Chapter 1

Inverse Iteration with GMRES and Galerkin Krylov Methods - March 5, 2012

1.1 Introduction and Theory

Inverse iteration can be used to solve eigenvalue problems such as

$$A\mathbf{v} = \lambda\mathbf{v}. \tag{1.1}$$

where $A \in \mathbb{R}^{n\times n}$, $\mathbf{v} \in \mathbb{R}^n$ and $\lambda \in \mathbb{R}$. The algorithm for carrying out inverse iteration requires a system to be solved at each iteration [1]. If we denote by bracketed superscript the overall inverse iterations, then the system is given by

$$(A - s^{(i)}I)\mathbf{y}^{(i)} = \mathbf{x}^{(i)}, \tag{1.2}$$

where the $s^{(i)}$ are defined below. We will look at solving (1.2) inexactly and will denote the related iterations of this inexact solve using a subscript, so the k^{th} approximation to $\mathbf{y}^{(i)}$ found by these iterations is denoted $\mathbf{y}_k^{(i)}$. To avoid confusion we will refer to '*inner*' iterations and '*outer*' iterations. Outer iterations refer to the main loop of inverse iteration, and vary i. Inner iterations are those contained within the process for solving (1.2) and vary k. In this way, we will look for inner solutions $\mathbf{y}_k^{(i)}$ for (1.2) that satisfy

$$\left\|\mathbf{r}_k^{(i)}\right\| \leq \tau_k^{(i)}, \tag{1.3}$$

where

$$\mathbf{r}_k^{(i)} \equiv (A - s^{(i)}I)\mathbf{y}_k^{(i)} - \mathbf{x}^{(i)} \tag{1.4}$$

defines the inner residual, and $\tau_k^{(i)}$ is a tolerance to be satisfied, at inner iteration k.

In (1.2) the $s^{(i)}$ are computed *shifts* which approximate the required eigenvalue, λ, at each outer iteration. Also, $\mathbf{x}^{(i+1)} = \mathbf{y}_{\text{final}}^{(i)} / \left\|\mathbf{y}_{\text{final}}^{(i)}\right\|$ is the next approximation to the eigenvector, $\mathbf{v}$, at each outer iteration using the final value of $\mathbf{y}_k^{(i)}$ found via the inner iteration.

In this experiment we look at solving (1.2) with GMRES or a Galerkin-Krylov (GK) method, however we fix the number of inner iterations these methods can carry out to a constant, m, meaning we have $1 \leq k \leq m$. This also means we will be working without a tolerance in these methods, since we ensure m inner iterations take place regardless of how small the inner residual, $\mathbf{r}_k^{(i)}$, becomes. The only tolerance will be in the outer inverse iteration loop. We will also keep the right hand side in (1.2) fixed to the initial guess $\mathbf{x}^{(0)}$ (not update it with each new guess), for which $\left\|\mathbf{x}^{(0)}\right\| = 1$. Consequently we are trying to solve the system

$$(A - s^{(i)}I)\mathbf{y}^{(i)} = \mathbf{x}^{(0)}, \qquad \text{with } \left\|\mathbf{x}^{(0)}\right\| = 1 \tag{1.5}$$

and have that $\mathbf{r}_k^{(i)} \equiv (A - s^{(i)}I)\mathbf{y}_k^{(i)} - \mathbf{x}^{(0)}$.

It was thought that this method would not yield approximations, $s^{(i)}$, in the outer iterations converging to λ. Instead it was expected that convergence would occur to some other value close to λ.

This stemmed from understanding the way that GMRES and GK methods work to find solutions. Among other things, a Krylov subspace is constructed each inner iteration [3], which at iteration k is given by

$$\mathcal{K}_k\left(A - s^{(i)}I, \mathbf{r}_0^{(i)}\right) = span\{\mathbf{r}_0^{(i)}, A\mathbf{r}_0^{(i)}, \ldots, A^{k-1}\mathbf{r}_0^{(i)}\}. \tag{1.6}$$

We define V_m to be the matrix whose columns are given by the spanning vectors of the subspace $\mathcal{K}_m\left(A - s^{(i)}I, \mathbf{r}_0^{(i)}\right)$, and so form a specific orthonormal basis. It was proposed that, if working with initial inner guess $\mathbf{y}_0 = 0$, the outer convergence of $s^{(i)}$ would be to eigenvalues of the matrix

$$H_m \equiv V_m^\top A V_m, \tag{1.7}$$

and not of A, but that as $m \to n$ (where n is the size of the system), the eigenvalues of H_m would converge to those of A. (When working to a tolerance, it would therefore be sufficient to use a large enough m such that the tolerance was reached.)

1.2 Galerkin-Krylov with a fixed number of iterations

If a Galerkin-Krylov (GK) solver is used instead of GMRES in inverse iteration (for example Conjugate Gradient methods) then it is fairly simple to show that limiting the number of inner iterations leads to convergence to something other than the smallest eigenvalue of A in (1.5).

Lemma 1.1:
If the inner system (1.5) *is solved iteratively using m steps of a Galerkin-Krylov subspace method with a fixed right hand side $\mathbf{x}^{(0)}$, and an initial inner guess $\mathbf{y}_0^{(i)} = 0$, then the convergence is to eigenpairs of $H_m \in \mathbb{R}^{m\times m}$ and not of $A \in \mathbb{R}^{n\times n}$ for $m < n$.*

Proof.
We consider the system

$$\left(A - s^{(i)}I\right)\mathbf{y}^{(i)} = \mathbf{x}^{(0)}, \tag{1.8}$$

which we want to solve iteratively using a Galerkin-Krylov subspace method. Since we take $\mathbf{y}_0 = 0$, we have that $\mathbf{r}_0^{(i)} = \mathbf{x}^{(0)}$, thus

$$\begin{aligned} \mathcal{K}_k\left(A - s^{(i)}I, \mathbf{r}_0^{(i)}\right) &= \mathcal{K}_k\left(A - s^{(i)}I, \mathbf{x}^{(0)}\right) \\ &= span\left\{\mathbf{x}^{(0)}, \left(A - s^{(i)}I\right)\mathbf{x}^{(0)}, \ldots, \left(A - s^{(i)}I\right)^{k-1}\mathbf{x}^{(0)}\right\}, \end{aligned} \tag{1.9}$$

so Galerkin methods compute the k^{th} estimate of $\mathbf{y}^{(i)}$ as $\mathbf{y}_k^{(i)} \in \mathbf{y}_0^{(i)} + \mathcal{K}_k\left(A - s^{(i)}I, \mathbf{x}^{(0)}\right)$ [4]. Now let V_m be the matrix whose columns are given by the spanning vectors of the Krylov subspace $\mathcal{K}_m\left(A - s^{(i)}I, \mathbf{x}^{(0)}\right)$. Specifically at inner iteration m, a GK method finds a $\mathbf{y}_m^{(i)}$ whose corresponding residual satisfies

$$\left(A - s^{(i)}I\right)\mathbf{y}_m^{(i)} - \mathbf{x}^{(0)} \perp V_m. \tag{1.10}$$

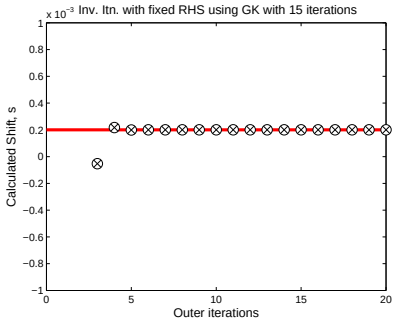
Premultiplying by $V_m^\top$ and using orthogonality, the following is satisfied

$$V_m^\top\left(A - s^{(i)}I\right)\mathbf{y}_m^{(i)} - V_m^\top\mathbf{x}^{(0)} = 0. \tag{1.11}$$

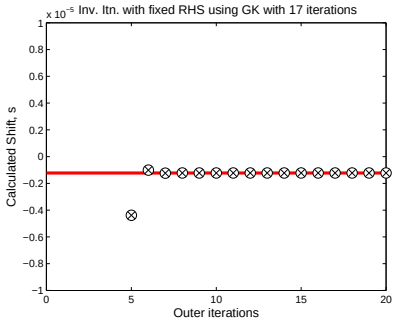
Writing $\mathbf{y}_m^{(i)} = V_m\boldsymbol{\alpha}$, where $\boldsymbol{\alpha} \in \mathbb{R}^m$, we proceed as follows

$$\begin{aligned} & V_m^\top\left(\, A - s^{(i)}I \,\right)V_m\boldsymbol{\alpha} &&= V_m^\top\mathbf{x}^{(0)}, \\ \Rightarrow\quad & V_m^\top A V_m\boldsymbol{\alpha} - V_m^\top s^{(i)} V_m\boldsymbol{\alpha} &&= \mathbf{e}_1, \\ \Rightarrow\quad & H_m\boldsymbol{\alpha} - s^{(i)}\boldsymbol{\alpha} &&= \mathbf{e}_1. \end{aligned} \tag{1.12}$$

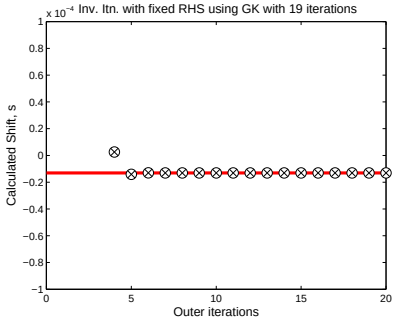
Here $\mathbf{e}_1$ denotes the unit vector $[1, 0, \ldots, 0] \in \mathbb{R}^m$. The right hand side follows since $\mathbf{x}^{(0)}$ is the first column of V_m, and we have used that $V_m^\top V_m = I$ on the left. This is



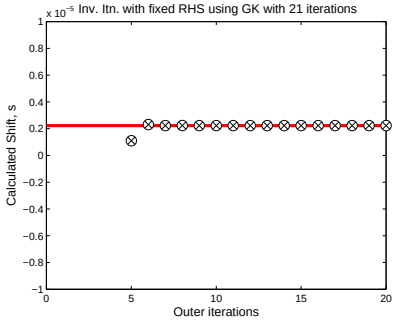
(a) GK with 15 inner iterations



(b) GK with 17 inner iterations



(c) GK with 19 inner iterations



(d) GK with 21 inner iterations

Figure 1-1: *The plotted points are the calculated shift $s^{(i)}$ at each outer iteration, i. They show the convergence of inverse iteration on a system of dimension 30 using inner solver GK with a fixed number of iterations, m, for four different values of m. The horizontal line shows the smallest eigenvalue of H_m, which Lemma 1.1 says should be the convergence limit of the calculated shifts $s^{(i)}$, as $i \to \infty$. (Note the varying y-axis scales.)*

solved at each iteration so we are conducting inverse iteration with exact solves and a fixed right hand side on the system $H_m\boldsymbol{\alpha} - s^{(i)}\boldsymbol{\alpha} = \mathbf{e}_1$, which will converge to eigenpairs of H_m as claimed.

Finally, since $H_m \in \mathbb{R}^{m\times m}$ and $A \in \mathbb{R}^{n\times n}$, for $m < n$ eigenpairs of H_m and A are distinct, unless V_m contains an invariant subspace of A. □

1.2.1 Numerical Examples

In this section we first look at results obtained by solving (1.5) (the inner solve of inverse iteration) using Galerkin-Krylov (GK) solvers with a fixed right hand side vector, $\mathbf{x}^{(0)}$, where $\left\|\mathbf{x}^{(0)}\right\| = 1$, and a fixed number of iterations m, (i.e. no tolerance). Then we will look at how many inner iterations are required to solve (1.5), for each outer iteration, using a fixed inner tolerance throughout: $\tau_k^{(i)} \equiv \tau$, $\forall i, \forall k$.

To do these tests we constructed an asymmetric 30×30 matrix, A, with random eigenvectors corresponding to eigenvalues $\lambda = 0, 1, \ldots, 29$. This was done using the formula

It^{n}s, m	Final E-Val Estimate	Smallest E-Val of H_m	Absolute Difference
7	-1.79(−3)	-1.79(−3)	5.0(−15)
9	5.22(−4)	5.22(−4)	3.0(−15)
11	-5.33(−5)	-5.33(−5)	3.0(−15)
13	2.19(−4)	2.19(−4)	0.0(−15)
15	2.00(−4)	2.00(−4)	4.0(−15)
17	-1.22(−6)	-1.22(−6)	9.0(−15)
19	-1.31(−5)	-1.31(−5)	3.0(−15)
21	2.23(−6)	2.23(−6)	0.0(−15)
23	-3.79(−8)	-3.79(−8)	1.0(−15)
25	-5.59(−8)	-5.59(−8)	1.0(−15)
27	2.27(−10)	2.27(−10)	1.0(−15)
29	7.00(−15)	7.00(−15)	3.0(−15)

Table 1.1: *Table showing the final shift estimate and the smallest eigenvalue of H_m when carrying out inverse iteration with a GK method, but specifying the number of iterations the method performs. Data for a 30×30 system, with m GK iterations.*

$$A = X\Lambda X^{-1},$$

where X was a random 30×30 matrix and Λ was a square matrix with $0, 1, \ldots, 29$ along the leading diagonal and zeros elsewhere. We used the zero vector as an initial guess for the inner GK process, and used a normalised perturbation of the first column of X as the initial guess, $\mathbf{x}^{(0)}$, in the outer inverse iteration loop.

We carried out inverse iteration to find the smallest eigenvalue of the matrix A (which had smallest eigenvalue $\lambda = 0$), and used a GK method for the inner solve but fixed the number of inner iterations to $m = 7, 9, 11, \ldots, 29$. The data in all of these cases are given in table 1.1, and is represented graphically for the cases $m = 15, 17, 19$ and 21 in figure 1-1 (note the varying scales of the y-axes). The behaviour observed was as predicted by Lemma 1.1 in that outer convergence was to eigenvalues of H_m.

A further interesting point that arose during this experiment was that the final inner residual error value (defined in (1.4)) actually increased dramatically as the outer iteration proceeded, despite convergence towards the true solution, $\mathbf{x}^{(i)} = \mathbf{v}$. A possible explanation of this relates to the nullspace of $A - s^{(i)}I$. For a matrix to have a non-empty nullspace it is necessarily singular. Since $A - s^{(i)}I$ is only approximately singular, becoming more so as $i \to \infty$, we can only say that there exist vectors $\boldsymbol{\phi} \neq 0$ such that

$$\left(A - s^{(i)}I\right)\boldsymbol{\phi} = \boldsymbol{\epsilon}, \tag{1.13}$$

where $\boldsymbol{\epsilon} \in \mathbb{R}^n$ has length $0 < \epsilon \in \mathbb{R}$, small. Now consider a solution to (1.5) of the form

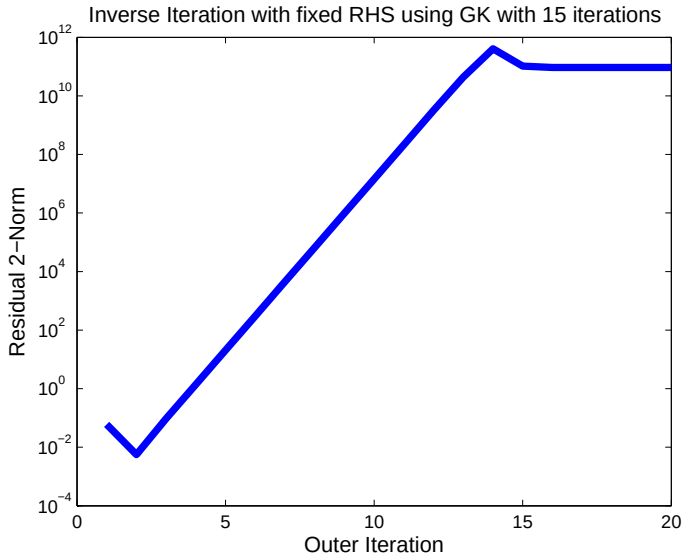


Figure 1-2: *Graph showing the 2-norm of the final inner residual error at each outer step of inverse iteration. Data for a* 30×30 *system, with 15 GK iterations*

$\mathbf{y}_m^{(i)} = \hat{\mathbf{y}} + \gamma\boldsymbol{\phi}$ where $\hat{\mathbf{y}}$ approximately solves (1.5), and $\gamma \in \mathbb{R}$ is such that

$$\begin{aligned} \left(A - s^{(i)}I\right)\left(\hat{\mathbf{y}} + \gamma\boldsymbol{\phi}\right) &\approx \mathbf{x}^{(0)} + \gamma\boldsymbol{\epsilon} \\ &\approx \mathbf{x}^{(0)}. \end{aligned} \tag{1.14}$$

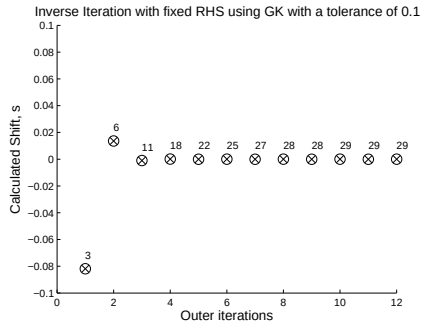
Then as i increases, $\boldsymbol{\phi}$ can be chosen with progrssively smaller ϵ values, allowing γ to be larger without affecting the validity of $\mathbf{y}_m^{(i)}$ as an approximate solution of (1.5). This means that for a large enough i, solutions can be found of this form with large values of γ, causing $\left\|\mathbf{y}_m^{(i)}\right\|$ to be large whilst still being a solution of (1.5). A plot of the final inner residual at each outer iteration in the case where $m = 15$ is given in Figure 1-2.

Instead of fixing the number of inner iterations to a constant, m, we now examine results obtained by fixing the inner tolerance to a constant: $\tau_k^{(i)} \equiv \tau$, $\forall i, \forall k$. So using the same system as before, at each inner step k we checked for convergence via the inner residual defined in (1.4), under the condition

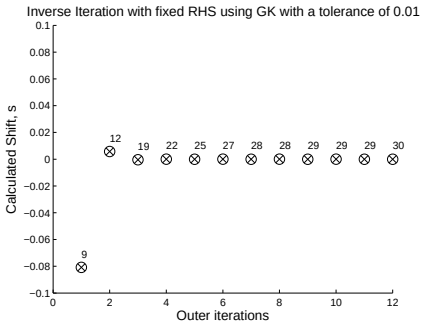
$$\left\|(A - s^{(i)}I)\mathbf{y}_k^{(i)} - \mathbf{x}^{(0)}\right\| \leq \tau, \tag{1.15}$$

where τ was a user defined constant. Moreover, we looked at how many inner iterations were needed to solve to the specified inner tolerance for each outer iteration. Figure 1-3 shows graphs of the convergence of the GK solve for four different inner tolerances.

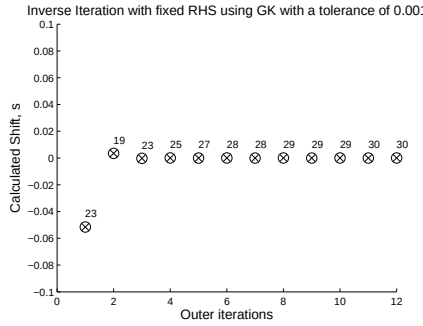
The data for $\tau = 10^{-1}$ and $\tau = 10^{-2}$ is given in table 1.2. From these it can be seen that for high inner tolerances, as inverse iteration proceeds the number of inner iterations performed approaches the system size. This is due to the shift $s^{(i)}$ approaching the true eigenvalue of A, causing $(A - s^{(i)}I)$ to approach singularity. Thus



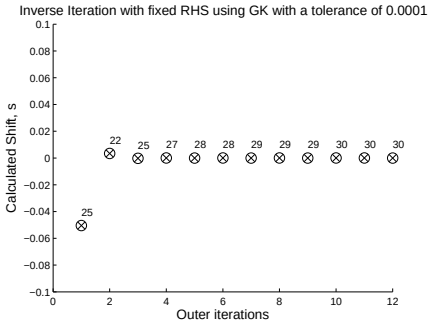
(a) GK with fixed tolerance $\tau = 10^{-1}$



(b) GK with fixed tolerance $\tau = 10^{-2}$



(c) GK with fixed tolerance $\tau = 10^{-3}$



(d) GK with fixed tolerance $\tau = 10^{-4}$

Figure 1-3: *The plotted points are the calculated shift $s^{(i)}$ at each outer iteration, i. They show the convergence of inverse iteration on a system of dimension 30 using inner solver GK with a fixed tolerance, τ, for four different values of τ. The numbers next to each point indicate how many inner iterations were required to reach the specified inner tolerance for each outer iteration.*

Outer	$\tau = 10^{-1}$		$\tau = 10^{-2}$		$\tau = 10^{-8}, 10^{-9}, \ldots$	
It^n, i	Shift, $s^{(i)}$	In. it^{n}s	Shift, $s^{(i)}$	In. it^{n}s	Shift, $s^{(i)}$	In. it^{n}s
1	-8.2(-2)	3	-8.1(-2)	9	-5.1(-2)	30
2	1.4(-2)	6	5.7(-3)	12	3.4(-3)	30
3	-9.8(-4)	11	-4.1(-4)	19	-2.3(-4)	30
4	6.5(-5)	18	2.9(-5)	22	1.6(-5)	30
5	-3.2(-6)	22	-2.0(-6)	25	-1.1(-6)	30
6	1.6(-7)	25	1.4(-7)	27	7.5(-8)	30
7	-1.1(-8)	27	-9.5(-9)	28	-5.1(-9)	30
8	7.3(-10)	28	6.6(-10)	28	3.5(-10)	30
9	-3.4(-11)	28	-4.5(-11)	29	-2.4(-11)	30
10	2.3(-12)	29	3.1(-12)	29	1.6(-12)	30
11	-1.6(-13)	29	-2.1(-13)	29	-1.1(-13)	30
12	8.9(-15)	29	-7.1(-15)	30	7.1(-15)	30

Table 1.2: *Table showing the final shift estimate and the number of inner iterations required to reach the inner tolerance when carrying out inverse iteration with a GK method, but fixing the inner tolerance to a constant, when solving* (1.5)*. Data for a 30×30 system, with four different inner tolerances.*

ultimately the inner system was being solved as if a very low tolerance was being used. Table 1.2 also contains the results for $\tau = 10^{-8}, 10^{-9}, \ldots$. It can be seen that there is very little difference between the eventual accuracy of the calculated shift using high or low tolerances, despite requiring far fewer inner iterations initially (and thus overall).

1.3 Galerkin-Krylov solves with a specific system

Lemma 1.2:
Consider a system

$$A\mathbf{x} = \mathbf{b}, \tag{1.16}$$

where $A \in \mathbb{R}^{n\times n}$ is nonsingular and $\mathbf{x}, \mathbf{b} \in \mathbb{R}^n$. Suppose that $\mathbf{b}$ is a linear combination of q eigenvectors of A, i.e.

$$\mathbf{b} = \sum_{i=1}^{q} \alpha_i \mathbf{w}_i, \tag{1.17}$$

where $\alpha_i \in \mathbb{R}$, $A\mathbf{w}_i = \lambda_i \mathbf{w}_i$, $\forall 1 \leq i \leq q$. Then solving the system iteratively using a Galerkin-Krylov solver with an initial guess $\mathbf{x}_0 = \mathbf{0}$ will give the true solution within q iterations.

Before proving this, we need a new definition.

Definition 1.3:
Take $A \in \mathbb{R}^{n\times n}$ and $\mathbf{v} \in \mathbb{R}^n$. let $p(A)$ be a polynomial in terms of A. Then the **grade** *of $\mathbf{v}$ with respect to A is the degree of the minimal nonzero monic polynomial p such that $p(A)\mathbf{v} = 0$.*

Proof.
We are solving (1.16) iteratively with $\mathbf{x}_0 = \mathbf{0}$, so we have that $\mathbf{r}_0 = \mathbf{b} - A\mathbf{x}_0 = \mathbf{b}$. Therefore

$$\begin{aligned} \mathcal{K}_k(A, \mathbf{r}_0) &= \mathcal{K}_k(A, \mathbf{b}) \\ &= span\left\{\mathbf{b}, A\mathbf{b}, \ldots, A^{k-1}\mathbf{b}\right\}. \end{aligned} \tag{1.18}$$

At iteration q this subspace will become $\mathcal{K}_q(A, \mathbf{b})$: the span of q vectors. We will first show that the grade of $\mathbf{b}$ with respect to A is at most q. Firstly, $\mathbf{b}$ is just a linear combination (henceforth 'LC') of q eigenvectors of A, denoted $\mathbf{w}_1, \ldots, \mathbf{w}_q$. It can be written as $\mathbf{b} = \sum_{i=1}^{q} \alpha_i \mathbf{w}_i$. Using this form and the notation $\alpha_{i,z} \equiv \alpha_i \lambda^z$, we get the following:

$$\begin{aligned} A\mathbf{b} = \textstyle\sum_{i=1}^{q} \alpha_i A\mathbf{w}_i &= \textstyle\sum_{i=1}^{q} \alpha_i \lambda_i \mathbf{w}_i &&= \textstyle\sum_{i=1}^{q} \alpha_{i,1}\mathbf{w}_i, \\ A^2\mathbf{b} = \textstyle\sum_{i=1}^{q} \alpha_i A^2\mathbf{w}_i &= \textstyle\sum_{i=1}^{q} \alpha_i \lambda_i^2 \mathbf{w}_i &&= \textstyle\sum_{i=1}^{q} \alpha_{i,2}\mathbf{w}_i, \\ &\vdots \\ A^{q-1}\mathbf{b} = \textstyle\sum_{i=1}^{q} \alpha_i A^{q-1}\mathbf{w}_i &= \textstyle\sum_{i=1}^{q} \alpha_i \lambda_i^{q-1} \mathbf{w}_i &&= \textstyle\sum_{i=1}^{q} \alpha_{i,q-1}\mathbf{w}_i. \end{aligned} \tag{1.19}$$

Thus the q spanning vectors of $\mathcal{K}_q(A, \mathbf{b})$ are just LCs of $\mathbf{w}_1, \ldots, \mathbf{w}_q$, and using them as a basis, any LC of $\mathbf{w}_1, \ldots, \mathbf{w}_q$ can be obtained. By extending (1.19) we know that $A^q\mathbf{b}$ is a LC of $\mathbf{w}_1, \ldots, \mathbf{w}_q$, therefore it must hold that $A^q\mathbf{b} \in \mathcal{K}_q(A, \mathbf{b})$, i.e. that $\mathcal{K}_q(A, \mathbf{b})$ is A-invariant. This implies that $\mathcal{K}_{q+1}(A, \mathbf{b}) = \mathcal{K}_q(A, \mathbf{b})$, and so by inductive reasoning

$\mathcal{K}_m(A, \mathbf{b}) = \mathcal{K}_q(A, \mathbf{b}), \forall m \geq q$.

Next we consider the true solution, $\hat{\mathbf{x}}$. Since the right hand side vector, $\mathbf{b}$, has such a nice form, it is easy to verify that

$$\hat{\mathbf{x}} = \sum_{i=1}^{q} \alpha_i \frac{1}{\lambda_i} \mathbf{w}_i, \tag{1.20}$$

where $\lambda_i \neq 0$ since A is nonsingular. Once more this is just an LC of $\mathbf{w}_1, \ldots, \mathbf{w}_q$, thus we know that $\hat{\mathbf{x}} \in \mathcal{K}_q(A, \mathbf{b})$. Now at iteration q of a Galerkin-Krylov method, the next approximation $\mathbf{x}_q$ is chosen from $(\mathbf{x}_0 + \mathcal{K}_q(A, \mathbf{r}_0)) \equiv \mathcal{K}_q(A, \mathbf{b})$ to be such that

$$\mathbf{b} - A\mathbf{x}_q \ \perp \ \mathcal{K}_q(A, \mathbf{b}). \tag{1.21}$$

If we define V_q to be the matrix whose columns are given by the spanning vectors of $\mathcal{K}_q(A, \mathbf{b})$, then this is equivalent to the condition that

$$V_q^\top (\mathbf{b} - A\mathbf{x}_q) = 0. \tag{1.22}$$

From earlier we know that $\mathcal{K}_q$ is A-invariant, so $A\mathbf{x}_q \in \mathcal{K}_q$, and by definition $\mathbf{b} \in \mathcal{K}_q$, so by subtracting we get that $(\mathbf{b} - A\mathbf{x}_q) \in \mathcal{K}_q$. Because of this, the condition (1.22) can only hold if $(\mathbf{b} - A\mathbf{x}_q) = 0$. This is satisfied by taking $\mathbf{x}_q \equiv \hat{\mathbf{x}}$, and so the true solution is obtained at least by iteration q, as required. □

Lemma 1.4:
Consider a system

$$A\mathbf{x} = \mathbf{b}, \tag{1.23}$$

where $A \in \mathbb{R}^{n \times n}$ is nonsingular and $\mathbf{x}, \mathbf{b} \in \mathbb{R}^n$. Suppose that $\mathbf{b}$ is of grade q with respect to A. Then solving the system iteratively using a Galerkin-Krylov (GK) solver with an initial guess $\mathbf{x}_0 = \mathbf{0}$ will give the true solution within q iterations.

Proof.
Since $\mathbf{b}$ is of grade q, Proposition 6.1 in [3] gives that $\mathcal{K}_q(A, \mathbf{b})$ is A-invariant. By extension this means that $\mathcal{K}_{q+k} \equiv \mathcal{K}_q, \ \forall k \in \mathbb{N}$. By step q of the GK method, the subspace $\mathcal{K}_q$ will have been built. Let us denote by V_q the matrix whose columns are the spanning vectors of $\mathcal{K}_q$. The new approximation, $\mathbf{x}_q$, to the solution is found by choosing a vector from $\mathcal{K}_q$ that satisfies

$$V_q^\top (\mathbf{b} - A\mathbf{x}_q) = 0. \tag{1.24}$$

We know that $A\mathbf{x}_q \in \mathcal{K}_q$, and by definition $\mathbf{b} \in \mathcal{K}_q$, so $\mathbf{b} - A\mathbf{x}_q \in \mathcal{K}_q$. This means there

exists some $\beta \in \mathbb{R}^q$ such that

$$\begin{aligned} & & \mathbf{b} - A\mathbf{x}_q &= V_q\beta \\ &\Rightarrow & V_q^\top(\mathbf{b} - A\mathbf{x}_q) &= V_q^\top V_q\beta \\ (1.24) &\Rightarrow & 0 &= V_q^\top V_q\beta \\ &\Rightarrow & 0 &= \beta \\ \\ &\Rightarrow & \mathbf{b} - A\mathbf{x}_q &= 0. \end{aligned}$$

Hence $\mathbf{x}_q$ is the solution as required. □

1.4 GMRES

Next we look at the equivalent theory when the inner solver used is GMRES.

Lemma 1.5:
If the inner system (1.5) *is solved iteratively using* m *steps of the GMRES method with a fixed right hand side,* $\mathbf{x}^{(0)}$*, and an initial inner guess* $\mathbf{y}_0^{(i)} = 0$*, then the convergence is to eigenpairs of* $H_m \in \mathbb{R}^{m\times m}$ *(defined as in* (1.7)*) and not of* $A \in \mathbb{R}^{n\times n}$ *for* $m < n$*.*

Proof.
We again consider the system

$$\left(A - s^{(i)}I\right)\mathbf{y}^{(i)} = \mathbf{x}^{(0)}, \tag{1.25}$$

and attempt to solve iteratively using the GMRES method. Suppose we have that V_m is the orthogonal basis for the Krylov subspace

$$\mathcal{K}_k\left(A - s^{(i)}I, \mathbf{x}^{(0)}\right) = span\left\{\mathbf{x}^{(0)}, \left(A - s^{(i)}I\right)\mathbf{x}^{(0)}, \ldots, \left(A - s^{(i)}I\right)^{k-1}\mathbf{x}^{(0)}\right\}, \tag{1.26}$$

whose columns are given by the spanning vectors of $\mathcal{K}_m\left(A - s^{(i)}I, \mathbf{x}^{(0)}\right)$. At each iteration, GMRES finds an estimate to the solution $\mathbf{y}^{(i)}$, say $\mathbf{y}_k^{(i)}$, such that $\mathbf{y}_k^{(i)} \in \mathbf{y}_0^{(i)} + \mathcal{K}_k\left(A - s^{(i)}I, \mathbf{x}^{(0)}\right)$ [2] (p39). To achieve this, method attempts to minimise the residual, i.e. GMRES solves

$$\min_{\mathbf{y}_k^{(i)}} \left\|(A - \sigma I)\,\mathbf{y}_k^{(i)} - \mathbf{x}^{(0)}\right\|. \tag{1.27}$$

Writing $\mathbf{y}_m^{(i)} = V_m\boldsymbol{\alpha}$, where $\boldsymbol{\alpha} \in \mathbb{R}^m$, and then premultiplying by $V_m^\top$ we have that, to find inner iteration m, we are minimising

$$\begin{aligned} & \min_{\boldsymbol{\alpha}} \left\|V_m^\top\left(A - s^{(i)}I\right)V_m\boldsymbol{\alpha} - V_m^\top\mathbf{x}_0\right\|, \\ \Rightarrow\quad & \min_{\boldsymbol{\alpha}} \left\|\left(V_m^\top A V_m - s^{(i)}V_m^\top V_m\right)\boldsymbol{\alpha} - \mathbf{e}_1\right\|, \\ \Rightarrow\quad & \min_{\boldsymbol{\alpha}} \left\|\left(H_m - s^{(i)}I\right)\boldsymbol{\alpha} - \mathbf{e}_1\right\|. \end{aligned} \tag{1.28}$$

Not complete or correct atm...

$$\left(H_m - s^{(i)}I\right)\boldsymbol{\alpha} = \mathbf{e}_1 \tag{1.29}$$

for $\boldsymbol{\alpha}$. As a result, by doing this at each iteration we are conducting inverse iteration on the system (1.29), and so will get convergence to eigenpairs $(\boldsymbol{\alpha}, \sigma)$ of H_m as required. As in the proof of Lemma 1.1, for $m < n$ eigenpairs of H_m and A are distinct. □

It^{n}s, m	Smallest E-Val of H_m	Limits of the oscillation Lower limit	Upper limit	Oscillation average	Tol being solved to: beginning	end
7	-1.8(−3)	-4.8(−3)	1.4(−2)	4.8(−3)	1.2(−2)	4.7(−1)
9	5.2(−4)	-3.4(−3)	6.7(−3)	1.6(−3)	6.9(−3)	4.2(−1)
11	-5.3(−5)	-2.1(−3)	1.9(−3)	-1.3(−4)	3.7(−3)	3.8(−1)
13	2.2(−4)	-8.7(−4)	1.1(−3)	1.0(−4)	2.7(−3)	3.8(−1)
15	2.0(−4)	-4.4(−4)	6.7(−4)	1.2(−4)	2.4(−3)	3.8(−1)
17	-1.2(−6)	-2.5(−4)	3.5(−4)	5.0(−5)	2.4(−3)	3.6(−1)
19	-1.3(−5)	-1.1(−4)	1.3(−4)	6.5(−6)	2.4(−3)	3.5(−1)
21	2.2(−6)	-2.7(−5)	3.0(−5)	1.7(−6)	1.9(−3)	3.4(−1)
23	-3.8(−8)	-5.3(−6)	8.2(−6)	1.4(−6)	8.5(−4)	3.4(−1)
25	-5.6(−8)	-9.1(−7)	8.8(−7)	-1.3(−8)	1.6(−4)	3.3(−1)
27	2.3(−10)	-6.0(−8)	5.7(−8)	-1.2(−9)	1.3(−5)	3.2(−1)
29	-1.8(−14)	-1.2(−10)	1.6(−10)	1.6(−11)	3.6(−8)	3.2(−1)

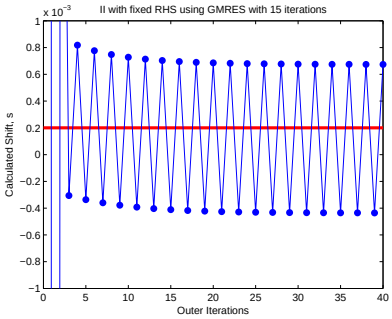
Table 1.3: *Table showing the limits of the oscillation observed when carrying out inverse iteration with GMRES, but specifying the number of iterations GMRES performs. Data for a* 30×30 *system, with 7 to 29 GMRES iterations in steps of 2.*

1.4.1 Numerical Example

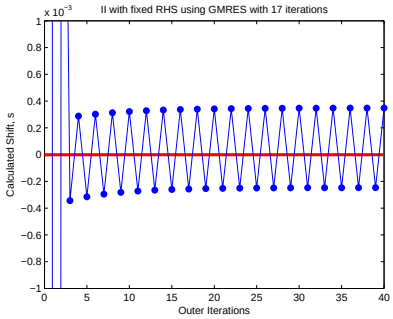
Using the same setup as defined in section 1.2.1, we will once again look at results obtained by solving (1.5) with a fixed right hand side vector, $\mathbf{x}^{(0)}$, and a fixed number of iterations, m, but this time using GMRES as the inner solver for inverse iteration. Then we will look at the number of inner iterations needed to solve (1.5) using GMRES again, but this time using a fixed inner tolerance, $\tau_k^{(i)} \equiv \tau$, $\forall i, \forall k$.

We first carried out inverse iteration to find the smallest eigenvalue of the matrix A (which had smallest eigenvalue $\lambda = 0$), and used GMRES as the inner solution method but with a fixed number of inner iterations. Fixing the number of inner iterations to $m = 15$, 17, 19 and 21, the method settled in to oscillations focussed around two values either side of the true eigenvalue. This behaviour can be seen in the respective graphs of figure 1-4. Further related data are given in Table 1.3 including the average of the upper and lower limits of the oscillations, which can be seen to be converging towards zero as $m \to n$.

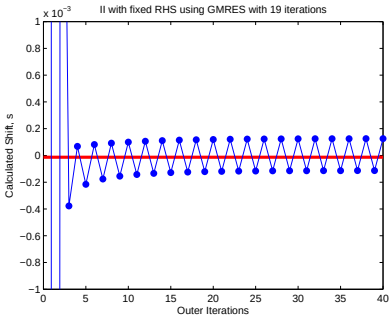
In all of these cases, the tolerance being solved to by GMRES was initially quite small (between 0.0019 and 0.0024), however by the time the oscillatory behaviour was reached, the tolerance being solved to was much larger (between 0.3391 and 0.3822). The reason for this is that as inverse iteration proceeds, the matrix $(A - s^{(i)}I)$ gets closer to being singular. This means that the solve becomes more and more inaccurate, leading to a higher tolerance being reached. This doesn't affect convergence to the true solution however, as the eigenvector estimate just gains magnitude in the same direction as the true solution. This suggests that faster solves could be carried out using larger inner tolerances without actually sacrificing accuracy.



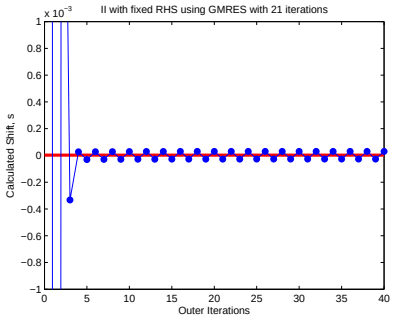
(a) GMRES with 15 inner iterations



(b) GMRES with 17 inner iterations



(c) GMRES with 19 inner iterations



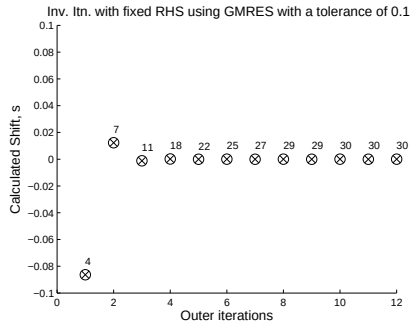
(d) GMRES with 21 inner iterations

Figure 1-4: *The plotted points are the calculated shift $s^{(i)}$ at each outer iteration, i. They show the convergence of inverse iteration on a system of dimension 30 using inner solver GMRES with a fixed number of iterations, m, for four different values of m. The horizontal lines show the smallest eigenvalue of H_m in each case.*

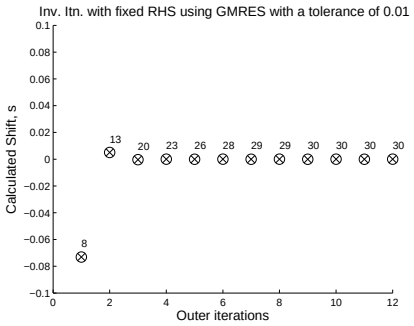
Another trend that can be seen from the graphs was that for values of m closer to the system's dimension, the oscillations were much more focussed about the true eigenvalue $\lambda = 0$. The limits of the oscillations are given in table 1.3 and can be seen to be converging around zero.

We now move on to examine results obtained by fixing the inner tolerance, $\tau_k^{(i)} \equiv \tau$, instead (as in section 1.2.1, but using GMRES as the inner solver). Once again we checked for inner convergence via (1.15), and the resulting data are represented graphically in figure 1-5 for four different inner tolerances. The numerical data are given in table 1.4 for two large tolerance cases, and also for very small tolerance cases.

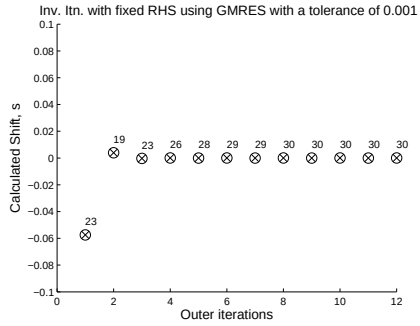
In the same way as seen in section 1.2.1, as the outer iteration proceeded, the number of inner iterations required to reach the inner tolerance approached the system size. This was due to the increased singularity of the matrix $(A - s^{(i)}I)$ as outer iteration proceeded and $s^{(i)}$ tended towards the true smallest eigenvalue of A. Once more, comparing the large and small tolerance cases given in table 1.4 shows very little difference between the final accuracy of the calculated shifts, despite the large tolerance cases needing far fewer inner iterations initially.



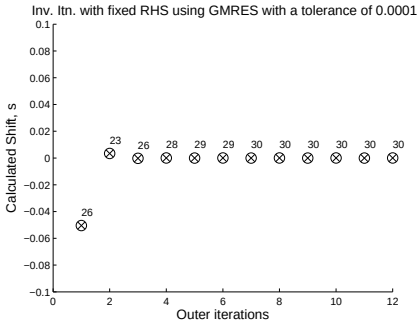
(a) GMRES with fixed tolerance $\tau = 10^{-1}$



(b) GMRES with fixed tolerance $\tau = 10^{-2}$



(c) GMRES with fixed tolerance $\tau = 10^{-3}$



(d) GMRES with fixed tolerance $\tau = 10^{-4}$

Figure 1-5: *The plotted points are the calculated shift $s^{(i)}$ at each outer iteration, i. They show the convergence of inverse iteration on a system of dimension 30 using inner solver GMRES with a fixed tolerance, τ, for four different values of τ. The numbers next to each point indicate how many inner iterations were required to reach the specified inner tolerance for each outer iteration.*

Outer	$\tau = 10^{-1}$		$\tau = 10^{-2}$		$\tau = 10^{-9}, 10^{-10}, \ldots$	
It^n, i	Shift, $s^{(i)}$	In. it^{n}s	Shift, $s^{(i)}$	In. it^{n}s	Shift, $s^{(i)}$	In. it^{n}s
1	-8.6(−2)	4	-7.3(−2)	8	-5.1(−2)	30
2	1.2(−2)	7	5.1(−3)	13	3.4(−3)	30
3	-1.2(−3)	11	-3.6(−4)	20	-2.3(−4)	30
4	1.4(−4)	18	2.6(−5)	23	1.6(−5)	30
5	-8.5(−6)	22	-1.8(−6)	26	-1.1(−6)	30
6	6.6(−7)	25	1.3(−7)	28	7.5(−8)	30
7	-5.1(−8)	27	-8.5(−9)	29	-5.1(−9)	30
8	3.5(−9)	29	6.0(−10)	29	3.5(−10)	30
9	-2.3(−10)	29	-4.1(−11)	30	-2.4(−11)	30
10	1.6(−11)	30	2.8(−12)	30	1.6(−12)	30
11	-1.1(−12)	30	-1.9(−13)	30	-1.1(−13)	30
12	7.1(−14)	30	-1.3(−14)	30	1.2(−14)	30

Table 1.4: *Table showing the final shift estimate and the number of inner iterations required to reach the inner tolerance when carrying out inverse iteration with a GMRES method, but fixing the inner tolerance to a constant, when solving* (1.5)*. Data for a 30×30 system, with four different inner tolerances.*

1.5 GMRES solves with a specific system

Lemma 1.6:
Consider a system

$$A\mathbf{x} = \mathbf{b}, \tag{1.30}$$

where $A \in \mathbb{R}^{n\times n}$ is nonsingular and $\mathbf{x}, \mathbf{b} \in \mathbb{R}^n$. Suppose that $\mathbf{b}$ is a linear combination of q eigenvectors of A, i.e.

$$\mathbf{b} = \sum_{i=1}^{q} \alpha_i \mathbf{w}_i, \tag{1.31}$$

where $\alpha_i \in \mathbb{R}$, $A\mathbf{w}_i = \lambda_i \mathbf{w}_i$, $\forall 1 \leq i \leq q$. Then solving the system iteratively using GMRES with an initial guess $\mathbf{x}_0 = \mathbf{0}$ will give the true solution within q iterations.

Proof.
Using the same initial arguement that was used in the proof of Lemma 1.2, we can similarly obtain that the subspace $\mathcal{K}_q(A, \mathbf{b})$ (constructed by GMRES at the qth iteration) is A-invariant. This again implies that $\mathcal{K}_m = \mathcal{K}_q, \forall m \geq q$. Further, the solution $\hat{\mathbf{x}}$ defined as

$$\hat{\mathbf{x}} = \sum_{i=1}^{q} \alpha_i \frac{1}{\lambda_i} \mathbf{w}_i, \tag{1.32}$$

still holds due to the structure of $\mathbf{b}$, and it is therefore still true that $\hat{\mathbf{x}} \in \mathcal{K}_q(A, \mathbf{b})$.

At this point the arguement varies due to the different nature in which GMRES chooses its approximate solutions at each iteration. At iteration q, GMRES chooses a vector $\mathbf{x}_q$ from $(\mathbf{x}_0 + \mathcal{K}_q(A, r_0)) \equiv \mathcal{K}_q(A, \mathbf{b})$ which satisfies

$$\min_{\mathbf{x}_q} \|A\mathbf{x}_q - \mathbf{b}\|. \tag{1.33}$$

Since $\hat{\mathbf{x}} \in \mathcal{K}_q$, and $\|A\hat{\mathbf{x}} - \mathbf{b}\| = 0$, this must be the minimiser of (1.33). Hence GMRES must choose $\mathbf{x}_q \equiv \hat{\mathbf{x}}$ at least at iteration q, thus we have convergence as required. □

Lemma 1.7:
Consider a system

$$A\mathbf{x} = \mathbf{b}, \tag{1.34}$$

where $A \in \mathbb{R}^{n\times n}$ is nonsingular and $\mathbf{x}, \mathbf{b} \in \mathbb{R}^n$. Suppose that $\mathbf{b}$ is of grade q with respect to A. Then solving the system iteratively using GMRES with an initial guess $\mathbf{x}_0 = \mathbf{0}$ will give the true solution within q iterations.

Proof.
By step q of GMRES, the subspace $\mathcal{K}_q(A, \mathbf{b})$ will have been built. Since $\mathbf{b}$ is of grade q, Proposition 6.1 in [3] gives that $\mathcal{K}_q(A, \mathbf{b})$ is A-invariant. By extension this means

that $\mathcal{K}_{q+k} \equiv \mathcal{K}_q$, $\forall k \in \mathbb{N}$. Even more simply, this gives us that

$$\mathcal{K}_q(A, \mathbf{b}) \equiv span\left\{\mathbf{b}, A\mathbf{b}, \ldots, A^{q-1}\mathbf{b}\right\} \equiv span\left\{A\mathbf{b}, A^2\mathbf{b}, \ldots, A^q\mathbf{b}\right\}, \tag{1.35}$$

and we note here that this shows $\mathbf{b} \in span\left\{A\mathbf{b}, A^2\mathbf{b}, \ldots, A^q\mathbf{b}\right\}$. Let us denote by V_q the matrix whose columns are the spanning vectors of $\mathcal{K}_q$. Further, let $V_q^{(A)}$ be the matrix whose columns are $A\mathbf{b}, A^2\mathbf{b}, \ldots, A^q\mathbf{b}$, and note the relationship that $V_q^{(A)} = AV_q$.

Since $\mathbf{b} \in span\left\{A\mathbf{b}, A^2\mathbf{b}, \ldots, A^q\mathbf{b}\right\}$, $\exists \beta \in \mathbb{R}^q$ such that

$$\mathbf{b} = V_q^{(A)}\beta = AV_q\beta. \tag{1.36}$$

Finally, if we define $\mathbf{x}_q \equiv V_q\beta$, then $\mathbf{x}_q \in \mathcal{K}_q$ and $\mathbf{b} = A\mathbf{x}_q$, i.e. $\|\mathbf{b} - A\mathbf{x}_q\| = 0$. This satisfies the criteria by which GMRES chooses its next approximation, and so will be chosen at step q as required. □

References

[1] Jörg Berns-Müller, Ivan G. Graham, and Alastair Spence. Inexact inverse iteration for symmetric matrices. *Linear Algebra and its Applications*, 416:389–413, 2006.

[2] Anne Greenbaum. *Iterative Methods for Solving Linear Systems.* SIAM, 1997.

[3] Yousef Saad. *Iterative Methods for Sparse Linear Systems, Second Edition.* Society for Industrial and Applied Mathematics, 2003.

[4] V Simoncini and L Elden. Inexact rayleigh quotient-type methods for eigenvalue computations. *BIT*, 42(1):159–182, 2002.