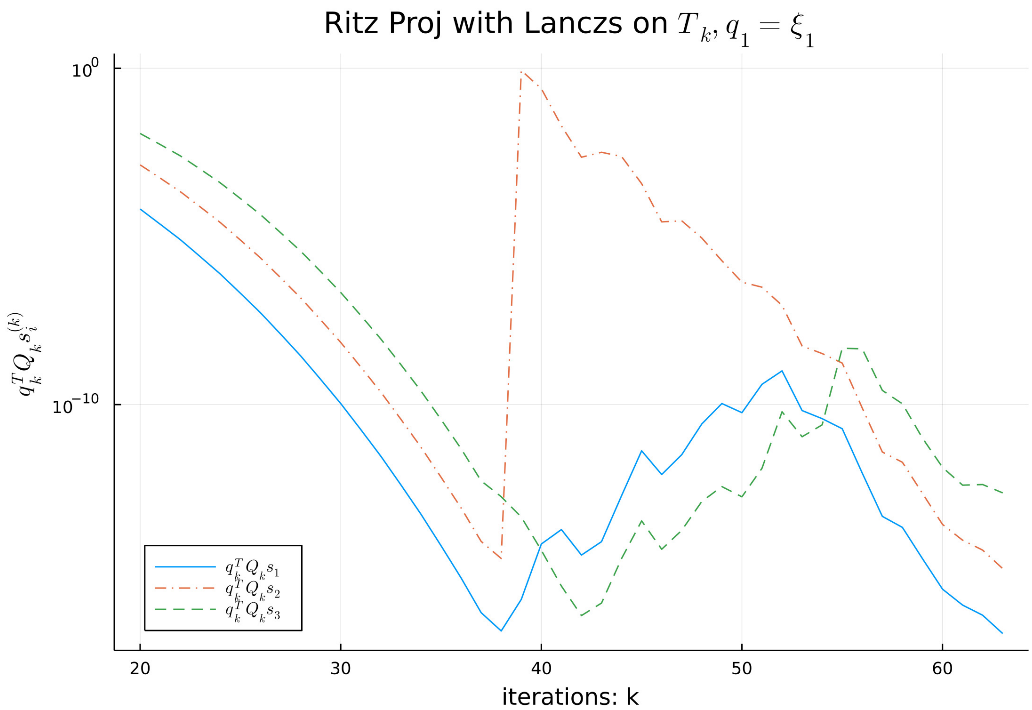


Figure 5.4.5: The projection of most recent Lanczos vector q_k onto the first 3 Ritz vectors: $Q_k s_i^{(k)}$ for $1 \leq i \leq 3$, it's performed on a tridiagonal matrix T_k generated by finite precision Lanczos with $q_1 = \xi_1$.

Remark 5.4.2 (Convergence Bounds on Ritz values)**.** The above presentation for the convergence of a Ritz Value and Ritz vector is an oversimplification. What happened is complicated. The characteristic polynomial of T_k minimizes under some weighted measured, hence the Ritz values tends to approximate the eigenvalues of A, but this characteristic alone cannot dictate the way certain Ritz values converges.

It's not always the case that $\theta_1^{(j)}$ for example, it's the best approximation for λ_1 of A, and it's especially true when iterations j is relative small compare to n. The theoretical importance is to find an interval of how far are the λ_i from $\theta_{i'}^{(k)}$, where λ_i denotes the actual eigenvalue in A where the Ritz value $\theta_{i'}^{(k)}$ is trying to approximate. The bound for the Ritz interval was refined by Y. Saad back in 1980[12] and first discovered by Shmuel Kaniel back in 1966[16].

5.4.3 Greenbaum's Tiny Interval Experiments

A smarter way of looking at the phenomenon of ghost eigenvalues (figure 5.4.1 left) is to take advantage of the clustering of the ghost eigenvalues and think of them as the eigenvalues of a potentially a larger matrix, denoted as $\tilde{A}$ whose eigenvalues are clustered around the eigenvalues of A within a tiny interval. The idea is if we perform exact Lanczos on A, then we get similar results for applying floating-point Lanczos on $\tilde{A}$. Simply put, due to the effect of round of errors, the floating-point Lanczos iterations can't see the spectrum of A clearly and instead, it sees $\tilde{A}$ whose eigenvalues are smeared out version of A, and there are many of them clustered around. More specifically, assuming A has eigenvalues: $\lambda_1, \cdots, \lambda_n$, the eigenvalues of $\tilde{A}$ lies in:

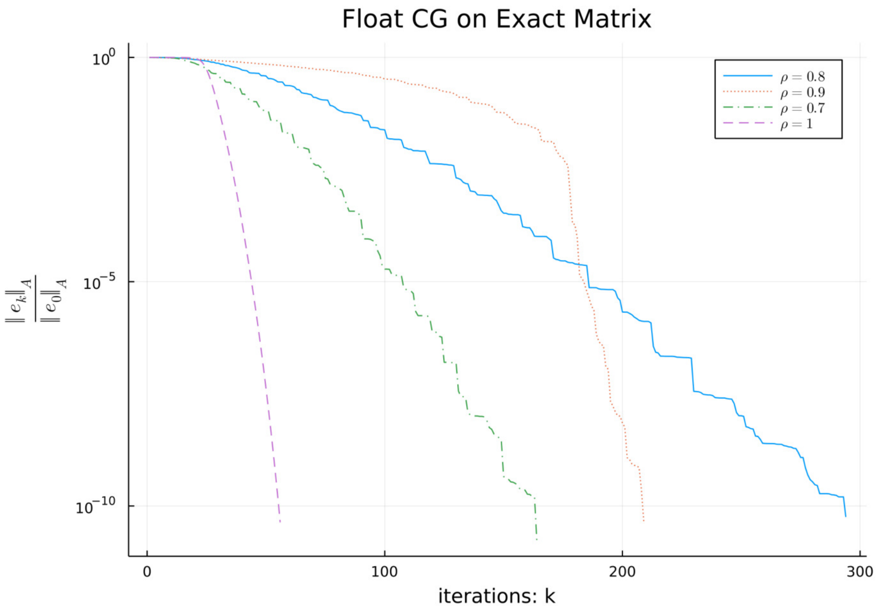
$$\bigcup_{n=1}^{n} [\lambda_i - \delta, \lambda_i + \delta] \tag{5.4.6}$$

As a result, running an exact Lanczos/CG on $\tilde{A}$ produces similar convergence compared to the floating-point version of the algorithm. Experiments where conducted by A. Greenbaum and Z. Strakos in 1992[5]. Here, we reproduce the experiments on CG and check on the convergence rate of the algorithm.

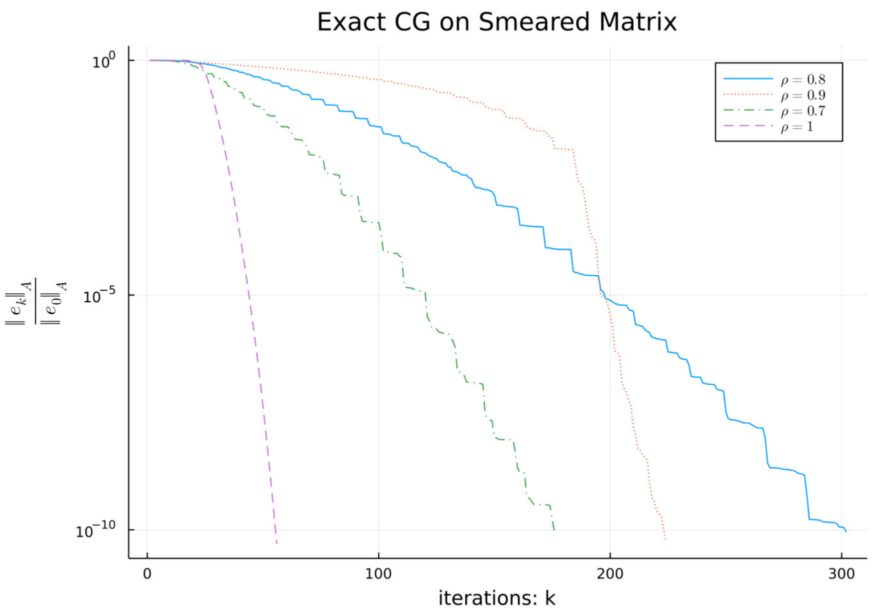
To reproduce the effects, The same matrix parameterized by ρ back in matrix 5.2.1. The tiny intervals are set by me via trials and errors. For the experiments, we set $\delta = 2\text{e-}5\|A\|\epsilon$ where ϵ is the machine epsilon for Float64; and 100 equally spaced eigenvalues on the spectrum for the matrix $\tilde{A}$ are clustered inside of the tiny intervals.

The right hand side vector $b, \tilde{b}$ are chosen to be a vector of all ones. The matrix A is chosen to be 64×64, and hence $\tilde{A}$ is 6400×6400.

Both exact and float CG are run and terminates once $\frac{\|e_k\|_A}{\|e_0\|_A}$ is less than 10^{-10}. By exact CG I mean CG with full re-orthogonalizations.



(a) Applying CG without re-orthogonalizations on $Ax = b$, the original matrix without the tiny intervals.



(b) Applying CG with full re-orthogonalizations on $\tilde{A}x = \tilde{b}$. $\tilde{A}$ has tiny intervals.

Figure 5.4.6

The results of the experiments are plotted out in fig 5.4.6. For a tolerance of 10^{-10} on the relative energy norm of the error, we reproduced the behaviors of the CG without re-orthogonalizations using the tiny intervals ideas. In fig 5.4.6a is the CG without any re-orthogonalizations applied on $Ax = b$ for different values of ρ, and in fig 5.4.6b, it's the convergence of the CG with full re-orthogonalizations on the system $\tilde{A}x = \tilde{b}$.

Remark 5.4.3 (Orhogonal in Another Measure, and an open Question)**.** The idea of tiny intervals allows for a good predictions for the behaviors of CG and Lanczos when finite precision arithmetic is involved. The underlying mechanism was shown by Greenbaum in 1989[3]. The Lanczos iterations generates tridiagonal matrix whose characteristic polynomial is orthogonal under a discrete measure at eigenvalues of A weighted by the vector $(U^H q_1)^2$, (appendix item B.4), however under finite arithmetic, they are no longer orthogonal under the original measure but instead, they are orthogonal under a new tiny intervals around the eigenvalues of A.

It's hypothesized that the tiny intervals are fixed, or grows slowly wrt to the number of iterations, however no current bounds are tight enough to show that's true.

5.5 Another Paige's Theorem

This other Paige theorem highlights the systematic ways of Ritz vector losing orthogonality. The theorem is stated in C.C Paige 1980 3.13[10], a more thorough proof is presented in Demmel's Book[2] theorem 7.3 on page 381. The original proof presented is succinct and required reader to read 2 of Paige's thesis. Here we present the thorough proof for the sake of appreciation.

The theorem highlights the fact that when the Ritz value converged $(\beta_k, (v_i^{(k)}))k$ is small), the Lanczos vector q_{k+1} loses orthogonality against the Ritz vector. It tells us that when under floating-point arithmetic, converged Ritz vector leads to lost of orthogonality of Lanczos vector, and they lose orthogonality along the direction of the converged Ritz vectors.

Theorem 5 (Another Paige's Theorem)**.**

$$(y_i^{(k)})^T q_{k+1} = \frac{\mathcal{O}(\epsilon \|A\|)}{\beta_k (v_i)_k} \tag{5.5.1}$$

$$y_i^{(k)} := Q_k (v_i^{(k)})_k \tag{5.5.2}$$

And we define the following quantities:

$$T_k :: \text{Tridiagonal at step k of Lanczos} \tag{5.5.3}$$

$$Q_k :: \text{Orthogonal matrix at step k of Lanczos} \tag{5.5.4}$$

$$V_k = [v_1^{(k)}\ v_2^{(k)}\ \cdots\ v_k^{(k)}] :: \text{Eigenbasis matrix atrix for } T_k \tag{5.5.5}$$

$$\theta_i^{(k)} :: \text{the eigenvalues for } v_i^{(k)},\ \text{Ritz Value} \tag{5.5.6}$$

$$F_k :: \text{The floats error matrix from Lanczos recurrence} \tag{5.5.7}$$

$$\epsilon :: \text{The machine Epsilon} \tag{5.5.8}$$

Proof. For simplicity, we ignore all the subscript goes under $Q_k, q_{k+1}, T_k, F_k, v_i^{(k)}, y_i^{(k)}$. Starting with the Lanczos recurrences under floating-point arithmetic:

$$AQ = AT + \beta q \xi_k^T + F \tag{5.5.9}$$

$$Q^T AQ = Q^T QT + Q^T \beta q \xi_k^T + Q^T F \tag{5.5.10}$$

$$Q^T AQ = (Q^T QT + Q^T \beta q \xi_k^T + Q^T F)^T \tag{5.5.11}$$

$$= T^T Q^T Q + \beta \xi_k q^T Q + F^T Q \tag{5.5.12}$$

The third line (5.5.12) is obtained by the fact that $Q^T AQ$ is symmetric. Takes the difference between the second line (5.5.11) and the third line(5.5.12) from above, we have:

$$\mathbf{0} = (Q^T QT - T^T Q^T Q) + \beta(Q^T q \xi_k^T - \xi_k q^T Q) + (Q^T F - F^T Q) \tag{5.5.13}$$

Here, we make the approximation that $\langle q_i, q_j \rangle = 0$ when $|i-j| \leq 2$ throughout the rest of the derivation, in theory, it should be $\mathcal{O}(\epsilon)$, but we ignore error of orthogonalizing the vector q_{j+1} against the vector q_j, q_{j-1} because it's small enough and doesn't change the final result.

As a result we obtained the factorization $Q^TQ = I + C^T + C$ where the matrix C is lower triangular with diagonal and sub-diagonals being all zeros, representing the Lanczos vectors losing orthogonality. Which means that $C^T + C$ is a matrix with zeros on the tridiagonal parts and all other entries are the floating point errors from lost of orthogonality. We proceed to simplify the first term from (5.5.14):

$$\begin{aligned}
Q^TQT - T^TQ^TQ &= (I + C^T + C)T - T^T(I + C^T + C) && (5.5.14)\\
&= T + C^TT + CT - T^T - T^TC^T - T^TC && (5.5.15)\\
&= (CT - TC) + (C^TT - TC^T) && (5.5.16)
\end{aligned}$$

CT is strictly lower triangular, TC is strictly lower triangular as well. This is true because a tridiagonal matrix only encodes interactions between adjacent rows/columns, and C has zeros on it's tridiagonal parts.

Consider adding back the subscript for $\xi_k q^TQ$, we have: $\xi_k q_{k+1}^T Q_k$, observe that $\xi_k q_{k+1}^T$ is a matrix whose last row is q_{k+1}^T. And because of the way that q_{k+1} is orthogonalized, the last 2 elements of the last row of $\xi_k q_{k+1} Q_k$ is zero, which is strictly lower triangular, therefore:

$$\mathbf{0} = (Q^TQT - T^TQ^TQ) + \beta(Q^Tq\xi_k^T - \xi_k q^TQ) + (Q^TF - F^TQ) \tag{5.5.17}$$

$$\mathbf{0} = -\underbrace{(CT - TC)}_{\text{strict tril}} + \underbrace{(C^TT - TC^T)}_{\text{strict triu}} + \beta(\underbrace{Q^Tq\xi_k^T}_{\text{strict triu}} - \underbrace{\xi_k q^TQ}_{\text{strict tril}}) - (Q^TF - F^TQ) \tag{5.5.18}$$

$$\implies \mathbf{0} = (CT - TC) - \beta\xi_k q^TQ + \underbrace{\text{tril}(Q^TF - F^TQ)}_{=:L} \tag{5.5.19}$$

From the second line (5.5.19) to the third line (5.5.20), we take triu (the upper triangular part of the matrix) on both side of the equation. Now consider multiplying by

$v^T(\bullet)v$ for each terms in the above expression and we have:

$$v^T(CT - TC)v = v^TCTv - v^TTCv \tag{5.5.20}$$

$$= v^TC\theta v - \theta v^TCv \tag{5.5.21}$$

$$= 0 \tag{5.5.22}$$

Therefore we are left with the equality:

$$v^T\beta\xi_k q^TQv = v^TLv \tag{5.5.23}$$

$$(\beta(v)_k)(q^TQv) = v^TLv \tag{5.5.24}$$

$$\beta(v)_k q^Ty = v^TLv \tag{5.5.25}$$

Adding back the subscripts we have: $\beta_k(v_i^{(k)})_k q_{k+1}^T y_i^{(k)} = v^TLv$, notice that $|v^TLv| = \mathcal{O}(\|L\|) = \mathcal{O}(\|Q^TF - F^TQ\|) = \mathcal{O}(\epsilon\|A\|)$, which obtains the formula for this theorem.

□

Remark 5.5.1 (Mitigating the Lost of Orthogonality)**.** For conjugate gradient, there is little needs for asserting orthogonality and A-Orthogonality between the vectors r_k and p_k unless ones need to emulate the behaviors of the algorithm under exact arithmetic. The Lanczos algorithm is sometimes used for symmetric eigenvalues problem, and in that case, making sure Q_k is orthogonal will eliminate ghost eigenvalues. Fortunately, there are ways where one can avoid the computational expense of full re-organization to eliminate ghost eigenvalues.

The implementations of such algorithm appears first back in 1979 by B. N. Parlett and D. S. Scott[11]. Later however, more sophisticated algorithms arised, and the state of the art Lanczos algorithm implementation can be found in a 1992 paper by Grimes, Roger G. and Lewis, John G. and Simon, Horst D.[7].

Appendices

A Useful Lemmas

A.1 Relative Energy Norm and Relative 2-Norm Conversions

Lemma A.1.1 (Relative Energy Norm and Relative 2-Norm Conversions)**.** Let A be a Symmetric Positive Definite Matrix, then:

$$\frac{\|Ax\|}{\|Ay\|} \le \kappa(A)\frac{\|x\|_A}{\|y\|_A}$$

Proof. From the definition of included 2-norm of matrices, assuming that λ_1 is the minimum eigenvalue of the matrix A, and λ_n the maximum, and the fact that matrix A has factorization $A^{1/2}A^{1/2}$:

$$\lambda_1\|x\| \le \|Ax\| \le \lambda_2\|x\| \tag{A.1.1}$$

$$\sqrt{\lambda_n}\|x\| \le \|A^{1/2}x\| \le \sqrt{\lambda_n}\|x\| \tag{A.1.2}$$

$$\implies \sqrt{\lambda_1} \le \frac{\|Ax\|}{\|A^{1/2}x\|} \le \sqrt{\lambda_n} \tag{A.1.3}$$

Consider another vector y:

$$\sqrt{\lambda_1} \le \frac{\|Ay\|}{\|A^{1/2}y\|} \le \sqrt{\lambda_n} \tag{A.1.4}$$

Combining the two we have:

$$\sqrt{\lambda_1}\frac{\|Ax\|}{\|A^{1/2}x\|} \leq \sqrt{\lambda_n}\sqrt{\lambda_1} \tag{A.1.5}$$

$$\sqrt{\lambda_1}\sqrt{\lambda_n} \geq \sqrt{\lambda_n}\frac{\|Ay\|}{\|A^{1/2}y\|} \tag{A.1.6}$$

$$\implies \sqrt{\lambda_1}\frac{\|Ax\|}{\|A^{1/2}x\|} \leq \sqrt{\lambda_n}\frac{\|Ay\|}{\|A^{1/2}y\|} \tag{A.1.7}$$

$$\frac{\|Ax\|}{\|A^{1/2}x\|} \leq \sqrt{\kappa(A)}\frac{\|Ay\|}{\|A^{1/2}y\|} \tag{A.1.8}$$

$$\frac{\|Ax\|}{\|Ay\|} \leq \sqrt{\kappa(A)}\frac{\|A^{1/2}x\|}{\|A^{1/2}y\|} \tag{A.1.9}$$

$$\frac{\|Ax\|}{\|Ay\|} \leq \sqrt{\kappa(A)}\frac{\|x\|_A}{\|y\|_A} \tag{A.1.10}$$

□

B Theorems, Propositions, Proofs

B.1 Krylov Subspace Grade Invariant Theorem

Proposition B.1 (Krylov Subspace Grade Invariant Theorem)**.** Once the subspace becomes linearly dependent, the subspace becomes invariant.

Proof.

$$K_k = \begin{bmatrix} b & AB & \cdots & A^{k-1}b \end{bmatrix} \tag{B.1.1}$$

$$K_k \text{ Lin Dep} \implies A^{k-1}b = K_{k-1}c_k \tag{B.1.2}$$

$$\implies AK_k = K_k \underbrace{\begin{bmatrix} e_2 & \cdots & e_k & c_k \end{bmatrix}}_{:=C_k} \tag{B.1.3}$$

$$\implies A^2K_k = AK_kC_k = K_kC_k^2 \tag{B.1.4}$$

A^2K_k will span the same space as the range of the matrix K_k. □

B.2 Cauchy Interlace Theorem for Tridiagonal Symmetric Matrices

Theorem 6 (Cauchy Interlace Theorem for Tridiagonal Symmetric Matrices)**.** Let T_k be a $k \times k$ symmetric tridiagonal matrix, then its top left upper submatrix: $T_{k-1} = (T_k)_{:k-1,:k-1}$ has eigenvalues interlaced between the eigenvalues of T_k. Denotes all k eigenvalues of T_k as $\theta_i^{(k)}$, and all $k-1$ eigenvalues of T_{k-1} as $\theta_i^{(k-1)}$. Order them so that: $\theta_1^{(k-1)} \le \cdots, \le \theta_i^{(k-1)}$, similarly: $\theta_1^{(k)} \le \cdots \le \theta_i^{(k)}$, then:

$$\theta_k^{(k)} \ge \theta_{k-1}^{(k-1)} \tag{B.2.1}$$

$$\theta_1^{(k)} \le \theta_1^{(k-1)} \tag{B.2.2}$$

$$\theta_{i-1}^{(k-1)} \le \theta_i^{(k)} \le \theta_i^{(k-1)} \tag{B.2.3}$$

Theorem taken from first chapter of Greenbuam's book[6] and it's adapted for symmetric tridiagonal matrix.

B.3 Orthogonal Polynomials and Lanczos

Proposition B.2 (Orthogonal Polynomials and Lanczos)**.** The Lanczos algorithm generates orthogonal polynomial under a discrete weighted measure covered by the eigenvalues of matrix A, the polynomial also represents the Lanczos vector q_k in the Krylov subspace.

Proof. Let $V_k^H A V_k = T_k$ be the tridiagonalization from Lanczos algorithm and we assume exact arithmetic, using the fact that each Lanczos vector v_k is an element from the Krylov subspace, we can represent it as a matrix polynomial multiplied by v_1:

$$\exists q_m \in \mathcal{P}_m : v_{m+1} = q_m(A)v_1 \in \mathcal{K}(A|v_1) \quad \forall\, m \le k-1 \tag{B.3.1}$$

Since the exact arithmetic generates orthogonal Lanczos vectors, let's consider v_i, v_j being represented by polynomial ϕ, φ, and we let $U\Lambda U^H = A$ be the eigendecomposition of matrix A then we have:

$$\langle v_i, v_j \rangle = 0 \tag{B.3.2}$$

$$\langle \phi(A)v_1, \varphi(A)v_1 \rangle = 0 \tag{B.3.3}$$

$$\langle U\phi(\Lambda)U^H v_1, U\varphi(\Lambda)U^H v_1 \rangle = 0 \tag{B.3.4}$$

$$\text{Let: } f_1 = U^H v_1 \text{ Then:} \tag{B.3.5}$$

$$\langle U\phi(\Lambda)f_1, U\varphi(\Lambda)f_1 \rangle = 0 \tag{B.3.6}$$

$$\langle \phi(\Lambda)f_1, \varphi(\Lambda)f_1 \rangle = 0 \tag{B.3.7}$$

$$\sum_{i=1}^{n} (f_1)_i^2 \phi(\lambda_i)\varphi(\lambda_i) = 0 \tag{B.3.8}$$

If we define an inner product between 2 functions $\langle \phi, \psi \rangle := \sum_{i=1}^{n} (f_1)_i^2 \phi(\lambda_i)\psi(\lambda_i)$, then the polynomial which represents the Lanczos vectors in the Krylov Subspace will be orthogonal under this inner product. □

B.4 Recursion of the Symmetric Tridiagonal Matrix Determinant

Proposition B.3 (Recursion of the Symmetric Tridiagonal Matrix Determinant)**.** Let T_k be a symmetric tridiagonal matrix in $\mathbb{R}^{k\times k}$ with α_i on its diagonal and β_i on its subdiagonal. Recursively, we define $T_{k-i} = (T_k)_{1:k-i,1:k-1}$. Using $|\cdot|$ to denote the determinant of a matrix, we have the recurrence relation:

$$|T_k| = \alpha_k |T_{k-1}| - \beta_{k-1}^2 |T_{k-2}|$$

Proof. Using the notation of $e_k^{(m)}$ to denote the k^{th} standard basis vector in $\mathbb{R}^m$, consider the Block Matrix:

$$T_k = \begin{bmatrix} T_{k-2} & \beta_{k-2} e_{k-1}^{(k-2)} & \\ \beta_{k-2} e_{k-2}^{(k-2)T} & \alpha_{k-1} & \beta_{k-1} e_{k-1}^{(k-1)} \\ & \beta_{k-1} e_{k-1}^{(k-1)T} & \alpha_k \end{bmatrix} \tag{B.4.1}$$

Now, we use the Laplace Expansion on the last row of T_k.

$$|T_k| = (-1)^{k+(k-1)}\beta_{k-1}\underbrace{\left|\begin{bmatrix} T_{k-2} & \\ \beta_{k-2}e_{k-2}^{(k-2)T} & \beta_{k-1}e_{k-1}^{(k-1)} \end{bmatrix}\right|}_{=(-1)^{2k-2}\beta_{k-1}|T_{k-2}|} + (-1)^{2k}\alpha_k\left|\underbrace{\begin{bmatrix} T_{k-2} & \beta_{k-2}e_{k-1}^{(k-2)} \\ \beta_{k-2}e_{k-2}^{(k-2)T} & \alpha_{k-1} \end{bmatrix}}_{=T_{k-1}}\right| \tag{B.4.2}$$

Substituting the last equation back to the first equation of the first term.

$$|T_k| = (-1)^{2k-2+2k-1}\beta_{k-1}^2|T_{k-2}| + \alpha_k|T_{k-1}| \tag{B.4.3}$$

$$= -\beta_{k-1}^2|T_{k-2}| + \alpha_k|T_{k-1}| \tag{B.4.4}$$

□

B.5 Recurrence of the Characteristic Polynomial of a Symmetric Tridiagonal Matrix

Theorem 7 (Recurrence of the Characteristic Polynomial of a Symmetric Tridiagonal Matrix)**.** The characteristic polynomial of a symmetric tridiagonal matrix satisfies the recurrences:

$$\begin{cases} p_k(x) = -\beta_{k-1}^2 p_{k-2}(x) + (\alpha_k - x)p_{k-1}(x) \\ p_0(x) = 1 \\ p_{-1}(x) = 0 \end{cases}$$

Where, $p_k(x) = |T_k - xI|$, and $p_{k-1}(x) := |(T_k)_{1:k-1,1:k-1}|$, and $p_{k-2} = |(T_k)_{1:k-2,1:k-2}|$.

Proof. Using Proposition B.3, but replacing α_k to be $\alpha_k - x$ due to the shifting introduced by $T_k - xI$, then:

$$|T_k - Ix| = (\alpha_k - x)|T_{k-1} - xI| - \beta_{k-1}^2|T_{k-2} - Ix| \tag{B.5.1}$$

$$\implies p_k(x) = -\beta_{k-1}^2 p_{k-2}(x) + (\alpha_k - x)p_{k-1}(x) \tag{B.5.2}$$

The recurrence is direct from the recurrences of the determinant of symmetric tridiagonal matrix, which is a polynomial with degree zero is just 1, therefore the base case matches up as well. □

B.6 Tridiagonal Characteristic Polynomials is Scaled Lanczos Orthgonal Polynomials

Proposition B.4 (Tridiagonal Characteristic Polynomials is Scaled Lanczos Orthgonal Polynomials)**.** The characteristic polynomial of T_k(with its recurrence justified in Theorem 7) is a scalar multiple of the same polynomial that represents the Lanczos vector q_{k+1} under the Krylov Subspace (from proposition B.2). Let $p_{j-1} = |T_{j-1}|$ be a $j-1$ degree monic polynomial, and let $\psi_j(x)$ represents Lanczos vector q_j under Krylov Subspace which is a $j-1$ degree polynomial, then:

$$\psi_j(x) = \left(\prod_{i=1}^{j-1}\beta_i\right)^{-1}(-1)^{j-1}p_{j-1}(x) \quad \forall\, 1 \le j \le k \tag{B.6.1}$$

Proof. To justify, we use the recurrence of the characteristic polynomial of the tridiagonal matrix together with the recurrence representing the q_k Lanczos vector. Inductively we assume the above (B.6.1) is true up to j. We make use of another recurrence relations of ψ_j, which is easy to prove using the recurrence relations of Lanczos vectors:

$$\begin{cases} \beta_j\psi_{j+1} = (x-\alpha_j)\psi_j - \beta_{j-1}\psi_{j-1} & \forall j \ge 2 \\ \psi_1 = 1 \\ \psi_0 = 0 \end{cases} \tag{B.6.2}$$

$$\begin{cases} p_j(x) = (\alpha_j - x)p_{j-1}(x) - \beta_{j-1}^2 p_{j-1}(x) & \forall j \ge 1 \\ p_0(x) = 1 \\ p_{-1}(x) = 0 \end{cases} \tag{B.6.3}$$

The base case matches up, consider:

$$\beta_j \psi_{j+1} = (x - \alpha_j)\psi_j + \beta_{j-1}\psi_{j-1} \tag{B.6.4}$$

$$= (x - \alpha_j)\left(\prod_{i=1}^{j-1}\beta_i\right)^{-1}(-1)^{j+1}p_{j-1} + \beta_{j-1}\left(\prod_{i=1}^{j-2}\beta_i\right)^{-1}(-1)^{j}p_{j-2} \tag{B.6.5}$$

$$= \left(\prod_{i=1}^{j-2}\beta_i\right)^{-1}\big((x - \alpha_j)\beta_{j-1}^{-1}(-1)^{j+1}p_{j+1} + \beta_{j-1}(-1)^{j}p_{j-2}\big) \tag{B.6.6}$$

$$= \left(\prod_{i=1}^{j-2}\beta_i\right)^{-1}(-1)^{j}\big((\alpha_j - x)\beta_{j-1}^{-1}p_{j+1} + \beta_{j-1}p_{j-2}\big) \tag{B.6.7}$$

$$= \left(\prod_{i=1}^{j-2}\beta_i\right)^{-1}(-1)^{j}\beta_{j-1}^{-1}\underbrace{\big((\alpha_j - x)p_{j+1} + \beta_{j-1}^{2}p_{j-2}\big)}_{=p_j(x)} \tag{B.6.8}$$

$$= \left(\prod_{i=1}^{j-1}\beta_i\right)^{-1}(-1)^{j+2}p_j(x) \tag{B.6.9}$$

$$\implies \beta_j \psi_{j+1} = \left(\prod_{i=1}^{j-1}\beta_i\right)^{-1}(-1)^{j+2}p_j(x) \tag{B.6.10}$$

Moves β_j to the RHS and we proved the statement for $j+1$ remains true. □

B.7 Irreducible Symmetric Tridiagonal Matrix

Proposition B.5. The tridiagonal matrix T_k generated by the Lanczos algorithm cannot have repeated eigenvalues. It's what referred to as an irreducible symmetric tridiagonal matrix in some literatures, such tridiagonal matrix must have non-zero elements on its sub-diagonals.

Proof. Let T_k be symmetric tridiaognal $k \times k$ matrix, its all sub/super diagonals are non-zeros. Consider the submatrix $(T_k - \lambda I)_{2:k,1:k-1}$ with the first row and last column removed. Regardless of λ, $(T_k - \lambda I)_{2:k,1:k-1}$ whose diagonals are the sub diagonals of T_k, which is all non-zero. Hence $\det((T_k - \lambda I)_{2:k,1:k-1}) \neq 0\ \forall \lambda$.

The determinant of $(T_k - \lambda I)_{2:k,1:k-1}$ is always nonzero implies that the full matrix $T_k - \lambda I$ has a rank of at least $k-1$ for all λ; which implies that all roots of $\det(T_k - \lambda I)$ has algebraic multiplicity of strictly 1.

Since the matrix is symmetric, it must be diagonalizable. For contradiction assuming that it has repeated eigenvalues and still diagonalizable, it must have repeated roots, which is a contradiction. Therefore all its eigenvalues are unique. □

B.8 From CG to Lanczos: The Proof

We will break the proof into several parts. Firstly we address the base case, and then we address the inductive case to establish the parameters between the tridiagonal matrix and a_k, b_k, finally we resolve the sign problem between the Lanczos vectors and the residual vectors.

B.8.1 The Base Case

Right from the start of the CG iteration we have:

$$r_0 = p_0 \tag{B.8.1}$$

$$r_1 = r_0 - a_0 A r_0 \tag{B.8.2}$$

$$A r_0 = a_0^{-1}(r_0 - r_1) \tag{B.8.3}$$

$$A r_0 = \frac{\|r_0\|_A^2}{\|r_0\|^2}(r_0 - r_1) \tag{B.8.4}$$

Consider substituting $r_0 = \|r_0\| q_1, r_1 = -\|r_1\| q_2$, then:

$$A\|r_0\|q_1 = \frac{\|r_0\|_A^2}{\|r_0\|^2}\left(\|r_0\|q_1 + \|r_1\|q_2\right) \tag{B.8.5}$$

$$= \frac{\|r_0\|_A^2}{\|r_0\|^2}\|r_0\|q_1 + \frac{\|r_1\|}{\|r_0\|}q_2 \tag{B.8.6}$$

And from this relation, using the Lanczos recurrence theorem would imply that $\alpha_1 = a_0^{-1}$; $\beta_1 = \frac{\sqrt{b_0}}{\alpha_0}$. So far so good, we have shown that there is an equivalence between the Lanczos and the CG for the first iterations of the CG algorithm.

B.8.2 The Inductive Case

Lemma B.8.1. Inductively we wish to show the relation that:

$$\begin{cases} \alpha_{j+1} = \frac{1}{a_j} + \frac{b_{j-1}}{a_{j-1}} & \forall 1 \leq j \leq n-1 \\ \beta_j = \frac{\sqrt{b_{j-1}}}{a_{j-1}} & \forall 2 \leq j \leq n-2 \end{cases} \tag{B.8.7}$$

Proof. We start by considering:

$$r_j = r_{j-1} - a_{j-1}Ap_{j-1} \tag{B.8.8}$$

$$= r_{j-1} - a_{j-1}A(r_{j-1} + b_{j-2}p_{j-1}) \tag{B.8.9}$$

$$= r_{j-1} - a_{j-1}Ar_{j-1} - a_{j-1}b_{j-2}Ap_{j-1} \tag{B.8.10}$$

We make use of the recurrence asserted by the CG algorithm, giving us:

$$r_{j-1} = r_{j-1} - a_{j-2}Ap_{j-1} \tag{B.8.11}$$

$$r_{j-1} - r_{j-1} = a_{j-2}Ap_{j-1} \tag{B.8.12}$$

$$Ap_{j-1} = a_{j-2}^{-1}(r_{j-2} - r_{j-1}) \tag{B.8.13}$$

Here, we can substitute the results for the term Ap_{j-1}, and then we can express the recurrence of residual purely in terms of residual. Consider:

$$r_j = r_{j-1} - a_{j-1}Ar_{j-1} - a_{j-1}b_{j-2}Ap_{j-2} \tag{B.8.14}$$

$$= r_{j-1} - a_{j-1}Ar_{j-1} - \frac{a_{j-1}b_{j-2}}{a_{j-2}}(r_{j-2} - r_{j-1}) \tag{B.8.15}$$

$$= \left(1 + \frac{a_{j-1}b_{j-2}}{a_{j-2}}r_{j-1}\right) - a_{j-1}Ar_{j-1} - \frac{a_{j-1}b_{j-2}}{a_{j-2}}r_{j-2} \tag{B.8.16}$$

$$a_{j-1}Ar_{j-1} = \left(1 + \frac{a_{j-1}b_{j-2}}{a_{j-2}}r_{j-1}\right) - \frac{a_{j-1}b_{j-2}}{a_{j-2}}r_{j-2} \tag{B.8.17}$$

$$Ar_{j-1} = \left(\frac{1}{a_{j-1}} + \frac{b_{j-2}}{a_{j-2}}\right)r_{j-1} + \frac{r_j}{a_{j-1}} - \frac{b_{j-2}}{a_{j-2}}r_{j-2} \tag{B.8.18}$$

Finally, we increment the index j by one for convenience, and therefore we establish the following relations between the residuals of the conjugate gradient algorithm:

$$Ar_j = \left(\frac{1}{a_j} + \frac{b_{j-1}}{a_{j-1}}\right) r_j + \frac{r_{j+1}}{a_j} - \frac{b_{j-1}}{a_{j-1}} r_{j-1} \tag{B.8.19}$$

Reader, please observe that this is somewhat similar to the recurrence relations between the Lanczos vectors, however it's failing to match the sign, at the same time, it's not quite matching the form of the recurrence of β_k from the Lanczos algorithm. To match it, we need the coefficients of r_{j-1} and r_{j+1} to be in the same form, parameterized by the same iterations parameter: j. To do that, consider the doing this:

$$\begin{aligned}
q_{j+1} &:= \frac{r_j}{\|r_j\|} && \text{(B.8.20)}\\
q_j &:= -\frac{r_{j-1}}{\|r_{j-1}\|} \quad \text{Note: This is Negative} && \text{(B.8.21)}\\
q_{j+2} &:= \frac{r_{j+1}}{\|r_{j+1}\|} && \text{(B.8.22)}\\
\implies A\|r_j\|q_{j+1} &= \left(\frac{1}{a_j} + \frac{b_{j-1}}{a_{j-1}}\right)\|r_j\|q_{j+1} + \frac{\|r_{j+1}\|q_{j+2}}{a_j} + \frac{b_{j-1}\|r_{j-1}\|}{a_{j-1}} q_j && \text{(B.8.23)}\\
Aq_{j+1} &= \left(\frac{1}{a_j} + \frac{b_{j-1}}{a_{j-1}}\right) q_{j+1} + \frac{\|r_{j+1}\|}{a_j\|r_j\|} q_{j+2} + \frac{b_{j-1}\|r_{j-1}\|}{a_{j-1}\|r_j\|} q_j && \text{(B.8.24)}
\end{aligned}$$

Recall that parameters from conjugate gradient, $\sqrt{b}_j = \|r_{j+1}\|/\|r_j\|$, and $a_j = \frac{\|r_j\|^2}{\|p_j\|_A^2}$, and we can use the substitution to match the coefficients for q_{j+2} and q_j, giving us:

$$\begin{aligned}
\frac{\|r_{j+1}\|}{a_j\|r_j\|} &= \frac{1}{a_j}\sqrt{b_j} && \text{(B.8.25)}\\
\frac{b_{j-1}\|r_{j-1}\|}{a_{j-1}\|r_j\|} &= \frac{b_{j-1}}{a_{j-1}} \frac{1}{\sqrt{b_{j-1}}} = \frac{\sqrt{b_{j-1}}}{a_{j-1}} && \text{(B.8.26)}\\
\implies & \begin{cases}
\alpha_{j+1} = \frac{1}{a_j} + \frac{b_{j-1}}{a_{j-1}} & \forall 1 \le j \le n-1\\
\beta_j = \frac{\sqrt{b_{j-1}}}{a_{j-1}} & \forall 2 \le j \le n-2
\end{cases} && \text{(B.8.27)}
\end{aligned}$$

Take notes that the form is now matched, but the expression for α_{j+1} has an extra b_{j-1}/a_{j-1}, to resolve that, we take the audacity to make b_0 so that it's consistent with the base case. □

B.8.3 Fixing the Sign

We need to take a more careful look into the sign between q_j the Lanczos Vector and its equivalence residual: r_{j-1} in CG. Here, I want to point out the fact that, there are potentially two substitutions possible for the above derivation for the inductive case and regardless of which one we use, it would still preserve the correctness for the proof. By which I mean the following substitutions would have both made it work:

$$\begin{cases} q_{j+1} := \pm\frac{r_j}{\|r_j\|} \\ q_j := \mp\frac{r_{j-1}}{\|r_{j-1}\|} \\ q_{j+2} := \pm\frac{r_{j+1}}{\|r_{j+1}\|} \end{cases} \tag{B.8.28}$$

Under the context, the operations $\pm, \mp$ are correlated, choose a sign for one, the other must be of opposite sign. In this case both substitutions work the same because multiplying the equation by -1 would give the same equality, and we can always multiply by another negative sign to get it back. The key here is that, the sign going from q_j to the next q_{j-1} will have to alternate. To find out precisely which one it is, we consider the base case for the Lanczos Vectors and Residuals:

$$q_1 = \hat{r}_0 \tag{B.8.29}$$

$$q_2 = -\hat{r}_1 \tag{B.8.30}$$

$$\vdots \tag{B.8.31}$$

$$q_j = (-1)^{j+1}\hat{r}_{j+1} \tag{B.8.32}$$

B.9 Derive CG using Lanczos: Proof

We made use of the fact that the matrix U_k is unit upper bidiagonal. We want to find the recurrences of the parameters u_k, l_k. Inductively assume $T_k = L_kU_k$ and using the block structure of the matrices:

$$T_k = L_k U_k \tag{B.9.1}$$

$$T_{k+1} = \begin{bmatrix} T_k & \beta_k \xi_k \\ \beta_k \xi_k^T & \alpha_{k+1} \end{bmatrix} = \begin{bmatrix} L_k & \mathbf{0} \\ l_k \xi_k^T & 1 \end{bmatrix} \begin{bmatrix} U_k & \eta_k \xi_k \\ \mathbf{0} & u_{k+1} \end{bmatrix} \tag{B.9.2}$$

$$= \begin{bmatrix} L_k U_k & \eta_k L_k \xi_k \\ l_k \xi_k^T U_k & \eta_k l_k \xi_k^T \xi_k + u_{k+1} \alpha_k \end{bmatrix} \tag{B.9.3}$$

$$= \begin{bmatrix} T_k & \eta_k (L_k)_{:,k} \\ l_k (U_k)_{k,:} & \eta_k l_k + u_{k+1} \end{bmatrix} \tag{B.9.4}$$

$$= \begin{bmatrix} T_k & \eta_k \xi_k \\ l_k u_k \xi_k^T & \eta_k l_k + u_{k+1} \end{bmatrix} \tag{B.9.5}$$

Assume matrix U at the top to be η_k, observe that β_k is indeed the same as the η_k for the upper diagonal of matrix U_k. From above, $\eta_k = \beta_k$, and $l_k = \beta_k / u_k$, $u_{k+1} = \alpha_{k+1} - \beta_k l_k$, and hence, to sum up the recurrence relation we have:

$$\begin{cases} u_{k+1} & = \alpha_{k+1} - \beta_k^2 / u_k \\ l_k & = \beta_k / u_k \end{cases} \tag{B.9.6}$$

The base case is $u_1 = \alpha_1$. The recurrence of the parameter u_k is useful for figuring out the recurrence for p_k, the recurrence for constructing x_k, we need to figure find out the recurrence relations of $(L_k^{-1})_{k,1}$ by consider:

$$L_k^{-1} L_k = I \tag{B.9.7}$$

$$\begin{bmatrix} L_k^{-1} & \mathbf{0} \\ s_k^T & d_{k+1} \end{bmatrix} \begin{bmatrix} L_k & \mathbf{0} \\ l_k \xi_k^T & 1 \end{bmatrix} = I \tag{B.9.8}$$

$$\begin{bmatrix} I & \mathbf{0} \\ s_k^T L_k + d_{k+1} l_k \xi_k^T & d_{k+1} \end{bmatrix} = I \tag{B.9.9}$$

Their product equals the identity matrix therefore $d_{k+1} = 1$, and it has to be that $s_k^T L_k + d_{k+1} l_k \xi_k^T$. For the lower unit bi-diagonal matrix L_k, its inverse is lower tridiagonal, and the left $k \times k$ principle submatrix of L_{k+1}^{-1} is L_k^{-1}. We can figure out s_k^T by considering:

$$s^T L_k + d_{k+1} l_k \xi_k^T = \mathbf{0} \tag{B.9.10}$$

$$L_k^T s_k + d_{k+1} l_k \xi_k = \mathbf{0} \tag{B.9.11}$$

$$s_k + L^{-T} d_{k+1} l_k \xi_k = \mathbf{0} \tag{B.9.12}$$

$$(s_k)_1 + d_{k+1} l_k ((L_k^{-1}) \xi_k)_1 = 0 \tag{B.9.13}$$

$$(s_k)_1 + d_{k+1} l_k (L_k^{-1})_{k,1} = 0 \tag{B.9.14}$$

$$\Longrightarrow (s_k)_1 = -l_k (L_k^{-1})_{k,1} \tag{B.9.15}$$

$$(s_k)_1 = (L_{k+1}^{-1})_{k+1,1} \quad \text{by definition} \tag{B.9.16}$$

$$\Longrightarrow (L_{k+1}^{-1})_{k+1,1} = -l_k (L_k^{-1})_{k,1} \tag{B.9.17}$$

The base case is $L_1 = 1$. The short recurrence of parameters for decomposing the tridiagonal matrix T_k allows for the Lanczos iterations to be mathematically equivalent to the CG.

C Algorithms

Definition 7 (Lanczos Iterations Variants).

$$
\begin{aligned}
&\text{Given arbitrary: } q_1 \text{ s.t: } \|q_1\| = 1 \\
&\alpha_1 := \langle q_1, Aq_1 \rangle \\
&\beta_0 := 0 \\
&\text{Memorize : } Aq_1 \\
&\text{For } j = 1, 2, \cdots \\
&\quad \tilde{q}_{j+1} := Aq_j - \beta_{j-1} q_{j-1} \\
&\quad \tilde{q}_{j+1} \leftarrow \tilde{q}_{j+1} - \alpha_j q_j \\
&\quad \beta_j = \|\tilde{q}_{j+1}\| \\
&\quad q_{j+1} := \tilde{q}_{j+1} / \beta_j \\
&\quad \alpha_{j+1} := \langle q_{j+1}, Aq_{j+1} \rangle \\
&\quad \text{Memorize: } Aq_{j+1}
\end{aligned}
\tag{C.0.1}
$$

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