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Using complex shifts in Rayleigh Quotient Iteration to compute close eigenvalues

Bachelor Thesis

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1 Introduction

This thesis introduces a novel shift-and-invert method to compute eigenvalues and eigenvectors of real symmetric matrices. The method is a modification of the *Rayleigh Quotient Iteration (RQI)*. Numerical examples suggest that our method overcomes some of the drawbacks of RQI at the expense of a slower convergence rate.

The thesis is structured as follows. In this chapter we collect some basic definitions and results from numerical linear algebra. We also review some simple iterative methods for eigenvalue problems. The second chapter is devoted to the study of the Rayleigh Quotient and Rayleigh Quotient Iteration. Among others, we give a proof for the property that makes RQI advantageous over other methods, viz., the local cubic convergence. In the third chapter we introduce our novel method that we call *Complex Rayleigh Quotient Iteration*. After motivating the method, different numerical experiments are carried out to better understand its behaviour.

1.1 The Symmetric Eigenvalue Problem

There is a plethora of examples which lead to eigenvalue problems in almost all of the natural sciences, engineering and many other disciplines. In many cases the matrix of which the eigenvalues are sought is real and symmetric. In this case, the task of finding eigenvalues and eigenvectors is referred to as the *symmetric eigenvalue problem*. For completeness, we collect some general facts from linear algebra on eigenvalues and eigenvectors below.

Definition 1.1. Let $\mathbf{A} \in \mathbb{C}^{n \times n}$. A scalar $\lambda \in \mathbb{C}$ is called *eigenvalue* of \mathbf{A} if

there exists a nonzero vector $\mathbf{v} \in \mathbb{C}^n$ such that

$$\mathbf{A}\mathbf{v} = \lambda\mathbf{v}. \quad (1.1)$$

The vector \mathbf{v} is called an *eigenvector* of \mathbf{A} associated with λ . The tuple (λ, \mathbf{v}) is called an *eigenpair*. The set of all eigenvalues of \mathbf{A} is referred to as the *spectrum* and is denoted by $\sigma(\mathbf{A})$. To indicate that eigenvalues belong to a particular matrix \mathbf{M} we sometimes write $\lambda(\mathbf{M})$.

Computing eigenpairs is a non-trivial task. Rewriting (1.1) gives $\mathbf{A}\mathbf{v} - \lambda\mathbf{v} = \mathbf{0}$ or $(\mathbf{A} - \lambda\mathbf{I})\mathbf{v} = \mathbf{0}$, where \mathbf{I} is the identity matrix. Since \mathbf{v} cannot be the zero vector, this equation has a solution if and only if the matrix $\mathbf{A} - \lambda\mathbf{I}$ is singular. Thus, eigenvalues of \mathbf{A} are exactly the roots of the *characteristic polynomial*

$$\chi_{\mathbf{A}}(t) := \det(\mathbf{A} - t\mathbf{I}).$$

This fact, despite being of theoretical importance, cannot be used to calculate eigenvalues numerically for two reasons. First, the computation of the coefficients of the polynomial is not stable [8, p. 37]. And even if it was, it is well-known that even small perturbations in the coefficients of $\chi_{\mathbf{A}}(t)$ can lead to devastating errors in the roots [cf. 32, p. 190]. Thus, other methods are necessary to solve (1.1) which gave rise to iterative algorithms. These methods date back to 1846 when Jacobi published a pioneering paper on a method to compute eigenvalues of symmetric matrices [12]. Below we present essential facts from linear algebra preparing us for discussing such iterative methods in Section 1.2.

Remark 1.2 (Generalisations of eigenvalue problems). The problem stated in Equation (1.1) can be generalised in multiple ways. Many problems from physics lead to the *generalised eigenvalue problem*

$$\mathbf{A}\mathbf{v} = \lambda\mathbf{M}\mathbf{v}. \quad (1.2)$$

In our case, we have $\mathbf{M} = \mathbf{I}$, the identity matrix. Many of the numerical algorithms for solving eigenvalue problems of the form (1.1) can be modified to solve (1.2); often certain assumptions have to be posed on \mathbf{M} such as positive definiteness.

Since matrices can be seen as representations of linear operators on finite-dimensional vector spaces, we can define eigenvalue problems for linear operators on more general spaces that are possibly of infinite dimension. The eigenvectors are then usually called *eigenfunctions*. Other generalisations include the *quadratic eigenvalue problem*

$$(\lambda^2 \mathbf{A}_2 + \lambda \mathbf{A}_1) \mathbf{v} = \mathbf{A}_0 \mathbf{v},$$

with matrix coefficients $\mathbf{A}_0, \mathbf{A}_1, \mathbf{A}_2 \in \mathbb{C}^{n \times n}$ or more general *nonlinear eigenproblems*

$$\mathbf{Q}(\lambda) \mathbf{v} = \mathbf{0},$$

where $\mathbf{Q}(\lambda)$ is a nonlinear matrix-valued function. In this thesis, we mostly consider problems of the form (1.1). We will briefly come back to problems of the form (1.2) in the last chapter.

In the following proposition we collect some basic facts on eigenvalues and eigenvectors. The results are shown under the assumption that $\mathbf{A} \in \mathbb{C}^{n \times n}$ is a complex Hermitian matrix, i. e., $\mathbf{A} = \mathbf{A}^* := \overline{\mathbf{A}}^T$, where the bar denotes the complex conjugate. If \mathbf{A} is a real matrix, we have $\overline{\mathbf{A}} = \mathbf{A}$ and thus the following facts hold in particular for real symmetric matrices.

Proposition 1.3. *Let $\mathbf{A} = \mathbf{A}^* \in \mathbb{C}^{n \times n}$ be a Hermitian matrix. Denote by $\lambda_1, \lambda_2, \dots, \lambda_n$ the eigenvalues¹ of \mathbf{A} with associated eigenvectors $\mathbf{v}_1, \dots, \mathbf{v}_n$.*

¹Of course, the eigenvalues need not be distinct. But since the eigenvalues of \mathbf{A} are the roots of the n -degree polynomial $\chi_{\mathbf{A}}(t)$, when counting these roots with their multiplicity, this polynomial has n roots over \mathbb{C} . Thus, we can label the eigenvalues from 1 to n .

- (i) All eigenvalues of \mathbf{A} are real.
- (ii) There exists an orthonormal basis of \mathbb{C}^n consisting of eigenvectors of \mathbf{A} .
If \mathbf{A} is a real symmetric matrix, the eigenvectors form an orthonormal basis of \mathbb{R}^n .
- (iii) If \mathbf{A} is non-singular the eigenvalues of \mathbf{A}^{-1} are given by $\lambda_1^{-1}, \dots, \lambda_n^{-1}$ with eigenvectors $\mathbf{v}_1, \dots, \mathbf{v}_n$.
- (iv) Let $\mu \in \mathbb{R}$ an arbitrary scalar. The eigenvalues of $\mathbf{A} - \mu\mathbf{I}$ are $\lambda_i - \mu$ with eigenvectors $\mathbf{v}_1, \dots, \mathbf{v}_n$.

Proof. Both (i) and (ii) are well-known results from linear algebra and the proofs can be found in most standard literature (see for example [10, Theorem 18 and Corollary, p. 314]).

- (iii) Suppose \mathbf{A} is invertible and let (λ, \mathbf{v}) be an eigenpair of \mathbf{A} (note that since \mathbf{A} is non-singular we have $\lambda \neq 0$). Then

$$\mathbf{A}\mathbf{v} = \lambda\mathbf{v} \quad \Leftrightarrow \quad \mathbf{A}^{-1}\mathbf{A}\mathbf{v} = \lambda\mathbf{A}^{-1}\mathbf{v} \quad \Leftrightarrow \quad \lambda^{-1}\mathbf{v} = \mathbf{A}^{-1}\mathbf{v},$$

hence $(\lambda^{-1}, \mathbf{v})$ is an eigenpair of \mathbf{A}^{-1} .

- (iv) For $\mu \in \mathbb{R}$ and (λ, \mathbf{v}) an eigenpair we have

$$\mathbf{A}\mathbf{v} = \lambda\mathbf{v} \quad \Leftrightarrow \quad \mathbf{A}\mathbf{v} - \mu\mathbf{v} = \lambda\mathbf{v} - \mu\mathbf{v} \quad \Leftrightarrow \quad (\mathbf{A} - \mu\mathbf{I})\mathbf{v} = (\lambda - \mu)\mathbf{v},$$

hence $(\lambda - \mu, \mathbf{v})$ is an eigenpair of $\mathbf{A} - \mu\mathbf{I}$.

□

In the following, we restrict our attention to the *symmetric eigenvalue problem*, i. e., we want to find solutions of equation (1.1) assuming \mathbf{A} is a real symmetric matrix. Thus, unless stated otherwise, for the remainder of the

thesis \mathbf{A} denotes a matrix of this type. The (real) eigenvalues are denoted by $\lambda_j(\mathbf{A}) = \lambda_j$ with corresponding (real) eigenvectors \mathbf{v}_j . Since any scalar multiple of an eigenvector is also an eigenvector, we assume that they are normalised w.r.t. the Euclidean norm, so that

$$\|\mathbf{v}_i\| := \|\mathbf{v}_i\|_2 := \sqrt{\mathbf{v}_i^\top \mathbf{v}_i} = 1 \quad \text{for all } i = 1, \dots, n.$$

Due to Proposition 1.3 (ii) we have

$$\langle \mathbf{v}_i, \mathbf{v}_j \rangle = \mathbf{v}_i^\top \mathbf{v}_j = 0 \quad \text{for } i \neq j,$$

where $\langle \cdot, \cdot \rangle$ denotes the Euclidean inner product on \mathbb{R}^n . Since all eigenvalues are real we can label them in increasing order of magnitude

$$|\lambda_1| \leq |\lambda_2| \leq \dots \leq |\lambda_n|.$$

The eigenvalues λ_1 and λ_n are called *extreme* eigenvalues. The remaining eigenvalues $\lambda_2, \dots, \lambda_{n-1}$ are called *interior* eigenvalues.

In addition to the assumption that the matrix we work with is real and symmetric, we are mainly interested in cases in which the target eigenvalue and its neighbours are very close. We usually do not have any a priori knowledge about their location. Also, the matrices are assumed to be large such that the computation of the complete set of eigenpairs is too expensive. However, we assume a good approximation of the target eigenvector is available. As we will see, traditional methods do not perform well when the gap between the wanted eigenvalue and adjacent eigenvalues is too small.

1.2 Iterative methods for eigenvalue problems

With the necessary facts from linear algebra at hand we can introduce some simple iterative methods for computing eigenpairs of symmetric matrices. We are always interested in how fast these methods produce good approximations of eigenvectors or eigenvalues (or both). The following definition provides us with a notion of the speed at which a sequence converges to its limit.

Definition 1.4 (Order of Convergence). Let $(\mathbf{x}^{(k)})_{k \in \mathbb{N}}$ be a sequence in \mathbb{C}^n that converges to $\mathbf{z} \in \mathbb{C}^n$.

- (i) The sequence is said to converge *linearly* to \mathbf{z} , if there exists a constant $0 < \rho < 1$ such that

$$\lim_{k \rightarrow \infty} \frac{\|\mathbf{x}^{(k+1)} - \mathbf{z}\|}{\|\mathbf{x}^{(k)} - \mathbf{z}\|} < \rho,$$

where ρ is called the *rate of convergence*.

- (ii) The sequence *converges with order q to \mathbf{z}* for $q > 1$ if

$$\lim_{k \rightarrow \infty} \frac{\|\mathbf{x}^{(k+1)} - \mathbf{z}\|}{\|\mathbf{x}^{(k)} - \mathbf{z}\|^q} < M,$$

for some $M > 0$. In particular, convergence with order

- $q = 2$ is called *quadratic convergence*,
- $q = 3$ is called *cubic convergence*

etc.

In some cases, in particular for sequences that approximate eigenvectors, the convergence behaviour is best studied in terms of the *error angle* between $\mathbf{x}^{(k)}$ and \mathbf{z} .

Definition 1.5 (Angle). The *angle* between two vectors $\mathbf{x}, \mathbf{y} \in \mathbb{C}^n \setminus \{\mathbf{0}\}$ is defined as

$$\angle(\mathbf{x}, \mathbf{y}) = \arccos \frac{|\langle \mathbf{x}, \mathbf{y} \rangle|}{\|\mathbf{x}\| \|\mathbf{y}\|}.$$

Often, the following identities are convenient

$$\sin \angle(\mathbf{x}, \mathbf{y}) := \sqrt{1 - \cos^2 \angle(\mathbf{x}, \mathbf{y})}, \quad \tan \angle(\mathbf{x}, \mathbf{y}) := \frac{\sin \angle(\mathbf{x}, \mathbf{y})}{\cos \angle(\mathbf{x}, \mathbf{y})}.$$

To see why also the angle can be used to measure the convergence speed, suppose $\mathbf{x}^{(k)}$ converges to the unit vector \mathbf{z} . Let $\mathbf{u}^{(k)}$ be the unit vector that lies in the span of $\mathbf{x}^{(k)}$ and \mathbf{z} and is orthogonal to \mathbf{z} and denote by $\phi^{(k)} = \angle(\mathbf{x}^{(k)}, \mathbf{z})$ the error angle between the current vector iterate and the limit. Now, write the vector iterate $\mathbf{x}^{(k)}$ as

$$\mathbf{x}^{(k)} = \mathbf{z} \cos \phi^{(k)} + \mathbf{u}^{(k)} \sin \phi^{(k)}.$$

We temporarily drop the superscripts and write $\mathbf{x} = \mathbf{x}^{(k)}$, $\mathbf{u} = \mathbf{u}^{(k)}$ and $\phi = \phi^{(k)}$. Then, using the identities $\sin^2(\phi/2) = \frac{1 - \cos \phi}{2}$, $\sin^2 \phi + \cos^2 \phi = 1$ and the Pythagorean theorem we obtain

$$\begin{aligned} \|\mathbf{x} - \mathbf{z}\|^2 &= \|\mathbf{z} \cos \phi + \mathbf{u} \sin \phi - \mathbf{z}\|^2 \\ &= \|\mathbf{z}(\cos \phi - 1)\|^2 + \|\mathbf{u} \sin \phi\|^2 \\ &= (\cos \phi - 1)^2 + 1 - \cos^2 \phi \\ &= 2(1 - \cos \phi) = 4 \sin^2(\phi/2). \end{aligned}$$

Thus, convergence orders w. r. t. the norm imply the same convergence orders in terms of the error angles and vice versa. Note that we did assume convergence of the sequence.

Power method

The *power method* is one of the oldest iterative methods for computing eigenvectors. It is based on generating the sequence $\mathbf{x}^{(k)} := \mathbf{A}^k \mathbf{x}^{(0)}$ where $\mathbf{x}^{(0)}$ is a non-zero unit vector. Of course, \mathbf{A}^k does not have to be computed explicitly at each step since

$$\mathbf{A}^k \mathbf{x} = \mathbf{A}(\mathbf{A}(\dots \mathbf{A}(\mathbf{A}\mathbf{x}) \dots)).$$

To prevent underflow and overflow errors, $\mathbf{x}^{(k)}$ is normalised at each step. In Algorithm 1.6 we normalise by ensuring that the largest component of the current approximation is equal to one. Of course, other norms can be used. The sequence $\mathbf{x}^{(k)}$ converges to the eigenvector associated with the eigenvalue λ_n under the assumptions that λ_n is dominant (i. e., $|\lambda_n|$ is strictly greater than $|\lambda_{n-1}|$) and that the starting vector $\mathbf{x}^{(0)}$ has a non-vanishing component in the direction of \mathbf{v}_n . The advantage of normalising w. r. t. the maximum norm is that the largest component of $|\mathbf{A}\mathbf{x}^{(k-1)}|$ converges to the eigenvalue λ_n . Regardless of the normalisation chosen, the method converges linearly with convergence rate

$$\rho = \frac{|\lambda_{n-1}|}{|\lambda_n|}. \quad (1.3)$$

Thus, the method can be very slow if the distance between the eigenvalues λ_n and λ_{n-1} is very small. For a detailed convergence proof, see [28, pp. 86 sq.].

Algorithm 1.6: Power method

```

begin
    Choose nonzero initial vector  $\mathbf{x}^{(0)}$ 
    for  $k = 1, 2, \dots$  until convergence do
         $\mathbf{x}^{(k)} = \frac{1}{\alpha^{(k)}} \mathbf{A}\mathbf{x}^{(k-1)}$ 
        /*  $\alpha^{(k)}$  is the component of  $\mathbf{A}\mathbf{x}^{(k-1)}$  with the maximum
           modulus */

```

Besides the possible slow convergence rate, the power method will always converge to an eigenvector associated with the dominant eigenvalue λ_n . In many applications, however, one already has a good approximation of another eigenvalue and wants to compute an eigenvector it belongs to. The following method allows for such computations.

(Shifted) Inverse Iteration

The *inverse iteration* is the power method applied to \mathbf{A}^{-1} (provided that the inverse exists). Due to Proposition 1.3 (iii) this will produce a sequence of vectors $\mathbf{x}^{(k)}$ converging to the eigenvector associated to the eigenvalue that is smallest in modulus λ_1 . Combining this idea with Proposition 1.3 (iv) yields the *shifted inverse iteration*. There, the iterates are defined by

$$\mathbf{x}^{(k)} = \beta(\mathbf{A} - \sigma\mathbf{I})^{-1}\mathbf{x}^{(k-1)},$$

where β is responsible for normalising $\mathbf{x}^{(k)}$. The smallest eigenvalue in modulus of the shifted matrix $\mathbf{A} - \sigma\mathbf{I}$ is the eigenvalue of \mathbf{A} that is closest to σ . Hence, this method converges to an eigenvector associated with this eigenvalue. Of course, the inverse need not be computed explicitly. Instead, before the loop we can compute the LU decomposition of $\mathbf{A} - \sigma\mathbf{I}$ (or any other factorisation, if applicable) and solve the system $(\mathbf{A} - \sigma\mathbf{I})\mathbf{x}^{(k)} = \mathbf{x}^{(k-1)}$ for $\mathbf{x}^{(k)}$. At each step then, only one backward and one forward substitution is required, reducing the complexity from $\mathcal{O}(n^3)$ to $\mathcal{O}(n^2)$. We summarise the results in Algorithm 1.7 (there, we normalise w. r. t. the Euclidean norm).²

Since this is essentially the power method (applied to the inverse of $\mathbf{A} - \sigma\mathbf{I}$) this algorithm still converges linearly. However, if we denote by μ_1 the eigenvalue that is closest to the shift σ and by μ_2 the one that is the next closest one, the eigenvalue of largest modulus of $(\mathbf{A} - \sigma\mathbf{I})^{-1}$ is $1/(\mu_1 - \sigma)$

²Note that we did not specify the “until convergence” criteria in neither of the algorithms introduced in this section. We postpone this discussion until Section 2.1.

Algorithm 1.7: Shifted inverse iteration

Input: Nonzero unit vector $\mathbf{x}^{(0)}$, shift $\sigma \in \mathbb{R}$
 Compute **LU** decomposition $\mathbf{A} - \sigma \mathbf{I} = \mathbf{LU}$
for $k = 1, 2, \dots$ *until convergence* **do**
 Solve $(\mathbf{A} - \sigma \mathbf{I})\tilde{\mathbf{x}}^{(k)} = \mathbf{x}^{(k-1)}$ for $\tilde{\mathbf{x}}^{(k)}$
 $\mathbf{x}^{(k)} \leftarrow \tilde{\mathbf{x}}^{(k)} / \|\tilde{\mathbf{x}}^{(k)}\|$

and (1.3) suggests that the convergence rate is

$$\rho = \frac{|\mu_1 - \sigma|}{|\mu_2 - \sigma|}.$$

Therefore, the method is often used to compute an eigenvector of \mathbf{A} if a good approximation of the corresponding eigenvalue is already available.

Note, however, that a shift which is very close to an eigenvalue produces a very ill-conditioned linear system and one might expect inverse iteration to fail in these cases since, in general, it is impossible to solve ill-conditioned systems accurately. Despite this seemingly sincere problem, in practice it was observed that the method produces good approximations even in these cases. According to Parlett [23, pp. 84 sq.], it was Wilkinson who elucidated why the ill-conditioning is not a problem in most cases. Suppose $\sigma \approx \lambda$ where λ is an eigenvalue of \mathbf{A} with corresponding eigenvector \mathbf{v} . Wilkinson illustrated that although $\tilde{\mathbf{x}}^{(k)}$ may be far from \mathbf{v} , the normalised solution $\mathbf{x}^{(k)} = \tilde{\mathbf{x}}^{(k)} / \|\tilde{\mathbf{x}}^{(k)}\|$ will not be far from \mathbf{v} , when the system is solved backwards-stably, for more details see [34, pp. 621–630], [23, pp. 68–71] and [25]. This will become important again later when we discuss Rayleigh Quotient Iteration. There, the system that is solved gets increasingly ill-conditioned at each step but for the same reason as above, in practice this poses no problem.

At each step in the shifted inverse iteration, better approximations for the target eigenvector are computed. One could try to use these approximations to compute approximations of the corresponding eigenvalue and replace oc-

asionally the shift. There are different techniques to obtain such estimates, e. g. the *Wielandt Shifted Inverse Iteration* or the *Rayleigh Quotient Iteration*, the latter of which is rigorously studied in the next chapter. For further discussion on the variants and developments of these so called *shift-and-invert* techniques see, e. g., the historic surveys [11] and [8] or Sections 2 and 3 of [31].

2 Classic Rayleigh Quotient Iteration

In this chapter we introduce the Rayleigh Quotient Iteration (or RQI, for short) and discuss some important results. Among others, we give a proof of the (local) cubic convergence of RQI. We provide numerical examples for the presented results and discuss some disadvantages.

Numerical
Examples?

As mentioned above, we assume that we have given an approximation of an eigenvector of a real symmetric matrix \mathbf{A} and we want to compute the exact eigenvector and corresponding eigenvalue.

2.1 The Rayleigh Quotient

In Chapter 1 we briefly introduced some simple iterative eigenvalue methods. In essence, RQI is shifted inverse iteration where the shift is replaced by the *Rayleigh quotient* at each step.

Definition 2.1 (Rayleigh Quotient). Let $\mathbf{A} \in \mathbb{C}^{n \times n}$. The mapping

$$\mathcal{R}_{\mathbf{A}} : \mathbb{C}^n \setminus \{\mathbf{0}\} \rightarrow \mathbb{C}, \quad \mathbf{x} \mapsto \frac{\mathbf{x}^* \mathbf{A} \mathbf{x}}{\mathbf{x}^* \mathbf{x}}$$

is called the *Rayleigh quotient* corresponding to the matrix \mathbf{A} .¹

For real vectors, we have

$$\mathcal{R}_{\mathbf{A}}(\mathbf{x}) = \frac{\mathbf{x}^{\top} \mathbf{A} \mathbf{x}}{\mathbf{x}^{\top} \mathbf{x}}.$$

¹Other notations that are popular in the literature include $R_{\mathbf{A}}(\mathbf{x})$, $R(\mathbf{A}, \mathbf{x})$, $r_{\mathbf{A}}(\mathbf{x})$, $\sigma_{\mathbf{A}}(\mathbf{x})$ or $\rho_{\mathbf{A}}(\mathbf{x})$.

We begin by discussing some basic facts.

Lemma 2.2. *Let $\mathbf{x} \in \mathbb{C}^n \setminus \{\mathbf{0}\}$, $0 \neq \alpha, \beta \in \mathbb{C}$ and $\mathbf{A} \in \mathbb{C}^{n \times n}$.*

(i) *If (λ, \mathbf{v}) is an eigenpair of \mathbf{A} , then $\mathcal{R}_{\mathbf{A}}(\mathbf{v}) = \lambda$.*

(ii) $\mathcal{R}_{\beta\mathbf{A}}(\alpha\mathbf{x}) = \beta\mathcal{R}_{\mathbf{A}}(\mathbf{x})$ (Homogeneity)

(iii) $\mathcal{R}_{\mathbf{A}-\alpha\mathbf{I}}(\mathbf{x}) = \mathcal{R}_{\mathbf{A}}(\mathbf{x}) - \alpha$ (Translation invariance)

Proof. (i) We can write the Rayleigh Quotient as

$$\mathcal{R}_{\mathbf{A}}(\mathbf{x}) = \frac{\langle \mathbf{x}, \mathbf{Ax} \rangle}{\langle \mathbf{x}, \mathbf{x} \rangle}, \quad (2.1)$$

where $\langle \mathbf{x}, \mathbf{y} \rangle = \mathbf{x}^* \mathbf{y}$ denotes the Euclidean inner product on \mathbb{C}^n . Due to the linearity in the second argument we obtain

$$\mathcal{R}_{\mathbf{A}}(\mathbf{v}) = \frac{\langle \mathbf{v}, \mathbf{Av} \rangle}{\langle \mathbf{v}, \mathbf{v} \rangle} = \frac{\langle \mathbf{v}, \lambda \mathbf{v} \rangle}{\langle \mathbf{v}, \mathbf{v} \rangle} = \lambda \frac{\langle \mathbf{v}, \mathbf{v} \rangle}{\langle \mathbf{v}, \mathbf{v} \rangle} = \lambda.$$

(ii) By again writing the Rayleigh Quotient as in (2.1) and using the semi-linearity in the first and linearity in the second argument of the inner product, we obtain

$$\mathcal{R}_{\beta\mathbf{A}}(\alpha\mathbf{x}) = \frac{\langle \alpha\mathbf{x}, \beta\mathbf{A}(\alpha\mathbf{x}) \rangle}{\langle \alpha\mathbf{x}, \alpha\mathbf{x} \rangle} = \beta \frac{\overline{\alpha}\alpha \langle \mathbf{x}, \mathbf{Ax} \rangle}{\overline{\alpha}\alpha \langle \mathbf{x}, \mathbf{x} \rangle} = \beta \mathcal{R}_{\mathbf{A}}(\mathbf{x}).$$

(iii)

$$\mathcal{R}_{\mathbf{A}-\alpha\mathbf{I}}(\mathbf{x}) = \frac{\mathbf{x}^*(\mathbf{A} - \alpha\mathbf{I})\mathbf{x}}{\mathbf{x}^*\mathbf{x}} = \frac{\mathbf{x}^*\mathbf{Ax} - \alpha\mathbf{x}^*\mathbf{x}}{\mathbf{x}^*\mathbf{x}} = \mathcal{R}_{\mathbf{A}}(\mathbf{x}) - \alpha.$$

□

Although the Rayleigh Quotient might look arbitrary at first sight, it occurs naturally as the solution of a least squares minimisation problem. First note

that if (λ, \mathbf{v}) is an eigenpair of \mathbf{A}

$$\|\mathbf{A}\mathbf{v} - \lambda\mathbf{v}\| = 0.$$

Now, suppose $\hat{\mathbf{v}}$ is an approximation for \mathbf{v} and we want to find the best approximation $\hat{\lambda}$ for λ in the sense that

$$\hat{\lambda} = \arg \min_{\mu \in \mathbb{C}} \|\mathbf{A}\hat{\mathbf{v}} - \mu\hat{\mathbf{v}}\|.$$

This is a linear least squares problem in μ with normal equations (see, e. g. [7, Theorem 6.12, p. 362])

$$(\hat{\mathbf{v}}^* \hat{\mathbf{v}}) \mu = \hat{\mathbf{v}}^* \mathbf{A} \hat{\mathbf{v}}$$

and dividing by $(\hat{\mathbf{v}}^* \hat{\mathbf{v}})$ yields the solution

$$\mu = \frac{\hat{\mathbf{v}}^* \mathbf{A} \hat{\mathbf{v}}}{\hat{\mathbf{v}}^* \hat{\mathbf{v}}} = \mathcal{R}_{\mathbf{A}}(\hat{\mathbf{v}}).$$

That is, the Rayleigh Quotient is the choice of μ that minimises the *residual* norm for the eigenvalue problem. The following result specifies how good of an estimate the Rayleigh Quotient is. According to Parlett this is the property to which “the phenomenal convergence rate [of RQI] can be attributed” [23, p. 77]. We postpone the proof of this statement until when we discuss the convergence behaviour of RQI.

Lemma 2.3 (Eigenvalue estimate). *Let $\mathbf{x} \in \mathbb{C}^n$ be an approximation of an eigenvector \mathbf{v} of a normal² matrix \mathbf{A} with corresponding eigenvalue λ . Then*

$$|\mathcal{R}_{\mathbf{A}}(\mathbf{x}) - \mathcal{R}_{\mathbf{A}}(\mathbf{v})| = |\mathcal{R}_{\mathbf{A}}(\mathbf{x}) - \lambda| = \mathcal{O}(\|\mathbf{x} - \mathbf{v}\|^2).$$

²A matrix \mathbf{A} is said to be *normal* if $\mathbf{A}^* \mathbf{A} = \mathbf{A} \mathbf{A}^*$. Note that for complex Hermitian (or real symmetric) matrices we have $\mathbf{A} = \mathbf{A}^*$, hence Hermitian (and thus symmetric) matrices are normal.

2 Classic Rayleigh Quotient Iteration

This result is often paraphrased as “the Rayleigh Quotient is a *quadratically accurate* estimate of an eigenvalue” (see for example [32, p. 204]). If \mathbf{A} is non-normal, the Rayleigh quotient is still an estimate of order one, i.e.,

$$|\mathcal{R}_{\mathbf{A}}(\mathbf{x}) - \mathcal{R}_{\mathbf{A}}(\mathbf{v})| = \mathcal{O}(\|\mathbf{x} - \mathbf{v}\|).$$

We now have a method that allows us to obtain an estimation of an *eigenvalue* from an *eigenvector*. With the Shifted Inverse Iteration (Algorithm 1.7) we have the converse: a method for obtaining an *eigenvector* estimate from an *eigenvalue* estimate. Rayleigh Quotient Iteration is essentially a combination of those two methods where each step consists of one step of Shifted Inverse Iteration and the computation of the Rayleigh Quotient.

Algorithm 2.4: Rayleigh Quotient Iteration

Input: Nonzero unit vector $\mathbf{x}^{(0)}$
 $\mu^{(0)} \leftarrow (\mathbf{x}^{(0)})^* \mathbf{A} \mathbf{x}^{(0)}$
for $k = 1, 2, \dots$ *until convergence* **do**
 Solve $(\mathbf{A} - \mu^{(k)} \mathbf{I}) \mathbf{y}^{(k)} = \mathbf{x}^{(k-1)}$ for $\mathbf{y}^{(k)}$
 $\mathbf{x}^{(k)} \leftarrow \mathbf{y}^{(k)} / \|\mathbf{y}^{(k)}\|$
 $\mu^{(k)} \leftarrow (\mathbf{x}^{(k)})^* \mathbf{A} \mathbf{x}^{(k)}$

We have yet to define what we mean by “until convergence” in this Algorithm but also in the simple vector iterations from Chapter 1. Now that we have defined the Rayleigh Quotient, we can define the following stopping criterion. Run the iteration until

$$\|\mathbf{r}^{(k)}\| = \|\mathbf{A} \mathbf{x}^{(k)} - \mu^{(k)} \mathbf{x}^{(k)}\| < \text{tol},$$

where $\mathbf{r}^{(k)} := \mathbf{A} \mathbf{x}^{(k)} - \mu^{(k)} \mathbf{x}^{(k)}$ is called the *residual vector* and tol is a user-given error tolerance. In Algorithm 1.6 (Power method) and Algorithm 1.7 (Inverse Iteration) the Rayleigh Quotient of the current vector iterate $\mu^{(k)} =$

$(\mathbf{x}^{(k)})^* \mathbf{A} \mathbf{x}^{(k)}$ is not computed. Therefore, for this *residual-based error control* to work, the computation of $\mu^{(k)}$ has to be added to these algorithms.

Obviously, if for some k the tuple $(\mu^{(k)}, \mathbf{x}^{(k)})$ is an eigenpair we have $\mathbf{r}^{(k)} = \mathbf{0}$. For approximate eigenpairs we expect a small residual to imply small errors in these approximations. Details on this residual-based error control can be found in [28, Section 3.2] or [3, Section 5.2]. Here, we give only some important results without proof. A popular result, usually referred to as the *Bauer-Fike theorem* (see, e. g. [28, p. 59]) states that there exists an eigenvalue λ of \mathbf{A} such that

$$|\lambda - \mu^{(k)}| \leq \|\mathbf{r}^{(k)}\|. \quad (2.2)$$

Thus, if the stopping criterion is fulfilled, we have $|\lambda - \mu^{(k)}| < \text{tol}$. For the eigenvector one can show [28, p. 63] that the following bound holds

$$\sin \angle(\mathbf{x}^{(k)}, \mathbf{v}) \leq \frac{\|\mathbf{r}^{(k)}\|}{\delta},$$

where \mathbf{v} is an eigenvector associated with λ and δ is the distance from $\mu^{(k)}$ to the rest of the spectrum, i. e.,

$$\delta := \min_i \{|\mu^{(k)} - \lambda_i| : \lambda_i \neq \lambda\}.$$

2.2 History and recent developments

Now that we have defined the Rayleigh Quotient and Rayleigh Quotient Iteration we give an overview of the historic developments of RQI. We also discuss recent contributions that are relevant to this thesis. Some of the results, mainly the ones that are concerned with the convergence of RQI, are discussed in more detail in Section 2.3.

2.2.1 Chronology of Rayleigh Quotient iteration

It took about 60 years from the first mention of what is now called the Rayleigh quotient until RQI was fully defined as it is given in Algorithm 2.4. In this section we give an overview of some important milestones within this 60 years. Large parts of this overview are based on Section 4 of [31].

1894 — Lord Rayleigh In the second edition of his book titled “The Theory of Sound” John William Strutt, 3rd Baron Rayleigh [26, p. 110], proposed the following iteration for improving an approximate eigenvector $\mathbf{x}^{(0)}$:

$$\text{Solve } (\mathbf{A} - \mathcal{R}_A(\mathbf{x}^{(i)})\mathbf{I})\mathbf{x}^{(i+1)} = \mathbf{e}_1, \quad (2.3)$$

where \mathbf{e}_1 denotes the first natural coordinate vector, i. e., the first column of the identity matrix and $\mathbf{x}^{(i)}$ and $\mathbf{x}^{(i+1)}$ denote the current and next iterate, respectively. In fact, Lord Rayleigh considered the generalised eigenvalue problem and so in his text, the iteration reads

$$\text{Solve } (\mathbf{A} - \mathcal{R}_A(\mathbf{x}^{(i)})\mathbf{M})\mathbf{x}^{(i+1)} = \mathbf{e}_1.$$

1949 — Kohn In a letter to the editor Walter Kohn [13] suggest the following iteration

$$\text{Solve } (\mathbf{A} - \mathcal{R}_A(\mathbf{x}^{(i)})\mathbf{I})\mathbf{x}^{(i+1)} = \mathbf{e}_k,$$

where \mathbf{e}_k is *any* of the natural coordinate vectors. Without a rigorous proof Kohn argues that $\mathcal{R}_A(\mathbf{x}^{(i)})$ converges quadratically to an eigenvalue of \mathbf{A} (provided that $\mathbf{x}^{(0)}$ is sufficiently close to an eigenvector of \mathbf{A}). Despite the similarity to (2.3), Kohn does not mention Lord Rayleigh’s method and it is not known whether or not he was aware of it.

1951 — Crandall In a text communicated to the Royal society of London Stephen Crandall [4] suggests

$$\text{Solve } (\mathbf{A} - \mathcal{R}_\mathbf{A}(\mathbf{x}^{(i)})\mathbf{I})\mathbf{x}^{(i+1)} = \mathbf{x}^{(i)} . \quad (2.4)$$

Actually, Crandall also considered the generalised eigenproblem but for our comparative purposes it is sufficient to consider the case $\mathbf{M} = \mathbf{I}$. Note, that this algorithm is RQI without the normalisation step. Based on the assumption that the sequence of vectors $\mathbf{x}^{(k)}$ converges, Crandall establishes cubic convergence in the this sequence and the approximate eigenvalue sequence. To see why the assumption is wrong, we assume the contrary, i. e., suppose that the sequence converges to an eigenvector, say \mathbf{v}_k . From (2.4) we have

$$\mathbf{A}\mathbf{v}_k - \mathcal{R}_\mathbf{A}(\mathbf{v}_k)\mathbf{v}_k = \mathbf{v}_k \quad \Leftrightarrow \quad \mathbf{A}\mathbf{v}_k = (1 + \mathcal{R}_\mathbf{A}(\mathbf{v}_k))\mathbf{v}_k ,$$

and so \mathbf{v}_k is an eigenvector of \mathbf{A} with corresponding eigenvalue $1 + \mathcal{R}_\mathbf{A}(\mathbf{v}_k)$. Since we know that for any eigenvector, the value of $\mathcal{R}_\mathbf{A}(\mathbf{v}_k)$ is the eigenvalue it belongs to, this implies

$$\mathcal{R}_\mathbf{A}(\mathbf{v}_k) = 1 + \mathcal{R}_\mathbf{A}(\mathbf{v}_k)$$

which is a contradiction.

Also, Crandall establishes what is usually referred to as r -cubic convergence. This is a weaker notion of convergence than the one defined earlier, which is called q -cubic convergence (see [31, Appendix A.1] for a detailed definition of these notions of convergence).

1957 – 59 — Ostrowski Alexander Ostrowski published a series of six papers titled “On the Convergence of the Rayleigh Quotient Iteration for the Computation of the Characteristic Roots and Vectors. I–VI” [15–20]. We mention the titles here, as they represent the first mention of the term

Rayleigh Quotient Iteration.

In the first paper the author suggests the iteration

$$\text{Solve } (\mathbf{A} - \mathcal{R}_{\mathbf{A}}(\mathbf{x}^{(i)})\mathbf{I})\mathbf{x}^{(i+1)} = \boldsymbol{\eta}, \quad \boldsymbol{\eta} \neq \mathbf{0}. \quad (2.5)$$

He rigorously establishes a *quadratic* convergence rate for the sequence of Rayleigh Quotients $\mathcal{R}_{\mathbf{A}}(\mathbf{x}^{(i)})$. He then refers to a paper of Wielandt [33] and his *fractional* or *broken iteration* (German: *gebrochene Iteration*). Inspired by Wielandt's method he suggests replacing the fixed vector $\boldsymbol{\eta}$ in the right hand side of (2.5) to the solution from the previous step

$$(\mathbf{A} - \mathcal{R}_{\mathbf{A}}(\mathbf{x}^{(i)})\mathbf{I})\mathbf{x}^{(i+1)} = \mathbf{x}^{(i)}, \quad (2.6)$$

starting with an arbitrary non-zero vector $\mathbf{x}^{(0)}$. He then gives a rigorous proof of the local *cubic* convergence of the sequence of Rayleigh quotients $\mu_i := \mathcal{R}_{\mathbf{A}}(\mathbf{x}^{(i)})$, i. e.,

$$\frac{\mu_{i+1} - \lambda}{(\mu_i - \lambda)^3} \longrightarrow \gamma \quad \text{as } i \rightarrow \infty, \quad (2.7)$$

where λ is an eigenvalue of \mathbf{A} and γ is a positive constant. Local convergence here means that $\mathbf{x}^{(0)}$ is assumed to be near the eigenvector corresponding to λ .

Note that (2.6) is the same algorithm previously proposed by Crandall given in Equation (2.4). Ostrowski was not aware of Crandall's method; however, while the first paper was in press the following note was added:

“Professor G. Forsythe has directed my attention to a paper by S. H. Crandall [...]. In particular, Professor Crandall establishes the *cubic character* of convergence of ξ_x in the rule (28), (29). However he does not arrive at our asymptotic formula (46), which

is the principal result of our paper.” [15, p. 241].³

In the beginning of the second paper [16] Ostrowski discusses this in more detail and remarks that Crandall proofed the r -cubic convergence of the sequence of eigenvalue iterates, while he showed q -cubic convergence.

More importantly, he also points out in §21 of the text that in order to assure convergence in the vector iterates (and not just the Rayleigh Quotients) one needs to normalise the vectors. With this small yet important modification of Crandall’s algorithm he fully defined RQI as it is known today.

The third paper [17] of the series addresses the non-symmetric case for which Ostrowski is also able to define a method that attains local cubic convergence. This method uses a generalised notion of the Rayleigh quotient and comes at the expense of solving two linear systems at each step instead of one. The remaining papers are also mainly concerned with the non-symmetric and non-Hermitian case and are thus not of particular interest for this thesis.

This concludes the overview of the development of RQI from Lord Rayleigh’s iteration that lacks the changing right hand side and the normalisation of the vector iterate to the complete definition of RQI by Ostrowski.

2.2.2 Further developments and recent contributions

We now give an overview of the developments and contributions after the introduction of RQI in 1958. We also look at some recent contributions.

After Ostrowski’s proof of the local cubic convergence, it took another ten years until a first important result concerning the *global* convergence behaviour of RQI was presented. In 1968 Parlett and Kahan [24] showed that RQI applied to symmetric matrices converges for almost all starting vectors and in 1974 Parlett [22] generalised the result for the case when \mathbf{A} is

³Here, ξ_x denotes the x -th iterate of the approximate eigenvector, i. e., in our notation $\mathbf{x}^{(x)}$. The rule (28), (29) in Ostrowski’s paper corresponds to our equation (2.6) and the asymptotic formula (46) he references is given in (2.7).

normal. A slightly more concise version of the proof has been again published in Parlett's book [23].

Of course, not only is it of interest *that* the method converges but also *which* eigenpair it converges to. The following example demonstrates that the convergence behaviour of RQI might sometimes be unexpected.

Example 2.5. This example is based on an example from [21, p. 254]. Let $\mathbf{A} = \text{diag}(1, 2, 4)$ with eigenvalues $\lambda_1 = 1$, $\lambda_2 = 2$, $\lambda_3 = 4$ and corresponding eigenvectors \mathbf{e}_i , the columns of the identity matrix.

(a) First consider RQI started with the vector

$$\mathbf{x}^{(0)} = \begin{pmatrix} 0.8163392507169525 \\ -0.0004821161298470036 \\ 0.5775725022046341 \end{pmatrix}.$$

This produces the eigenpair $(1, \mathbf{e}_1)$ although

$$\mathcal{R}_{\mathbf{A}}(\mathbf{x}^{(0)}) = 2.000770218344729.$$

Note, however, that computing the angle between $\mathbf{x}^{(0)}$ and the eigenvectors gives

$$\angle(\mathbf{x}^{(0)}, \mathbf{e}_1) \approx 0.61575, \quad \angle(\mathbf{x}^{(0)}, \mathbf{e}_2) \approx 1.57128, \quad \angle(\mathbf{x}^{(0)}, \mathbf{e}_3) \approx 0.95504,$$

that is, the angle between the initial vector and the resulting eigenvector is smallest.

(b) Now take

$$\mathbf{x}^{(0)} = (0.74278, 0.55709, 0.37139)^\top$$

the angles are

$$\angle(\mathbf{x}^{(0)}, \mathbf{e}_1) \approx 0.73358, \quad \angle(\mathbf{x}^{(0)}, \mathbf{e}_2) \approx 0.97992, \quad \angle(\mathbf{x}^{(0)}, \mathbf{e}_3) \approx 1.19029$$

and the initial shift is $\mathcal{R}_A(\mathbf{x}^{(0)}) \approx 1.7241$. In this case, RQI converges to the eigenpair $(2, \mathbf{e}_2)$, i. e., not the eigenvector that has the smallest angle with $\mathbf{x}^{(0)}$ but rather the one that corresponds to the eigenvalue to which the initial shift is closest.

This example shows that there seems to be no obvious way how the computed eigenpair depends on $\mathbf{x}^{(0)}$ or $\mathcal{R}_A(\mathbf{x}^{(0)})$, and indeed the characterisation of the global convergence behaviour of RQI is not straightforward. In contrast, the local convergence behaviour is better understood. Ostrowski [15] defined explicit estimates of *convergence neighbourhoods* for the shift, i. e., intervals around an eigenvalue in which convergence to this eigenvalue is assured. However, these intervals depend on quantities that are not known beforehand so they are of little practical use.

Efforts have been made to obtain local convergence regions with as little knowledge about the spectrum as possible. For example, Beattie and Fox [2] derive conditions under which convergence is assured to be in a given interval assuming the number of eigenvalues contained in the interval is known. Recently, Rommes [27] derived sharper bounds for local convergence neighbourhoods. He compares RQI to a related algorithm, called the Dominant Pole Algorithm (DPA). Further, he observes that RQI does not take much advantage of the information in the initial vector $\mathbf{x}^{(0)}$. In other words, even if the initial vector is a very good approximation of the wanted eigenvector, RQI might fail. We will come back to this observation in the next chapter.

Szyld [30] suggests combining shifted inverse iteration and RQI to ensure that the computed eigenvalue lies in a given interval. He obtains criteria to switch back and forth between the two algorithms to benefit from their respective advantages (inverse iteration is guaranteed to converge to the nearest eigenvalue but convergence is merely linear; RQI possesses local cubic convergence but the global convergence behaviour is possibly erratic).

The task of identifying global convergence regions in terms of the initial

vector seems to be more difficult. Parlett noted in 1980 that “[t]here appears to be no simple description of how \mathbf{v} depends on $\mathbf{x}^{(0)}$ ” [23, p. 82] and it looks as if this statement still holds true today. Pantazis and Szyld [21] and Batterson and Smillie [1] studied *basins of attraction*, i. e., regions in the unit sphere from which RQI will converge to a specific eigenvector. They did, however, only consider the three-dimensional case.

Besides the unpredictability of the outcome of RQI another major drawback is its high cost. At every iteration a linear system has to be solved and since the system changes at each step one cannot factorise the matrix beforehand as was the case in inverse iteration. There are several obvious possibilities to reduce the cost such as to change the shift only occasionally. Sometimes, inverse iteration is run a fixed number of steps before changing the shift to the Rayleigh Quotient and Szyld’s paper [30] that was mentioned above can also be interpreted as a method that reduces the computational cost for large problems. Another approach that was first studied for inverse iteration is to solve the linear system itself iteratively leading to an *inexact shift-and-invert method*. The use of iterative inner solvers in RQI (for Hermitian matrices) was studied by Simoncini and Eldén in [29] and Notay in [14]. They both analyse how the convergence of RQI is affected by solving the linear systems only approximately. This means at each iteration an approximate solution $\mathbf{y}^{(k)}$ to

$$\left(\mathbf{A} - \mu^{(k)} \mathbf{I}\right) \mathbf{y}^{(k)} = \mathbf{x}^{(k)}$$

is sought that satisfies

$$\left\| \left(\mathbf{A} - \mu^{(k)} \mathbf{I}\right) \mathbf{y}^{(k)} - \mathbf{x}^{(k)} \right\| \leq \tau^{(k)},$$

where $\tau^{(k)}$ is a tolerance that might change at each step. Also [29] shows the equivalence of inexact RQI and another iterative eigenvalue method called the *Jacobi-Davidson method*. This result is extended to the non-Hermitian case by

Freitag and Spence in [6]. They also study how different preconditioners for the linear system can be used and “tuned” to improve the outer convergence. We will briefly come back to the idea of solving the inner system inexactly when discussing our new method in the next chapter.

2.3 Convergence Analysis

We have mentioned on several occasions the local cubic convergence of RQI. In this section we give a proof of this property and we also discuss some results concerning the global convergence behaviour. We do not give a full proof of the global convergence, since parts of it are very technical and, at least for our purposes, it does not give much insight in the method.

As we have seen in the previous section, the first rigorous proof of the cubic convergence of RQI was given by Ostrowski [15] but over time a number of different, simpler proofs were presented. The one we give below follows closely the one given by Demmel [5, pp. 215 sq.].

Theorem 2.6 (Cubic convergence). *Rayleigh Quotient Iteration is locally cubically convergent.*

Before giving the proof, we make some remarks. *Locally* here means that

1. it is assumed that the sequence $(\mathbf{x}^{(i)})_i$ does converge to an eigenvector of \mathbf{A} and
2. there is a finite number of iterations for which convergence might not be cubic (the *preasymptotic phase*). For some $j \in \mathbb{N}$, however, the j -th iterate is a sufficiently good approximation of the target eigenvector, such that the sequence of subsequent iterates does converge cubically.

We defined the notion of cubic convergence in the first chapter, nonetheless we remark again here that this means the number of correct digits *triples* at

each step once the error is small enough. And even if the method might not converge cubically from the beginning, in practice the preasymptotic phase rarely takes more than three steps.

Citation
[Parlett]

Some of the proofs in the literature are given under the assumption that \mathbf{A} is diagonal. To see why no generality is lost with this assumption, consider the eigendecomposition of \mathbf{A} and write $\mathbf{Q}^\top \mathbf{A} \mathbf{Q} = \mathbf{\Lambda}$, where \mathbf{Q} is an orthogonal matrix consisting of the eigenvectors of \mathbf{A} as its columns and $\mathbf{\Lambda} = \text{diag}(\lambda_1, \dots, \lambda_n)$ is the diagonal matrix of eigenvalues. We discard the superscripts for a moment and change variables in RQI⁴ to $\hat{\mathbf{x}} := \mathbf{Q}^\top \mathbf{x}$ and $\hat{\mathbf{y}} := \mathbf{Q}^\top \mathbf{y}$. Then

$$\mu^{(i)} = \mu = \mathcal{R}_{\mathbf{A}}(\mathbf{x}) = \frac{\mathbf{x}^\top \mathbf{A} \mathbf{x}}{\mathbf{x}^\top \mathbf{x}} = \frac{\hat{\mathbf{x}}^\top \mathbf{Q}^\top \mathbf{A} \mathbf{Q} \hat{\mathbf{x}}}{\hat{\mathbf{x}}^\top \mathbf{Q}^\top \mathbf{Q} \hat{\mathbf{x}}} = \frac{\hat{\mathbf{x}}^\top \mathbf{\Lambda} \hat{\mathbf{x}}}{\hat{\mathbf{x}}^\top \hat{\mathbf{x}}} = \mathcal{R}_{\mathbf{\Lambda}}(\hat{\mathbf{x}}) = \mathcal{R}_{\mathbf{\Lambda}}(\hat{\mathbf{x}}^{(i)}),$$

and $\mathbf{Q} \hat{\mathbf{y}}^{(i+1)} = (\mathbf{A} - \mu^{(i)} \mathbf{I})^{-1} \mathbf{Q} \hat{\mathbf{x}}^{(i)}$. Hence,

$$\hat{\mathbf{y}}^{(i+1)} = \mathbf{Q}^\top (\mathbf{A} - \mu^{(i)} \mathbf{I})^{-1} \mathbf{Q} \hat{\mathbf{x}}^{(i)} = (\mathbf{Q}^\top \mathbf{A} \mathbf{Q} - \mu^{(i)} \mathbf{I})^{-1} \hat{\mathbf{x}}^{(i)} = (\mathbf{\Lambda} - \mu^{(i)} \mathbf{I})^{-1} \hat{\mathbf{x}}^{(i)},$$

where we used $\mathbf{Q}^\top = \mathbf{Q}^{-1}$, the orthogonality of \mathbf{Q} . We see that running RQI with \mathbf{A} and $\mathbf{x}^{(0)}$ is equivalent to running RQI with $\mathbf{\Lambda}$ and $\hat{\mathbf{x}}^{(0)}$. Thus, we assume that $\mathbf{A} = \mathbf{\Lambda}$ is already diagonal which in particular implies that the eigenvectors of \mathbf{A} are \mathbf{e}_i , the natural coordinate vectors.

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Proof of Theorem 2.6. Suppose without loss of generality that $\mathbf{x}^{(i)}$ converges to \mathbf{e}_1 . Remember that we assume that the current iterate is a sufficiently good estimate of \mathbf{e}_1 , such that for some i we can write $\mathbf{x}^{(i)} = \mathbf{e}_1 + \mathbf{d}^{(i)}$ with $\|\mathbf{d}^{(i)}\| = \epsilon \ll 1$. To show cubic convergence, we have to verify that

$$\lim_{i \rightarrow \infty} \frac{\|\mathbf{x}^{(i+1)} - \mathbf{e}_1\|}{\|\mathbf{x}^{(i)} - \mathbf{e}_1\|^3} < M,$$

⁴Recall the notation from Algorithm 2.4 where $\mathbf{y} = \mathbf{y}^{(i)}$ denotes the unnormalised i -th iterate and $\mathbf{x} = \mathbf{x}^{(i)}$ denotes the same iterate after normalisation.

for some positive constant M . We know that $\|\mathbf{x}^{(i)} - \mathbf{e}_1\|^3 = \epsilon^3$, hence it suffices to show that $\|\mathbf{x}^{(i+1)} - \mathbf{e}_1\| = \mathcal{O}(\epsilon^3)$. In other words we have to show that $\mathbf{x}^{(i+1)} = \mathbf{e}_1 + \mathbf{d}^{(i+1)}$ with $\|\mathbf{d}^{(i+1)}\| = \mathcal{O}(\epsilon^3)$.

Since the vectors are normalised at each step we have

$$\begin{aligned} 1 &= (\mathbf{x}^{(i)})^\top (\mathbf{x}^{(i)}) = (\mathbf{e}_1 + \mathbf{d}^{(i)})^\top (\mathbf{e}_1 + \mathbf{d}^{(i)}) = \mathbf{e}_1^\top \mathbf{e}_1 + 2\mathbf{e}_1^\top \mathbf{d}^{(i)} + (\mathbf{d}^{(i)})^\top \mathbf{d}^{(i)} \\ &= 1 + 2d_1^{(i)} + \epsilon^2. \end{aligned}$$

where $d_1^{(i)}$ denotes the first component of the vector $\mathbf{d}^{(i)}$. Rewriting gives $d_1^{(i)} = -\epsilon^2/2$ and using the symmetry⁵ of $\mathbf{\Lambda}$ we obtain

$$\begin{aligned} \mu^{(i)} &= (\mathbf{x}^{(i)})^\top \mathbf{\Lambda} \mathbf{x}^{(i)} = (\mathbf{e}_1 + \mathbf{d}^{(i)})^\top \mathbf{\Lambda} (\mathbf{e}_1 + \mathbf{d}^{(i)}) \\ &= \mathbf{e}_1^\top \mathbf{\Lambda} \mathbf{e}_1 + 2\mathbf{e}_1^\top \mathbf{\Lambda} \mathbf{d}^{(i)} + (\mathbf{d}^{(i)})^\top \mathbf{\Lambda} \mathbf{d}^{(i)} = \lambda_1 - \eta, \end{aligned}$$

where $\eta := -2\mathbf{e}_1^\top \mathbf{\Lambda} \mathbf{d}^{(i)} - (\mathbf{d}^{(i)})^\top \mathbf{\Lambda} \mathbf{d}^{(i)} = \lambda_1 \epsilon^2 - (\mathbf{d}^{(i)})^\top \mathbf{\Lambda} \mathbf{d}^{(i)}$. Using the fact that the spectral norm of a symmetric matrix is equal to its spectral radius, i.e., the absolute value of the largest eigenvalue λ_{\max} , we can bound $|\eta|$ as follows

$$|\eta| \leq |\lambda_1| \epsilon^2 + \|\mathbf{\Lambda}\| \|\mathbf{d}^{(i)}\|^2 \leq |\lambda_{\max}| \epsilon^2 + \|\mathbf{\Lambda}\| \epsilon^2 = 2\|\mathbf{\Lambda}\| \epsilon^2 \quad (2.8)$$

and we see that $\mu^{(i)} = \lambda_1 - \eta = \lambda_1 + \mathcal{O}(\epsilon^2)$ (note that this proves Lemma 2.3).

⁵For a symmetric matrix $\mathbf{B} = \mathbf{B}^\top$ holds

$$\mathbf{u}^\top \mathbf{B} \mathbf{w} = (\mathbf{u}^\top \mathbf{B} \mathbf{w})^\top = \mathbf{w}^\top (\mathbf{u}^\top \mathbf{B})^\top = \mathbf{w}^\top \mathbf{B}^\top \mathbf{u} = \mathbf{w}^\top \mathbf{B} \mathbf{u}.$$

We obtain

$$\begin{aligned}
 \mathbf{y}^{(i+1)} &= (\mathbf{\Lambda} - \mu^{(i)})^{-1} \mathbf{x}^{(i)} \\
 &= \left(\frac{x_1^{(i)}}{\lambda_1 - \mu^{(i)}}, \frac{x_2^{(i)}}{\lambda_2 - \mu^{(i)}}, \dots, \frac{x_n^{(i)}}{\lambda_n - \mu^{(i)}} \right)^\top \quad (\text{since } (\mathbf{\Lambda} - \mu^{(i)} \mathbf{I})^{-1} = \text{diag} \left(\frac{1}{(\lambda_j - \mu^{(i)})} \right)) \\
 &= \left(\frac{1 + d_1^{(i)}}{\lambda_1 - \mu^{(i)}}, \frac{d_2^{(i)}}{\lambda_2 - \mu^{(i)}}, \dots, \frac{d_n^{(i)}}{\lambda_n - \mu^{(i)}} \right)^\top \quad (\text{since } \mathbf{x}^{(i)} = \mathbf{e}_1 + \mathbf{d}^{(i)}) \\
 &= \left(\frac{1 - \epsilon^2/2}{\eta}, \frac{d_2^{(i)}}{\lambda_2 - \lambda_1 + \eta}, \dots, \frac{d_n^{(i)}}{\lambda_n - \lambda_1 + \eta} \right)^\top \quad (\text{since } \mu^{(i)} = \lambda_1 - \eta, d_1^{(i)} = -\epsilon^2/2) \\
 &= \frac{1 - \epsilon^2/2}{\eta} \left(1, \frac{d_2^{(i)} \eta}{(1 - \epsilon^2/2)(\lambda_2 - \lambda_1 + \eta)}, \dots, \frac{d_n^{(i)} \eta}{(1 - \epsilon^2/2)(\lambda_n - \lambda_1 + \eta)} \right)^\top \\
 &=: \frac{1 - \epsilon^2/2}{\eta} (\mathbf{e}_1 + \hat{\mathbf{d}}^{(i+1)}).
 \end{aligned}$$

If we denote by δ the gap between λ_1 and the rest of the spectrum, i.e.,

$$\delta := \min_{j=2}^n |\lambda_j - \lambda_1|,$$

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we can bound the denominators of $\hat{\mathbf{d}}^{(i+1)}$ using $|\lambda_j - \lambda_1 + \eta| \geq \delta - |\eta|$, and in conjunction with (2.8) we get

$$\|\hat{\mathbf{d}}^{(i+1)}\| \leq \frac{\|\mathbf{d}^{(i)}\| |\eta|}{(1 - \epsilon^2/2)(\delta - |\eta|)} \leq \frac{2\|\mathbf{\Lambda}\|\epsilon^3}{(1 - \epsilon^2/2)(\delta - 2\|\mathbf{\Lambda}\|\epsilon^2)}$$

or $\|\hat{\mathbf{d}}^{(i+1)}\| = \mathcal{O}(\epsilon^3)$. Finally, since $\mathbf{x}^{(i+1)} = \mathbf{e}_1 + \mathbf{d}^{(i+1)} = \mathbf{y}^{(i+1)} / \|\mathbf{y}^{(i+1)}\|$ and

$$\frac{\mathbf{y}^{(i+1)}}{\|\mathbf{y}^{(i+1)}\|} = \frac{\frac{1-\epsilon^2/2}{\eta} (\mathbf{e}_1 + \hat{\mathbf{d}}^{(i+1)})}{\left\| \frac{1-\epsilon^2/2}{\eta} (\mathbf{e}_1 + \hat{\mathbf{d}}^{(i+1)}) \right\|} = \frac{\mathbf{e}_1 + \hat{\mathbf{d}}^{(i+1)}}{\|\mathbf{e}_1 + \hat{\mathbf{d}}^{(i+1)}\|}$$

we see that also $\mathbf{d}^{(i+1)} = \mathcal{O}(\epsilon^3)$, which concludes the proof. \square

We see that the property that the Rayleigh Quotient yields quadratically accurate approximations of eigenvalues is indeed crucial in the derivation of the cubic convergence. Some other proofs, for example the one given by Parlett [23, p. 77], proof convergence of the *error angle* $\phi^{(k)} = \angle(\mathbf{x}^{(k)}, \mathbf{v})$, i. e., he shows

$$\lim_{k \rightarrow \infty} \left| \frac{\phi^{(k+1)}}{(\phi^{(k)})^3} \right| \leq 1.$$

In some texts that study inverse iteration in a more particularised fashion, cubic convergence is proofed by combining the quadratic accuracy of the Rayleigh Quotient together with convergence results from inverse iteration (since a single step of RQI is equivalent to a single step of inverse iteration with the Rayleigh quotient of the current iterate vector chosen as the shift), see for example [32, p. 208] or [3, pp. 89 sq.].

To conclude this chapter we briefly discuss some of the results concerning the global convergence behaviour of RQI. Essential for showing that RQI is globally convergent is the following fact which, according to Parlett [23, p. 85], is due to Kahan [24]. We recall that $\mathbf{r}^{(k)}$ denotes the residual at step k in RQI, i. e.,

$$\mathbf{r}^{(k)} = (\mathbf{A} - \mu^{(k)} \mathbf{I}) \mathbf{x}^{(k)}.$$

Lemma 2.7 (Monotonic residuals). *For every k it holds*

$$\|\mathbf{r}^{(k+1)}\| \leq \|\mathbf{r}^{(k)}\|.$$

Before giving the proof, we note that we can relate the k -th and $k + 1$ -th iterate of RQI by

$$\mathbf{x}^{(k)} = \beta (\mathbf{A} - \mu^{(k)} \mathbf{I}) \mathbf{x}^{(k+1)},$$

for some β which implies

$$\begin{aligned} \left| \left(\mathbf{x}^{(k)} \right)^* \left(\mathbf{A} - \mu^{(k)} \mathbf{I} \right) \mathbf{x}^{(k+1)} \right| &= \left| \beta^{-1} \left(\mathbf{x}^{(k)} \right)^* \mathbf{x}^{(k)} \right| \\ &= |\beta^{-1}| \left\| \mathbf{x}^{(k)} \right\| \\ &= |\beta^{-1}| \left\| \beta \left(\mathbf{A} - \mu^{(k)} \mathbf{I} \right) \mathbf{x}^{(k+1)} \right\| \end{aligned}$$

and thus

$$\left\| \left(\mathbf{A} - \mu^{(k)} \mathbf{I} \right) \mathbf{x}^{(k+1)} \right\| = \left| \left(\mathbf{x}^{(k)} \right)^* \left(\mathbf{A} - \mu^{(k)} \mathbf{I} \right) \mathbf{x}^{(k+1)} \right|. \quad (2.9)$$

Proof of Lemma 2.7.

$$\begin{aligned} \left\| \mathbf{r}^{(k+1)} \right\| &= \left\| \left(\mathbf{A} - \mu^{(k+1)} \mathbf{I} \right) \mathbf{x}^{(k+1)} \right\| \\ &\leq \left\| \left(\mathbf{A} - \mu^{(k)} \mathbf{I} \right) \mathbf{x}^{(k+1)} \right\| && \text{(Since } \mu^{(k+1)} \text{ minimises the residual norm)} \\ &= \left| \left(\mathbf{x}^{(k)} \right)^* \left(\mathbf{A} - \mu^{(k)} \mathbf{I} \right) \mathbf{x}^{(k+1)} \right| && \text{(by (2.9))} \\ &\leq \left\| \left(\mathbf{x}^{(k)} \right)^* \left(\mathbf{A} - \mu^{(k)} \mathbf{I} \right) \right\| \left\| \mathbf{x}^{(k+1)} \right\| && \text{(by the Cauchy-Schwarz inequality)} \\ &= \left\| \left(\mathbf{x}^{(k)} \right)^* \left(\mathbf{A} - \mu^{(k)} \mathbf{I} \right) \right\| && \text{(since } \mathbf{x}^{(k+1)} \text{ is a unit vector)} \\ &= \left\| \left(\mathbf{A} - \mu^{(k)} \mathbf{I} \right) \mathbf{x}^{(k)} \right\| && \text{(since } \mathbf{A} \text{ is symmetric)} \\ &= \left\| \mathbf{r}^{(k)} \right\|. \end{aligned}$$

□

Theorem 2.8 (Global convergence of RQI). *Let the RQI be applied to a normal matrix started with an arbitrary unit vector $\mathbf{x}^{(0)}$. Then, as $k \rightarrow \infty$, the eigenvalue sequence $\mu^{(k)}$ converges and either*

1. $(\mu^{(k)}, \mathbf{x}^{(k)})$ converges to an eigenpair (λ, \mathbf{v}) , or
2. the sequence $\mu^{(k)}$ converges to $(\lambda_p + \lambda_q)/2$ and $\mathbf{x}^{(k)}$ oscillates between vectors converging to \mathbf{v}_{pq}^+ and vectors converging to \mathbf{v}_{pq}^- , where $\mathbf{v}_{pq}^\pm =$

$(\mathbf{v}_p \pm \mathbf{q})/\sqrt{2}$, where λ_p and λ_q are eigenvalues of \mathbf{A} with corresponding eigenvectors \mathbf{v}_p and \mathbf{v}_q .

The latter is unstable under perturbations of $\mathbf{x}^{(k)}$.

As mentioned above, we do not give a complete proof of this result; below we outline a rough sketch of the first statement based on the proof by Parlett in [23].

We begin by observing that the monotonicity of the residuals implies

$$\|\mathbf{r}^{(k)}\| \rightarrow \tau \geq 0 \quad \text{as } k \rightarrow \infty.$$

Now, note that the sequence of vector iterates $\mathbf{x}^{(k)}$ is confined in the unit sphere, a compact subset of \mathbb{R}^n . One can also show that the sequence of the Rayleigh Quotients $\mathcal{R}_\mathbf{A}(\mathbf{x}^{(k)})$ is confined in a compact set and thus, the sequence $(\mathcal{R}_\mathbf{A}(\mathbf{x}^{(k)}), \mathbf{x}^{(k)})_{k \in \mathbb{N}}$ has at least one limit point. Call this point (ρ, \mathbf{z}) . This point is the limit of a subsequence $(\mathcal{R}_\mathbf{A}(\mathbf{x}^{(j)}), \mathbf{x}^{(j)})_{j \in \mathcal{J}}$ for some index set \mathcal{J} . Using the fact that the Rayleigh Quotient is a continuous function on the unit sphere we see that

$$\mathcal{R}_\mathbf{A}(\mathbf{z}) = \lim_j \mathcal{R}_\mathbf{A}(\mathbf{x}^{(j)}) = \rho$$

and thus

$$\|(\mathbf{A} - \rho)\mathbf{z}\| = \lim_j \|\mathbf{r}^{(j)}\| = \tau,$$

where the limits are for $j \rightarrow \infty$ in \mathcal{J} . If we assume $\tau = 0$, this shows that (ρ, \mathbf{z}) must be an eigenpair of \mathbf{A} . Parlett then proceeds to use the local convergence theorem to conclude that indeed $\lim_{k \rightarrow \infty} \mathbf{x}^{(k)} = \mathbf{z}$.

The second case $\tau > 0$ is much harder to analyse and does also require a number of auxiliary results relating the eigenvectors of a matrix \mathbf{A} to its square \mathbf{A}^2 . Therefore, as mentioned above, we do not discuss this part of the

proof here.

Parlett states in [23, p. 61] and in [22, p. 680] that RQI converges for almost all starting vectors but Batterson and Smillie claim that this assertion is not proved [1, p. 625]. They proceed to give a proof of this fact which is formulated in their paper as follows.

Theorem 2.9. *The set of unit vectors for which RQI does not converge to an eigenvector is a set of measure zero.*

Concluding
remarks

3 Complex Rayleigh Quotient Iteration

In this chapter we introduce *Complex Rayleigh Quotient Iteration* (CRQI¹). This is a novel shift-and-invert algorithm similar to classic RQI. Numerical experiments suggest that this new method overcomes some of the disadvantages of classic RQI. In particular, it seems to perform well in cases when there are eigenvalues very close to the target eigenvalue but a good approximation of the eigenvector is known.

3.1 Motivation

As was the case in the previous chapters we fix a real symmetric matrix $\mathbf{A} \in \mathbb{R}^{n \times n}$. Recall that since the eigenvectors $\mathbf{v}_1, \dots, \mathbf{v}_n$ of \mathbf{A} form an orthonormal basis of \mathbb{R}^n we can write every $\mathbf{u} \in \mathbb{R}^n$ as

$$\mathbf{u} = \sum_{i=1}^n \alpha_i \mathbf{v}_i$$

for certain $\alpha_1, \dots, \alpha_n \in \mathbb{R}$. Suppose now, that \mathbf{u} is a good approximation for one of the eigenvectors, say for \mathbf{v}_k . Then

$$\alpha_k \approx 1 \quad \text{and} \quad \alpha_j \approx 0 \quad \text{for } j \neq k.$$

¹We abbreviate the classic Rayleigh Quotient Iteration that was discussed in the previous chapter by *RQI* or *classic RQI* and the method introduced in this chapter by *CRQI*.

Due to the pairwise orthogonality of the eigenvectors this implies

$$\mathbf{u}^\top \mathbf{v}_j \approx \begin{cases} 1 & \text{if } j = k, \\ 0 & \text{if } j \neq k. \end{cases} \quad (3.1)$$

As already mentioned previously, when using classic RQI even good approximations of eigenvectors can lead to convergence to the wrong eigenpair when the gap between the target eigenvalue and eigenvalues nearby is very small. We will illustrate this behaviour in different examples in the next section. There, we will see that the reason for this seems to be that classic RQI does not “incorporate” the information in the initial vector. The main purpose of complex RQI is to fix this, i.e., to alter classic RQI in such a way that for sufficiently good approximations of eigenvectors convergence to this very eigenvector is guaranteed.

To that end, the linear system that is solved at each step in RQI is perturbed in such a way that the wanted eigenvalue gets “isolated”. Of course this perturbed linear system will lead to wrong solutions and so we will decrease this perturbation successively until we arrive at the unperturbed problem.

Explain a bit more

We make use of the fact that all eigenvalues of \mathbf{A} are real and perturb the matrix in such a way that the eigenvalues are “raised” into the complex plane. Of course, we do not want to raise them all equally but rather in such a way that the Euclidean distance between the target eigenvalue and the other eigenvalue is increased. This is done by incorporating the approximation \mathbf{u} of the target eigenvector \mathbf{v}_k into the perturbed matrix. Let

$$\tilde{\mathbf{A}} := \mathbf{A} - \gamma i (\mathbf{I} - \mathbf{u}\mathbf{u}^\top), \quad (3.2)$$

where $\gamma > 0$ is positive real number and i denotes the imaginary unit. Note that the matrix $\mathbf{I} - \mathbf{u}\mathbf{u}^\top$ defines the orthogonal projection onto the span of \mathbf{u} . Therefore, a vector \mathbf{x} that is almost parallel to \mathbf{u} will barely see the

imaginary part $\gamma i(\mathbf{I} - \mathbf{u}\mathbf{u}^\top)$ when multiplied with $\tilde{\mathbf{A}}$ and so $\tilde{\mathbf{A}}\mathbf{x} \approx \mathbf{A}\mathbf{x}$. If, however, the vector \mathbf{x} is almost perpendicular to \mathbf{u} we have

$$\tilde{\mathbf{A}}\mathbf{x} = \mathbf{A}\mathbf{x} - \gamma i\mathbf{x} - \underbrace{\mathbf{u}\mathbf{u}^\top\mathbf{x}}_{\approx 0} \approx (\mathbf{A} - \gamma i\mathbf{I})\mathbf{x}. \quad (3.3)$$

Since \mathbf{u} approximates \mathbf{v}_k , the orthogonal complement of the span of \mathbf{u} approximates the orthogonal complement of the span of \mathbf{v}_k . Note that the latter is the subspace spanned by the remaining eigenvectors. Therefore, we expect that the eigenvectors of $\tilde{\mathbf{A}}$ are similar to those of \mathbf{A} and that the eigenvalues corresponding to eigenvectors \mathbf{v}_j , $j \neq k$ to approximately be $\lambda_j - \gamma i$ due to (3.3). The eigenvalue corresponding to \mathbf{v}_k would then be approximately equal to λ_k since $\tilde{\mathbf{A}}\mathbf{v}_k \approx \mathbf{A}\mathbf{v}_k = \lambda_k\mathbf{v}_k$.

To make this intuition more quantitative, we first need the following result where we replace \mathbf{u} by the exact target eigenvector \mathbf{v}_k . The proofs for the following results can be found in Appendix A.

Lemma 3.1. *The matrix*

$$\tilde{\mathbf{A}}_{(0)} := \mathbf{A} - \gamma i(\mathbf{I} - \mathbf{v}_k\mathbf{v}_k^\top) \quad (3.4)$$

has the same eigenvectors as \mathbf{A} with corresponding eigenvalues $\lambda_j(\tilde{\mathbf{A}}_{(0)}) = \lambda_j(\mathbf{A}) - \gamma i$ for $j \neq k$ and $\lambda_k(\tilde{\mathbf{A}}_{(0)}) = \lambda_k(\mathbf{A})$.

To derive estimations for the eigenvalues of $\tilde{\mathbf{A}}$, we decompose it into the sum $\tilde{\mathbf{A}} = \tilde{\mathbf{A}}_{(0)} + \tilde{\mathbf{A}}_{(1)}$, where $\tilde{\mathbf{A}}_{(0)}$ is defined in (3.4) and $\tilde{\mathbf{A}}_{(1)}$ is given by

$$\tilde{\mathbf{A}}_{(1)} := \gamma i(\mathbf{u}\mathbf{u}^\top - \mathbf{v}_k\mathbf{v}_k^\top). \quad (3.5)$$

Since \mathbf{u} approximates \mathbf{v}_k we expect the effect on the eigenvalues of $\tilde{\mathbf{A}}_{(0)}$ due to the perturbation $\tilde{\mathbf{A}}_{(1)}$ to be small. The following lemma answers how “big” this perturbation is.

Replace
effect

Lemma 3.2. *Let $\tilde{\mathbf{A}}_{(1)}$ be the matrix defined in Equation (3.5). Then*

$$\|\tilde{\mathbf{A}}_{(1)}\| = \gamma \sqrt{1 - \langle \mathbf{u}, \mathbf{v}_k \rangle^2}, \quad (3.6)$$

where $\|\cdot\|$ denotes the spectral norm of a matrix.

For good approximations \mathbf{u} we have $\langle \mathbf{u}, \mathbf{v}_k \rangle^2 \approx 1$ and thus, if γ is sufficiently small, $\|\tilde{\mathbf{A}}_{(1)}\| \ll 1$. We can now estimate the eigenvalues of $\tilde{\mathbf{A}}$.

Proposition 3.3. *The eigenvalues of $\tilde{\mathbf{A}}$ satisfy*

$$\lambda_j(\tilde{\mathbf{A}}) = \lambda_j(\mathbf{A}) + \gamma i \left(\langle \mathbf{v}_j, \mathbf{u} \rangle^2 - 1 \right) + \mathcal{O} \left(\|\tilde{\mathbf{A}}_{(1)}\|^2 \right), \quad (3.7)$$

As mentioned above the proof can be found in the Appendix. It uses classic results from analytic perturbation theory. To understand why this matches our intuitive arguments from above we consider the middle part of (3.7). For $j \neq k$ the scalar product is approximately zero and thus, if we ignore the last term of the sum (which is small according to the previous lemma), we get

$$\lambda_j(\tilde{\mathbf{A}}) \approx \lambda_j(\mathbf{A}) - \gamma i.$$

For $j = k$ the middle part is negligible due to the scalar product being approximately one and so $\lambda_k(\tilde{\mathbf{A}}) \approx \lambda_k(\mathbf{A})$. In summary, the eigenvalue corresponding to the wanted eigenvector stays near the real line whereas the remaining eigenvalues are raised into the lower complex half-plane.

If we would use this matrix in RQI, the results would of course not be the target eigenpair but an eigenpair of $\tilde{\mathbf{A}}$. Thus, instead of keeping this matrix fixed, we replace the vector \mathbf{u} by the current iterate $\mathbf{x}^{(k)}$ and the scalar γ by a sequence $\gamma^{(k)}$ that converges to zero. Ideally, in the beginning of the iteration $\gamma^{(k)}$ should be sufficiently large such that the target eigenvalue is properly isolated. As the iterates get closer to the target eigenpair, $\gamma^{(k)}$ should decrease such that in the end $\tilde{\mathbf{A}} \approx \mathbf{A}$. A possibly choice that comes

to mind is the norm of the current residual $\mathbf{r}^{(k)}$ or related quantities such as the square of the residual norm. How the choice of this shift influences the convergence behaviour is discussed in the next first example of Section 3.3. Obviously, we cannot expect this method to attain local cubic convergence. The matrix $\tilde{\mathbf{A}}$ is neither symmetric nor Hermitian but of complex symmetric type. As we will see shortly, however, if good approximations of the wanted eigenvector are used for the initial vector the method often requires merely three or four additional steps compared to classic RQI.

Another problem seems to be that if \mathbf{A} is sparse, $\tilde{\mathbf{A}}$ will in general not be sparse. In fact, the perturbed matrix will quite possibly possess only few, if any, zero entries. This seemingly severe disadvantage will shortly be resolved. We will see that it is in fact not necessary to perturb the matrix by $\gamma i(\mathbf{I} - \mathbf{u}\mathbf{u}^\top)$. It suffices to subtract from \mathbf{A} the diagonal matrix $\gamma i\mathbf{I}$ and the method presented above was merely for motivational purposes. The resulting matrix is still complex symmetric but now only the diagonal entries are altered and sparsity is preserved.

3.2 Implementation

Although we will soon slightly change the matrix $\tilde{\mathbf{A}}$ defined in (3.2) again, we summarise the discussion up to this point in Algorithm 3.4.²

Strictly speaking, this algorithm is not a Rayleigh Quotient Iteration as the matrix changes at each step. Obviously, the method is strongly linked to RQI so we still refer to it as Complex Rayleigh Quotient Iteration. As mentioned above, this is not the final version as we wish to present it. The following lemma allows for a small simplification of the algorithm.

Sign of shift in Algo step should be +?

Lemma 3.5. *Let $\mathbf{A} \in \mathbb{R}^{n \times n}$ be a non-singular real symmetric matrix. Let*

²By $\Re(\mathbf{x})$ we denote the real part of the complex vector \mathbf{x} .

Algorithm 3.4: Complex Rayleigh Quotient Iteration, First Version

Input: Nonzero initial vector $\mathbf{x}^{(0)}$ with $\|\mathbf{x}^{(0)}\| = 1$

begin

```

     $\mu^{(0)} \leftarrow (\mathbf{x}^{(0)})^* \mathbf{A} \mathbf{x}^{(0)}$ 
     $r^{(0)} \leftarrow \|(\mathbf{A} - \mu^{(0)} \mathbf{I}) \mathbf{x}^{(0)}\|$ 
     $\gamma^{(0)} \leftarrow r^{(0)}$ 
    for  $k = 1, 2, \dots$  until convergence do
         $\tilde{\mathbf{A}} \leftarrow \mathbf{A} - \gamma^{(k)} i (\mathbf{I} - \mathbf{x}^{(k)} (\mathbf{x}^{(k)})^*)$ 
        Solve  $(\tilde{\mathbf{A}} - \mu^{(k)} \mathbf{I}) \tilde{\mathbf{x}}^{(k+1)} = \mathbf{x}^{(k)}$ 
         $\mathbf{x}^{(k+1)} \leftarrow \tilde{\mathbf{x}}^{(k+1)} / \|\tilde{\mathbf{x}}^{(k+1)}\|$ 
         $\mu^{(k+1)} \leftarrow (\mathbf{x}^{(k+1)})^* \mathbf{A} \mathbf{x}^{(k+1)}$ 
         $r^{(k+1)} \leftarrow \|(\mathbf{A} - \mu^{(k+1)} \mathbf{I}) \mathbf{x}^{(k+1)}\|$ 
         $\gamma^{(k+1)} \leftarrow r^{(k+1)}$ 
     $\mathbf{x} \leftarrow \Re(\mathbf{x}^{(k+1)})$ 
     $\mathbf{x} \leftarrow \mathbf{x} / \|\mathbf{x}\|$ 

```

$\mathbf{u} \in \mathbb{C}^n$ be a unit vector. We define the matrices

$$\mathbf{B} := \mathbf{A} - (\sigma - \gamma i) \mathbf{I} \quad (3.8)$$

and

$$\mathbf{C} := \mathbf{A} - \sigma \mathbf{I} + \gamma i (\mathbf{I} - \mathbf{u} \mathbf{u}^*), \quad (3.9)$$

where i is the imaginary unit and $\sigma, \gamma > 0$ are positive real numbers such that σ is not an eigenvalue of \mathbf{A} . Then

$$\mathcal{R}_{\mathbf{A}}(\mathbf{B}^{-1} \mathbf{u}) = \mathcal{R}_{\mathbf{A}}(\mathbf{C}^{-1} \mathbf{u}). \quad (3.10)$$

Proof. Without loss of generality, we can assume $\sigma = 0$. Otherwise, set $\tilde{\mathbf{A}} = \mathbf{A} - \sigma \mathbf{I}$ and use this matrix instead of \mathbf{A} ($\tilde{\mathbf{A}}$ is obviously still real and symmetric and invertible since σ is not an eigenvalue of \mathbf{A}). First, observe that $\mathbf{C} = \mathbf{B} - \gamma i \mathbf{u} \mathbf{u}^*$. Using the Sherman-Morrison formula [9] and letting

$\alpha := 1 - \gamma i \mathbf{u}^* \mathbf{B}^{-1} \mathbf{u} \in \mathbb{C}$ we obtain

$$\begin{aligned} \mathbf{C}^{-1} \mathbf{u} &= (\mathbf{B} - \gamma i \mathbf{u} \mathbf{u}^*)^{-1} \mathbf{u} \\ &= (\mathbf{B}^{-1} + \alpha^{-1} \mathbf{B}^{-1} \mathbf{u} \gamma i \mathbf{u}^* \mathbf{B}^{-1}) \mathbf{u} \\ &= \mathbf{B}^{-1} \mathbf{u} + \mathbf{B}^{-1} \mathbf{u} \underbrace{\alpha^{-1} \gamma i \mathbf{u}^* \mathbf{B}^{-1} \mathbf{u}}_{\in \mathbb{C}} \\ &= \mathbf{B}^{-1} \mathbf{u} (1 + \alpha^{-1} \gamma i \mathbf{u}^* \mathbf{B}^{-1} \mathbf{u}). \end{aligned}$$

Thus, the vector $\mathbf{C}^{-1} \mathbf{u}$ is a scalar multiple of $\mathbf{B}^{-1} \mathbf{u}$ and the result follows from Lemma 2.2 (i) (the Homogeneity of the Rayleigh Quotient). \square

Immediately, the following result follows.

Corollary 3.6. *Algorithm 3.4 produces the same results when $\tilde{\mathbf{A}}$ is replaced with $\hat{\mathbf{A}} = \mathbf{A} + \gamma i \mathbf{I}$.*

Proof. \square

This result allows for a simplification of the algorithm. We combine the real shift $\mu^{(k)}$ and the imaginary shift $i\gamma^{(k)}$ into a new shift $\sigma^{(k)} := \mu^{(k)} - i\gamma^{(k)}$ and solve the system

$$(\mathbf{A} - \sigma^{(k)} \mathbf{I}) \mathbf{x}^{(k+1)} = \mathbf{x}^{(k)}$$

for $\mathbf{x}^{(k+1)}$ at each step.

3.3 Numerical Experiments

In this section we discuss different numerical examples to better understand the behaviour of CRQI. Throughout the section we will always compare the method to classic RQI. All experiments were executed in Matlab 9. The criterion for convergence was $\|\mathbf{r}^{(k)}\| = \|\mathbf{A} \mathbf{x}^{(k)} - \mu^{(k)} \mathbf{x}^{(k)}\| < 10^{-8}$. The source codes for both classic and complex RQI can be found in the Appendix. The

Where is the non-singularity needed?

Cite matlab

methods are defined slightly differently from the Algorithms given above. They both allow to explicitly set the initial shifts $\mu^{(0)}$ and $\gamma^{(0)}$ to specific values whereas in Algorithm 2.4 and Algorithm 3.4 the initial shifts are always initialised as the Rayleigh Quotient of the initial vector and the initial residual, respectively. In most of the examples below the matrix \mathbf{A} was a randomly generated sparse symmetric 200×200 matrix. To simulate that a good approximation of the initial vector is available we computed the full set of eigenvectors collected as columns of the matrix \mathbf{V} . Next, a weight vector \mathbf{w} of uniformly distributed numbers between 0 and 1 is created. One of the components is set to a higher value than the others, e. g. $w_{50} = 10$ (in most examples the index of the component was also chosen randomly). The initial vector is then set to a weighted linear combination of the eigenvectors, i. e., $\mathbf{x}^{(0)} = \beta \mathbf{V} \mathbf{w}$, where β has to be chosen such that $\mathbf{x}^{(0)}$ is normalised. Now, $\mathbf{x}^{(0)}$ is a vector with a strong component in the direction of the target eigenvector and random (smaller) contributions in the directions of the other eigenvectors.

The first example demonstrates the influence of the imaginary shift $\gamma^{(k)}i$ on the convergence speed. We started by running two versions of CRQI. The first uses $\gamma^{(k)} = \|\mathbf{r}^{(k)}\|$, the second uses the square of the residual norm. A plot of the residuals against the iteration number of both these approaches together with the results using classic RQI³ and a third approach described shortly is given in Figure 3.1.

We observe that in the initial phase of the iteration, the second variant seems to be slower than the first. Although it is not clearly observable in the figure below, further investigation of other examples suggested that during the final steps of the iterations the second version was faster than the first. Consequently, by combining both approaches and thus changing the shift

³Classic RQI is merely included for speed comparison. Since the eigenvalues of the test problem are closely spaced, in almost all of the examples classic RQI failed to converge to the right eigenvalue.

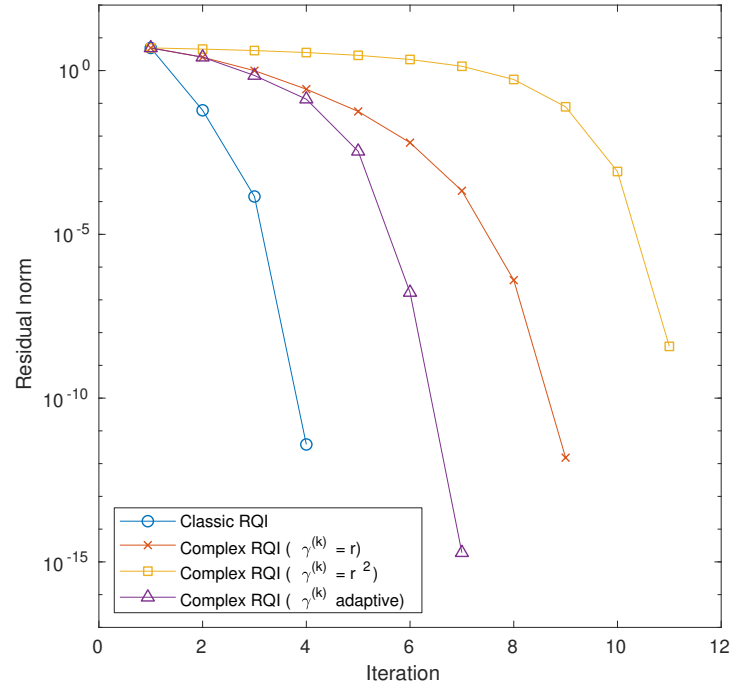


Figure 3.1: Plot of residuals of Classic RQI, Complex RQI with $\gamma^{(k)} = \|\mathbf{r}^{(k)}\|$, Complex RQI with $\gamma^{(k)} = \|\mathbf{r}^{(k)}\|^2$ and Complex RQI with the imaginary shift chosen adaptively (see text). The last variant seems to combine the advantages of the second and third alternatives.

adaptively we expect faster convergence. The results are also plotted in Figure 3.1 and are in accordance with the expectation. In this particular case, the shift was changed according to

$$\gamma = \begin{cases} \|\mathbf{r}\| & \text{if } \|\mathbf{r}\| \geq 1, \\ \|\mathbf{r}\|^2 & \text{if } \|\mathbf{r}\| < 1, \end{cases}$$

where we dropped the superscripts from $\gamma = \gamma^{(k)}$ and $\mathbf{r} = \mathbf{r}^{(k)}$. In the following, when we speak of CRQI we mean CRQI performed with this adaptive choice of imaginary shifts.

Running the same experiment but increasing the component of the initial vector in the direction of the target eigenvector led to a decrease of the number of additional steps required by CRQI. For eigenvectors that were very close to the target sometimes both classic RQI and complex RQI even finished within the same number of iterations. Still, even in these cases, classic RQI usually failed to converge to the right eigenpair.

In the next examples we will examine how the initial vector and initial (real) shift affect the results of RQI and CRQI. We have already discussed the sometimes erratic behaviour of classic RQI. As we will shortly see, a main problem of RQI is convergence often hardly depends on the initial vector but rather on the initial shift. This is why especially for eigenvalue problems with closely spaced eigenvalues RQI fails to compute the right eigenpair even if the method is started with a good approximation of the eigenvector. We start with an example where the algorithm was run many times with a fixed initial vector but varying initial shifts. To obtain the shifts we computed the spectrum of the matrix using built-in functions of Matlab and then extracted 100 evenly spaced values from the interval $[\lambda_{\min} - 10, \lambda_{\max} + 10]$, where λ_{\min} and λ_{\max} are the smallest and largest eigenvalue of \mathbf{A} , respectively. The results are plotted in Figure 3.2. The initial vector was set to a weighted combination of the exact eigenvectors as described above. The component

Finish discussing this example?

in the target direction was small in the first two examples (Figure 3.2(a) and 3.2(b)), big in the third example (Figure 3.2(c)) and not larger than the remaining components in the last example (i. e., there was no weight set to a larger value than the other, Figure 3.2(d)).

We immediately observe that RQI seems to depend heavily on the choice of the initial shift, especially when the shift lies between the upper and lower bound of the spectrum (indicated by the dotted area in the plots). This does not change even for initial vectors that are very close approximations of an eigenvector as we have already seen earlier, in Section 2.2.2. In contrast, it appears that CRQI does not depend so much on the shift but rather on the initial vector. In the first two examples, it seems as if in some cases the result of CRQI depends on the sign of the target eigenvalue. If the eigenvalue is negative, shifts below this eigenvalue produced the correct result whereas shifts above the eigenvalue did not and analogously for positive eigenvalues. Further investigation revealed that this has actually nothing to do with the target eigenvalue being negative or positive but rather its location in the spectrum. If it is below the centre of the spectrum the behaviour is as in Figure 3.2(a) and for eigenvalues above the centre the method acts as in Figure 3.2(b). This observation could possibly be used if the initial vector is not that good of an approximation but some knowledge of the spectrum is available so that the initial shifts could be chosen accordingly.

3 Complex Rayleigh Quotient Iteration

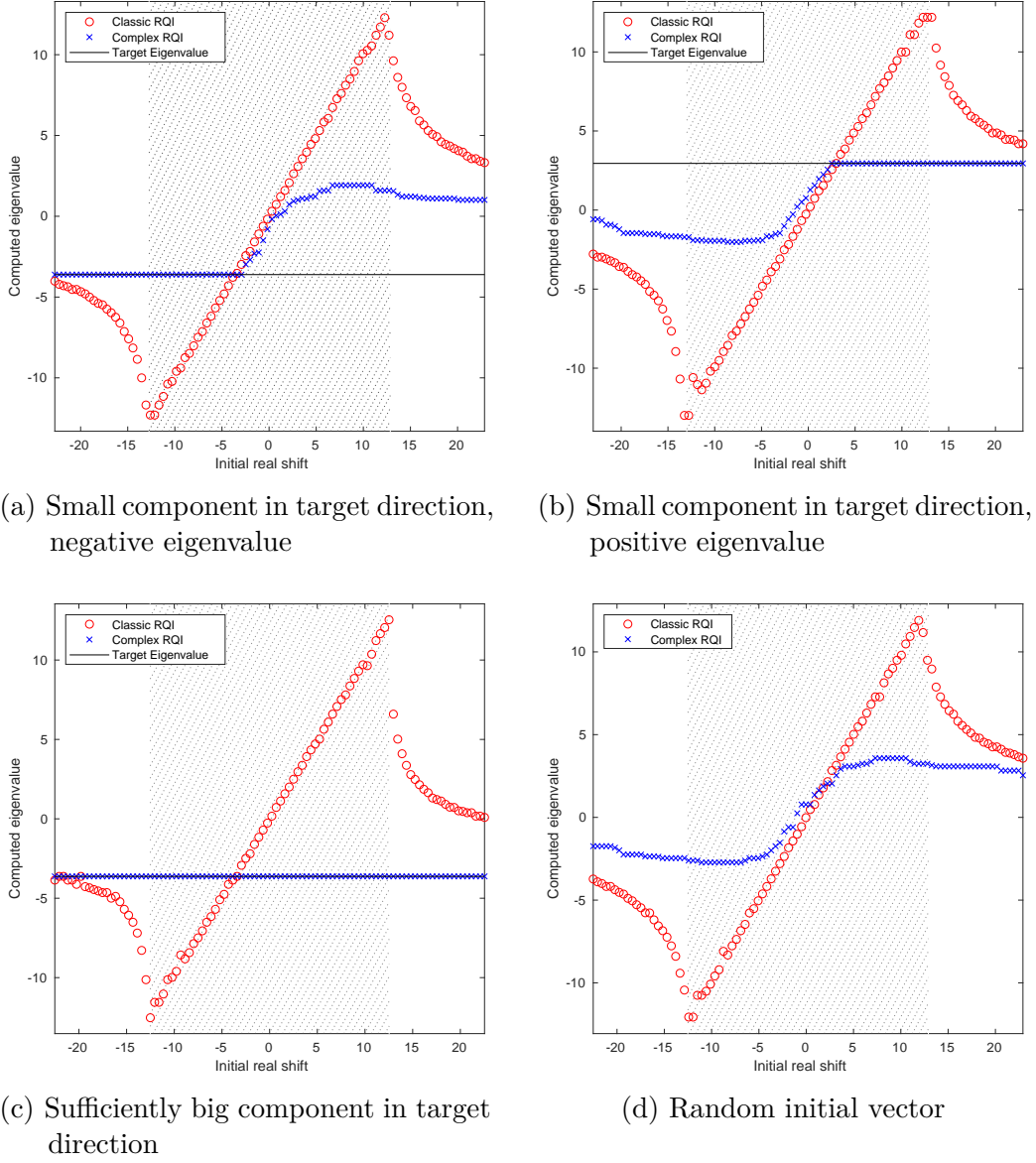


Figure 3.2: Plot of initial real shift against the computed eigenvalue using classic RQI and CRQI. The dotted area encloses the initial shifts that lie in the spectrum of \mathbf{A} . In the first two examples the initial vector had only a small component in the direction of the target eigenvector.

Appendices

A Proofs

Proof of Lemma 3.1. First consider $j \neq k$. Using the orthogonality of the eigenvectors

$$(\mathbf{A} - \gamma i(\mathbf{I} - \mathbf{v}_k \mathbf{v}_k^\top)) \mathbf{v}_j = \mathbf{A} \mathbf{v}_j - \gamma i \mathbf{v}_j + \gamma i \mathbf{v}_k \underbrace{\mathbf{v}_k^\top \mathbf{v}_j}_{=0} = \lambda_j \mathbf{v}_j - \gamma i \mathbf{v}_j = (\lambda_j - \gamma i) \mathbf{v}_j.$$

For $j = k$ we have $\mathbf{v}_k^\top \mathbf{v}_j = \mathbf{v}_k^\top \mathbf{v}_k = 1$ and thus

$$(\mathbf{A} - \gamma i(\mathbf{I} - \mathbf{v}_k \mathbf{v}_k^\top)) \mathbf{v}_k = \lambda_k \mathbf{v}_k - \gamma i \mathbf{v}_k + \gamma i \mathbf{v}_k = \lambda_k \mathbf{v}_k.$$

□

Proof of Lemma 3.2. Since

$$\|\tilde{\mathbf{A}}_{(1)}\| = \|\gamma i(\mathbf{u} \mathbf{u}^\top - \mathbf{v}_k \mathbf{v}_k^\top)\| = \gamma \|\underbrace{\mathbf{u} \mathbf{u}^\top - \mathbf{v}_k \mathbf{v}_k^\top}_{=\mathbf{E}}\|$$

it suffices to compute the norm of \mathbf{E} . Additionally, \mathbf{E} is symmetric (since it is a sum of two symmetric matrices) and thus its spectral norm coincides with its spectral radius. The matrices $\mathbf{u} \mathbf{u}^\top$ and $\mathbf{v}_k \mathbf{v}_k^\top$ have both rank one and therefore \mathbf{E} is at most of rank two. This implies that it has at most two non-zero eigenvalues, denoted by μ_1 and μ_2 , and we can therefore compute both of them and take the one that is larger in modulus.

To compute the eigenvalues of \mathbf{A} we use the following two well-known facts from linear algebra. Here, $\text{tr}(\mathbf{E})$ denotes the trace of \mathbf{E} defined as the sum of the diagonal entries of the matrix.

1. The trace is the sum of the eigenvalues of \mathbf{E} , i. e.,

$$\text{tr}(\mathbf{E}) = \mu_1 + \mu_2. \tag{A.1}$$

2. The eigenvalues of the square of \mathbf{E} are μ_1^2 and μ_2^2 and thus, using the previous fact,

$$\text{tr}(\mathbf{E}^2) = \mu_1^2 + \mu_2^2. \quad (\text{A.2})$$

The diagonal entries of the matrices $\mathbf{u}\mathbf{u}^\top$ and $\mathbf{v}_k\mathbf{v}_k^\top$ consist of the squares of their respective entries and thus, using the additivity of the trace, we get

$$\text{tr}(\mathbf{E}) = \|\mathbf{u}\| - \|\mathbf{v}_k\| = 0$$

which in conjunction with (A.1) implies $\mu_1 = -\mu_2$. We expand \mathbf{E}^2 and obtain

$$\begin{aligned} \mathbf{E}^2 &= (\mathbf{u}\mathbf{u}^\top - \mathbf{v}_k\mathbf{v}_k^\top)(\mathbf{u}\mathbf{u}^\top - \mathbf{v}_k\mathbf{v}_k^\top) \\ &= \mathbf{u}\mathbf{u}^\top\mathbf{u}\mathbf{u}^\top - \mathbf{v}_k\mathbf{v}_k^\top\mathbf{u}\mathbf{u}^\top - \mathbf{u}\mathbf{u}^\top\mathbf{v}_k\mathbf{v}_k^\top + \mathbf{v}_k\mathbf{v}_k^\top\mathbf{v}_k\mathbf{v}_k^\top \\ &= \mathbf{u}\mathbf{u}^\top + \mathbf{v}_k\mathbf{v}_k^\top - \langle \mathbf{u}, \mathbf{v}_k \rangle (\mathbf{u}\mathbf{v}_k^\top + \mathbf{v}_k\mathbf{u}^\top). \end{aligned}$$

Therefore,

$$\begin{aligned} \text{tr}(\mathbf{E}^2) &= \|\mathbf{u}\| + \|\mathbf{v}_k\| - \langle \mathbf{u}, \mathbf{v}_k \rangle (\langle \mathbf{u}, \mathbf{v}_k \rangle + \langle \mathbf{u}, \mathbf{v}_k \rangle) \\ &= 2 - 2\langle \mathbf{u}, \mathbf{v}_k \rangle^2. \end{aligned}$$

However, we also have $\text{tr}(\mathbf{E}^2) = 2\mu_1^2$ due to (A.2) and so

$$\mu_1 = \sqrt{1 - \langle \mathbf{u}, \mathbf{v}_k \rangle^2}$$

from which the result follows. □

Proof of Proposition 3.3. For this proof we treat $\tilde{\mathbf{A}}_{(1)}$ as a perturbation of $\tilde{\mathbf{A}}_{(0)}$ and a result from [REFERENCE] which states that the eigenvalues of $\tilde{\mathbf{A}} = \tilde{\mathbf{A}}_{(0)} + \tilde{\mathbf{A}}_{(1)}$ satisfy

$$\lambda_j(\tilde{\mathbf{A}}) = \lambda_j(\tilde{\mathbf{A}}_{(0)}) + \mathbf{w}_j^* \tilde{\mathbf{A}}_{(1)} \mathbf{w}_j + \mathcal{O}\left(\|\tilde{\mathbf{A}}_{(1)}\|^2\right), \quad (\text{A.3})$$

where \mathbf{w}_j is an eigenvector belonging to $\lambda_j(\tilde{\mathbf{A}}_{(0)})$. We expand the middle part and obtain

$$\begin{aligned} \mathbf{w}_j^* \tilde{\mathbf{A}}_{(0)} \mathbf{w}_j &= \gamma i \mathbf{w}_j^* (\mathbf{u} \mathbf{u}^* - \mathbf{v}_k \mathbf{v}_k^*) \mathbf{w}_j \\ &= \gamma i (\mathbf{w}_j^* \mathbf{u} \mathbf{u}^* \mathbf{w}_j - \mathbf{w}_j^* \mathbf{v}_k \mathbf{v}_k^* \mathbf{w}_j) \\ &= \gamma i (\langle \mathbf{w}_j, \mathbf{u} \rangle^2 - \langle \mathbf{w}_j, \mathbf{v}_k \rangle^2) \\ &= \begin{cases} \gamma i \langle \mathbf{v}_j, \mathbf{u} \rangle^2 & \text{if } j \neq k, \\ \gamma i (\langle \mathbf{v}_j, \mathbf{u} \rangle^2 - 1) & \text{if } j = k, \end{cases} \end{aligned}$$

where we used Lemma 3.1 in the last step, which states that in fact $\mathbf{w}_j = \mathbf{v}_j$ with \mathbf{v}_j being the eigenvectors of \mathbf{A} . Adding this to the first part of (A.3) yields

$$\begin{aligned} \lambda_j(\tilde{\mathbf{A}}_{(0)}) + \mathbf{w}_j^* \tilde{\mathbf{A}}_{(0)} \mathbf{w}_j &= \lambda_j(\mathbf{A}) - \gamma i + \gamma i \langle \mathbf{v}_j, \mathbf{u} \rangle^2 \\ &= \lambda_j(\mathbf{A}) + \gamma i (\langle \mathbf{v}_j, \mathbf{u} \rangle^2 - 1) \end{aligned}$$

for $j \neq k$ and

$$\lambda_j(\tilde{\mathbf{A}}_{(0)}) + \mathbf{w}_j^* \tilde{\mathbf{A}}_{(0)} \mathbf{w}_j = \lambda_k(\mathbf{A}) + \gamma i (\langle \mathbf{v}_k, \mathbf{u} \rangle^2 - 1)$$

for $j = k$ and thus

$$\lambda_j(\tilde{\mathbf{A}}) = \lambda_j(\mathbf{A}) + \gamma i (\langle \mathbf{v}_j, \mathbf{u} \rangle^2 - 1) + \mathcal{O}(\|\tilde{\mathbf{A}}_{(1)}\|^2),$$

for all $j = 1, \dots, n$, which concludes the proof. □

B Implementation of the Numerical Algorithms

B.1 Matlab code of classic Rayleigh Quotient
Iteration

B.2 Matlab code of complex Rayleigh
Quotient Iteration

B.3 Sampling from a cone inside the
 n -dimensional unit sphere

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