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# Using Complex Shifts in Rayleigh Quotient Iteration to Compute Interior Eigenvalues

*Bachelor Thesis*

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**Abstract** This thesis presents a novel iterative method for computing interior eigenvalues of real symmetric matrices.

**Zusammenfassung** In dieser Arbeit wird eine neue iterative Methode zur Berechnung innerer Eigenwerte reeller symmetrischer Matrizen vorgestellt.

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# 1 Introduction

{chapter:intro

This thesis introduces a novel shift-and-invert-type method that is similar to the *Rayleigh Quotient Iteration (RQI)*. Numerical examples suggest that this method overcomes some of the drawbacks of RQI. Before we introduce this new method we collect all the necessary definitions and results from numerical linear algebra in the next section. We will finish off this introductory chapter by reviewing some of the most basic iterative methods to compute eigenvalues.

In the next chapter we study the classic Rayleigh Quotient Iteration. Among others, we give a proof for the property that makes it so popular, namely the local cubic convergence.

Rewrite

The third chapter is devoted to the novel method that we call *Complex Rayleigh Quotient Iteration*. We give many different numerical examples and carefully analyse them.

## 1.1 Motivation

The following example introduces a physical problem that requires the solution of an eigenvalue problem. There is a plethora of problems which lead to eigenvalue problems in almost all of the natural sciences but also in finance and other social sciences (see, for example, ).

References  
for eigen-  
value  
problems

**Example 1.1** (Photonic Crystal Fibres).

## 1.2 Results from (numerical) linear algebra

In this section we introduce the definitions and results from linear algebra that will be needed later. We also introduce the most basic iterative eigenvalue algorithms.

### 1.2.1 The Symmetric Eigenvalue Problem

{sec:symmetri

In Example 1.1 a problem of the form

$$\text{“Find } \mathbf{v} \in \mathbb{R}^n \setminus \{\mathbf{0}\}, \lambda \in \mathbb{R}, \text{ such that } \mathbf{A}\mathbf{v} = \lambda\mathbf{v} \text{”}$$

arised, where  $\mathbf{A}$  was a real symmetric matrix. This problem is referred to as the *symmetric eigenvalue problem*. A more general definition is given in the following.

**Definition 1.2.** 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

$$\mathbf{A}\mathbf{v} = \lambda\mathbf{v}. \quad (1.1) \quad \text{\texttt{eq:eigvalpro}}$$

The vector  $\mathbf{v}$  is called an *eigenvector* of  $\mathbf{A}$  associated with  $\lambda$ . The tuple  $(\lambda, \mathbf{v})$  is called an *eigenpair*. The set of all eigenvalues of  $\mathbf{A}$  is referred to as the *spectrum* and is denoted by  $\sigma(\mathbf{A})$ .

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 holds 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, although being of theoretical significance, cannot be used to calculate eigenvalues numerically for two reasons. First, the computation of the coefficients of the polynomial is not stable [4, 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. 20, 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 [7]. Below we present essential facts from linear algebra preparing us for discussing such iterative methods in Section 1.2.2.

**Remark 1.3** (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*

$$\mathbf{A}\mathbf{v} = \lambda\mathbf{M}\mathbf{v}. \quad (1.2) \quad \text{\texttt{eq:eigvalpro}}$$

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.

Citation  
needed.

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 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.,  $\mathbf{A} = \mathbf{A}^* := \overline{\mathbf{A}}^\top$ , 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.

{prop:eigval:}

**Proposition 1.4.** *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 eigenvalues<sup>1</sup> of  $\mathbf{A}$  with associated eigenvectors  $\mathbf{v}_1, \dots, \mathbf{v}_n$ .*

- (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  $\mathbf{v}_1, \dots, \mathbf{v}_n$ .*

<sup>1</sup>Of 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  $n$ .

*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 [5, Theorem 18 and Corollary, p. 314]).

(iii) Suppose  $\mathbf{A}$  is invertible and let  $(\lambda, \mathbf{v})$  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  $(\lambda, \mathbf{v})$  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) given  $\mathbf{A} \in \mathbb{R}^{n \times n}$  is a real symmetric matrix. The (real) eigenvalues and associated (real) eigenvectors of  $\mathbf{A}$  are denoted by  $\lambda_1, \dots, \lambda_n$  and  $\mathbf{v}_1, \dots, \mathbf{v}_n$ , respectively. Since for any eigenvector  $\mathbf{v}$  also any scalar multiple of  $\mathbf{v}$  is also an eigenvector, we assume that the eigenvectors are normalised w.r.t. the Euclidean norm, so that

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

Note, that due to Proposition 1.4 (ii) we have

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

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  $\lambda_1$  and  $\lambda_n$  are called *extreme* eigenvalues. The remaining eigenvalues  $\lambda_2, \dots, \lambda_{n-1}$  are called *interior* eigenvalues. Sometimes we will make the assumption that



$\mathbf{A}$  is positive definite, i. e., that

$$x^\top \mathbf{A} x > 0 \quad \text{for all } x \in \mathbb{R}^n \setminus \{\mathbf{0}\}.$$

Given an eigenvalue  $\lambda$  and an associated normalised eigenvector  $\mathbf{v}$  we then have

$$\lambda = \mathbf{v}^\top \lambda \mathbf{v} = \mathbf{v}^\top \mathbf{A} \mathbf{v} > 0,$$

i. e., eigenvalues of symmetric positive definite matrices are positive.

To indicate that eigenvalues belong to a particular matrix  $\mathbf{M}$  we sometimes write  $\lambda(\mathbf{M})$  or  $\lambda_j(\mathbf{M})$ . If not stated otherwise, for the remainder of the thesis  $\mathbf{A}$  denotes a symmetric  $n \times n$  matrix with eigenvalues  $\lambda_j(\mathbf{A}) = \lambda_j$  and corresponding eigenvectors  $\mathbf{v}_j$  for  $j = 1, \dots, n$ .

### 1.2.2 Iterative methods for eigenvalue problems

{sec:iterativ

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 the sequence converges to its limit.

**Definition 1.5** (Order of Convergence). Let  $(\mathbf{x}^{(k)})_{k \in \mathbb{N}}$  be a sequence in  $\mathbb{R}^n$  that converges to  $\mathbf{z} \in \mathbb{R}^n$ .

- (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  $\rho$  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 convergence behaviour is best studied in terms of the *error angle* between  $\mathbf{x}^{(k)}$  and  $\mathbf{z}$ .

**Definition 1.6** (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

$$\begin{aligned} \cos \angle(\mathbf{x}, \mathbf{y}) &= \frac{|\langle \mathbf{x}, \mathbf{y} \rangle|}{\|\mathbf{x}\| \|\mathbf{y}\|}, \\ \sin \angle(\mathbf{x}, \mathbf{y}) &:= \sqrt{1 - \cos^2 \angle(\mathbf{x}, \mathbf{y})}, \\ \tan \angle(\mathbf{x}, \mathbf{y}) &:= \frac{\sin \angle(\mathbf{x}, \mathbf{y})}{\cos \angle(\mathbf{x}, \mathbf{y})}. \end{aligned}$$

## Power method

The *power method* is probably the simplest iterative method 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 under- and overflow errors  $\mathbf{x}^{(k)}$  is normalised at each step. Although the vectors are usually normalised w.r.t. the Euclidean norm, in Algorithm 1.7 we normalise by ensuring that the largest component of the current approximation is equal to one (i.e., we normalise w.r.t. to the maximum norm) as proposed in [18]. The sequence  $\mathbf{x}^{(k)}$  converges to the eigenvector associated with the eigenvalue  $\lambda_n$  under the assumptions that  $\lambda_n$  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  $\lambda_n$ .

Regardless of the normalisation choosen, the method converges linearly with convergence rate

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

Thus, the method can be very slow if the distance between the eigenvalues  $\lambda_n$  and  $\lambda_{n-1}$  is very small. For more details, see [18, pp. 85 sqq.].

---

**Algorithm 1.7:** 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 */
    {alg:power:method}

```

---

Besides the possible slow convergence rate, the power method will always converge to an eigenvector associated with the dominant eigenvalue  $\lambda_n$ . 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 1.4 (iii) this will produce a sequence of vectors  $\mathbf{x}^{(k)}$  converging to the eigenvector associated to the smallest eigenvalue  $\lambda_1$ . Combining this idea with Proposition 1.4 (iv) produces the *shifted inverse iteration*.<sup>2</sup> There, the iterates are defined by

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

where we omitted the normalisation step. The scalar  $\sigma \in \mathbb{R}$  is often called the *shift* since it shifts the eigenvalues of  $\mathbf{A}^{-1}$  by  $\sigma$  on the real axis. Of course, we do not have to compute the inverse explicitly. Instead, before the loop we can compute the **LU** decomposition of  $\mathbf{A} - \sigma \mathbf{I}$  and solve the system

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

---

<sup>2</sup>Note that some authors call this the inverse iteration and do not make a distinction of a shift being used or not.

Check  
this  
again

for  $\mathbf{x}^{(k)}$  reducing the complexity from  $\mathcal{O}(n^3)$  to  $\mathcal{O}(n^2)$  at each step. We summarise the results in Algorithm 1.8 (there, we normalise w. r. t. the Euclidean norm such that at every step  $\|\mathbf{v}^{(k)}\| = 1$  holds).

---

**Algorithm 1.8:** Shifted inverse iteration

---

**Input:** Nonzero unit vector  $\mathbf{x}^{(0)}$ , shift  $\sigma \in \mathbb{R}$

Compute  $\mathbf{LU}$  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  $\tilde{\mathbf{x}}^{(k)}$   
     $\mathbf{x}^{(k)} \leftarrow \tilde{\mathbf{x}}^{(k)} / \|\tilde{\mathbf{x}}^{(k)}\|$

---

{alg:sii}

---

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  $\mu_1$  the eigenvalue that is closest to the shift  $\sigma$  and by  $\mu_2$  the one that is the next closest one, the eigenvalue of largest modulus of  $(\mathbf{A} - \sigma \mathbf{I})^{-1}$  is  $1/(\mu_1 - \sigma)$  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 while a shift that is very close to an eigenvalue increases the convergence rate, at the same time leads to a more and more ill-conditioned linear system. In the case when  $\sigma$  is exactly an eigenvalue the system is even singular and one might expect the method to fail in these cases. It took some time from when inverse iteration was first defined until Wilkinson established that this is merely a problem in exact arithmetic and it was fully understood what was observed in practice for many years, namely that this poses no problem when the linear system is solved numerically using a backwards stably method, see [22, pp. 620 sq.] and [16].

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

We now give two examples for both the power method and the shifted inverse iteration.

**Example 1.9.** Consider the matrix

$$\mathbf{A} = \begin{pmatrix} 1 & 2 & 3 \\ 2 & 5 & 6 \\ 3 & 6 & 8 \end{pmatrix}.$$

At each step in the shifted inverse iteration, better approximations for the target eigenvector are computed. One could try to use these approximations to replace occasionally the shift by an approximation of the corresponding eigenvalue. 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. [4, 6, 19].

Example  
of Power  
method  
and in-  
verse  
iteration

## 2 Classic Rayleigh Quotient Iteration

{chapter:rqi}

In this chapter we thoroughly 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 disadvantages and shortcomings.

In the following, 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

{sec:rqi:rqi}

In Chapter 1 we briefly introduced iterative methods for computing eigenpairs. In essence, RQI is shifted inverse iteration where the shift is replaced by the *Rayleigh quotient* at each step. As we will see, the Rayleigh Quotient can be used to obtain good estimates of an eigenvalue given an approximation of an eigenvector.

**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*<sup>1</sup> corresponding to the matrix  $\mathbf{A}$ .

Note that for real matrices, we have

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

We begin by discussing some basic facts.

{lem:rqi:prop}

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

---

<sup>1</sup>Other 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  $\rho_{\mathbf{A}}(\mathbf{x})$ .

(i) If  $(\lambda, \mathbf{v})$  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

$$\mathcal{R}_{\mathbf{A}}(\mathbf{x}) = \frac{\langle \mathbf{x}, \mathbf{Ax} \rangle}{\langle \mathbf{x}, \mathbf{x} \rangle}, \quad (2.1) \quad \text{\texttt{feq:rq:innerp}}$$

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

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

(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  $(\lambda, \mathbf{v})$  is an eigenpair of  $\mathbf{A}$ , then

$$\|\mathbf{Av} - \lambda\mathbf{v}\|^2 = 0.$$

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

$$\hat{\lambda} = \arg \min_{\mu \in \mathbb{C}} \|\mathbf{A}\hat{\mathbf{v}} - \mu\hat{\mathbf{v}}\|^2.$$

This is a linear least squares problem in  $\mu$  with normal equations (cf. [3, p. 106])

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

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

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

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” [15, p. 77].

{lem:rq:quade

**Lemma 2.3** (Eigenvalue estimate). *Let  $\mathbf{x} \in \mathbb{C}^n$  be an approximation of an eigenvector  $\mathbf{v}$  of a normal<sup>2</sup> matrix  $\mathbf{A}$  with corresponding eigenvalue  $\lambda$ . Then*

$$|\mathcal{R}_{\mathbf{A}}(\mathbf{x}) - \lambda| \leq \|\mathbf{A} - \lambda \mathbf{I}\| \sin^2 \angle(\mathbf{x}, \mathbf{v}) \leq \|\mathbf{A} - \lambda \mathbf{I}\| \left( \frac{\|\mathbf{x} - \alpha \mathbf{v}\|}{\|\mathbf{x}\|} \right)^2 \quad \text{for all } \alpha \in \mathbb{C}.$$

The proof is given in Appendix A. □

This result is often paraphrased as “the Rayleigh Quotient is a *quadratically accurate* estimate of an eigenvalue” (see for example [20, p. 204]) and is often presented in the following shorter form

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

cite ex-  
amples

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 1.8) 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.

<sup>2</sup>A 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.



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**Algorithm 2.4:** Rayleigh Quotient Iteration

---

**Input:** Nonzero unit vector  $\mathbf{x}^{(0)}$

$$\mu^{(0)} \leftarrow \left( \mathbf{x}^{(0)} \right)^* \mathbf{A} \mathbf{x}^{(0)}$$

**for**  $k = 1, 2, \dots$  *until convergence* **do**

Solve  $(\mathbf{A} - \mu^{(k)} \mathbf{I}) \mathbf{y}^{(k)} = \mathbf{x}^{(k-1)}$  for  $\mathbf{y}^{(k)}$

$$\mathbf{x}^{(k)} \leftarrow \mathbf{y}^{(k)} / \|\mathbf{y}^{(k)}\|$$

$$\mu^{(k)} \leftarrow \left( \mathbf{x}^{(k)} \right)^* \mathbf{A} \mathbf{x}^{(k)}$$

{alg:rqi}

---

We have yet to define what we mean by “until convergence” (cf. the algorithms persented in Section 1.2.2). Now that we the 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  $\text{tol}$  is a user-given error tolerance. 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. A rigorous justification is given in [18, pp. 59 sqq.]. Here, we give only some important results without proof for the case when  $\mathbf{A}$  is symmetric. A popular result, usually referred to as the *Bauer-Fike theorem* (see, e.g. [18, p. 59]) states that there exists an eigenvalue  $\lambda$  of  $\mathbf{A}$  such that

$$|\lambda - \mu^{(k)}| \leq \kappa(\mathbf{Q}) \|\mathbf{r}^{(k)}\|, \tag{2.2} \quad \text{\texttt{eq:bauer-fike}}$$

where  $\mathbf{Q}$  is a matrix that transforms  $\mathbf{A}$  into diagonal form (i. e.,  $\mathbf{Q}$  is such that  $\mathbf{Q}^{-1} \mathbf{A} \mathbf{Q}$  is diagonal) and  $\kappa(\mathbf{Q}) := \|\mathbf{Q}\| \|\mathbf{Q}^{-1}\|$  is the *condition number* of  $\mathbf{Q}$ . Such a matrix exists due to the *spectral theorem* [5, Theorem 18 and Corollary, p. 314]. Since  $\mathbf{A}$  is real and symmetric  $\mathbf{Q}$  is an *orthogonal* matrix. In particular  $\|\mathbf{Q}\| = \|\mathbf{Q}^{-1}\| = 1$  and thus

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

Therefore, if the stopping criterion is fulfilled, we have  $|\lambda - \mu^{(k)}| < \text{tol}$ . For the eigenvector

Rewrite

one can show [18, 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  $\lambda$  and  $\delta$  is the distance from  $\mu^{(k)}$  to the rest of the spectrum, i.e.,

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

These results hold if  $\mu^{(k)} = (\mathbf{x}^{(k)})^* \mathbf{A}(\mathbf{x}^{(k)})$  (Rayleigh Quotient).

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## 2.2 History and recent developments

Now that we have defined the Rayleigh Quotient and Rayleigh Quotient Iteration we give an overview on 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 on some important milestones within this 60 years. Large parts of this overview are based on [19].

Page

**1894 — Lord Rayleigh** In the second edition of his book titled “The Theory of Sound” John William Strutt, 3rd Baron Rayleigh [17, p. 110], proposed the following iteration for improving an approximate eigenvector  $\mathbf{x}^{(0)}$ :

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

where  $\mathbf{e}_1$  denotes the first natural coordinate vector, i.e., the first column of the  $n \times n$  identity matrix and  $\mathbf{x}^{(i)}$  and  $\mathbf{x}^{(i+1)}$  denote the current and next iterate, respectively. To

be precise, Lord Rayleigh considered the *generalised eigenvalue problem*

$$\mathbf{A}\mathbf{v} = \lambda \mathbf{M}\mathbf{v} \quad (2.4) \quad \text{eq:general:e}$$

and so in his text, the iteration reads

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

**1949 — Kohn** In a letter to the editor Walter Kohn [8] suggest the following iteration

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

where  $\mathbf{e}_k$  is *any* of the natural coordinate vectors. Without a rigorous proof Kohn argues that  $\mathcal{R}_{\mathbf{A}}(\mathbf{x}^{(i)})$  converges quadratically to an eigenvalue of  $\mathbf{A}$  (given 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 Crandall [2] suggests

$$\text{Solve } (\mathbf{A} - \mathcal{R}_{\mathbf{A}}(\mathbf{x}^{(i)})\mathbf{I})\mathbf{x}^{(i+1)} = \mathbf{x}^{(i)} . \quad (2.5) \quad \text{eq:unnormali}$$

Actually, Crandall also considered the generalised eigenproblem (2.4) 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 (wrong) assumption that the sequence of vectors  $\mathbf{x}^{(k)}$  converges, Crandall establishes cubic convergence for this sequence. To see why the assumption is wrong, we assume the contrary, i. e., suppose  $\mathbf{x}^{(i)} \rightarrow \mathbf{v}_k$  for some  $k = 1, \dots, n$ . From (2.5) we have

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

i. e.,  $\mathbf{v}_k$  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 we have

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

which is a contradiction.

Define  
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(linear,  
quadratic,  
cubic)  
conver-  
gence

Full  
name

**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” [9–14]. We mention the titles here, since it is the first mention of the term *Rayleigh Quotient Iteration*.

In the first paper the author suggests the iteration

$$\text{Solve } (\mathbf{A} - \mathcal{R}_{\mathbf{A}}(\mathbf{x}^{(i)})\mathbf{I})\mathbf{x}^{(i+1)} = \boldsymbol{\eta}, \quad \boldsymbol{\eta} \neq \mathbf{0}. \quad (2.6) \quad \text{feq:rqi:ostro}$$

He rigorously establishes a *quadratic* convergence rate for the sequence  $\{\mathcal{R}_{\mathbf{A}}(\mathbf{x}^{(i)})\}$ . He then refers to a paper of Wielandt [21] and his *fractional* or *broken iteration* (German: *gebrochene Iteration*). Inspired by Wielandt’s method he suggests replacing the fixed vector  $\mathbf{e}_1$  in the right hand side of (2.6) to the solution from the previous step

$$(\mathbf{A} - \mathcal{R}_{\mathbf{A}}(\mathbf{x}^{(i)})\mathbf{I})\mathbf{x}^{(i+1)} = \mathbf{x}^{(i)}, \quad (2.7) \quad \text{feq:rqi:unnor}$$

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.,

$$\frac{\mu_{i+1} - \lambda}{(\mu_i - \lambda)^3} \longrightarrow \gamma \quad \text{as } i \rightarrow \infty, \quad (2.8) \quad \text{feq:rqi:cubic}$$

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

Note that (2.7) is the same algorithm previously proposed by Crandall given in Equation (2.5). 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  $\xi_x$  in the rule (28), (29). However he does not arrive at our asymptotic formula (46), which is the principal result of our paper.” [9, p. 241].<sup>3</sup>

In the beginning of the second paper [10] Ostrowski discusses this in more detail. More importantly, he also points out in §21 of the text that in order to assure convergence

---

<sup>3</sup>Here,  $\xi_x$  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 (2.7) and the asymptotic formula (46) he references is given in (2.8).

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. This was all shown under the assumption that the matrix  $\mathbf{A}$  is real symmetric and Ostrowski mentions that all results remain valid in the complex Hermitian case.

The third paper [11] of the series addresses the non-symmetric (or non-Hermitian) 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.

This concludes the overview on the development of RQI from the first mention of the Rayleigh Quotient by Lord Rayleigh to the first definition of RQI and the first rigorous proof of what makes it so appealing, namely the (local) cubic convergence.

Read Ostrowski's other papers

### 2.2.2 Further developments and recent contributions

## 2.3 Convergence Analysis

{sec:convergence}

We mentioned earlier the local cubic convergence of RQI. In this section we give a proof of this claim and we also show that RQI converges globally.

As we have seen in the previous section the first rigorous proof of the cubic convergence of RQI was given by Ostrowski [9] but over time a number of different, simpler proofs were presented. We start by stating the result we want to proof and then sketch a few of the different approaches.

{thm:rqi:cubic}

**Theorem 2.5** (Cubic convergence). *Rayleigh Quotient Iteration is locally cubically convergent.*

Locally here means that

1. we assume that the sequence  $(\mathbf{x}^{(i)})$  does converge to an eigenvector of  $\mathbf{A}$  and
2. the current iterate is a sufficiently good approximation of the target eigenvector, i. e., the error between the current iterate and the target is small enough.

It suffices to make these assumptions for the eigenvectors only since if the vector iterates converge to an eigenvector, the eigenvalue approximations (given by the Rayleigh Quotient of the vector iterates) must also converge due to Lemma 2.2 (ii). Furthermore, we have already seen in Lemma 2.3 that the Rayleigh Quotient of good eigenvector estimates yields even better eigenvalue estimates.

Some of the proofs are given under the assumption that  $\mathbf{A}$  is diagonal. To see why no generality is lost with this assumption, 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 temporarily drop the superscripts that denote the current iteration and change variables in RQI<sup>4</sup> 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,

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

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 will assume that  $\mathbf{A} = \mathbf{\Lambda}$  is already diagonal which in particular implies that the eigenvectors of  $\mathbf{A}$  are  $\mathbf{e}_i$ , the columns of the identity matrix.

Check if this is right

*Proof 1*. This proof is due to Demmel [3, pp. 215 sq.]. Assume that the eigenvalue that is computed is *simple* (cf. Definition ??). 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

Rewrite, too close to [Demmel]

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

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  $\|\mathbf{d}^{(i+1)}\| = \mathcal{O}(\epsilon^3)$ .

<sup>4</sup>Recall 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.

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 symmetry<sup>5</sup> 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  $\lambda_{\max}$ , we can bound  $|\eta|$  as follows

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

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

---

<sup>5</sup>For a symmetric matrix  $\mathbf{B} = \mathbf{B}^\top$  we have

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

# 3 Complex Rayleigh Quotient Iteration

In this chapter we introduce *Complex Rayleigh Quotient Iteration* (CRQI<sup>1</sup>). This is a novel shift and invert type algorithm similar to classic RQI that overcomes some of its disadvantages. .

Finish  
intro for  
chapter

## 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

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

Due to the pairwise orthogonality of the eigenvectors this implies

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

As we have seen before, 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. The main idea of CRQI is now to use the approximation  $\mathbf{u}$  of  $\mathbf{v}_k$  to perturb the linear system that is solved at each step in RQI in such a way that the distance between the target eigenvalue  $\lambda_k$  and the neighboring eigenvalues is increased. 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. We make use of the fact that all eigenvalues of  $\mathbf{A}$  are real and perturb this matrix in such

Rewrite

<sup>1</sup>We 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*.



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.

The idea is now to apply Rayleigh Quotient iteration to the matrix

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

instead of  $\mathbf{A}$ , where  $\gamma > 0$  is positive real number and  $i$  denotes the imaginary unit. To get an intuition on why we choose this matrix, we first note that the matrix  $\mathbf{I} - \mathbf{u}\mathbf{u}^\top$ , interpreted as a linear mapping, defines the orthogonal projection onto the span of  $\mathbf{u}$ . Of course, this works for any vector  $\mathbf{v} \in \mathbb{R}^n$  and can be seen as follows. Given a vector  $\mathbf{x} \in \mathbb{R}^n$ , the projection of  $\mathbf{x} \in \mathbb{R}^n$  onto the span of  $\mathbf{v}$  is

$$\frac{\langle \mathbf{v}, \mathbf{x} \rangle}{\langle \mathbf{v}, \mathbf{v} \rangle} \mathbf{v},$$

where  $\langle \cdot, \cdot \rangle$  denotes the Euclidean inner product on  $\mathbb{R}^n$ . Thus, the projection onto the orthogonal complement of the span of  $\mathbf{v}$  is

$$\mathbf{x} - (\mathbf{v}^\top \mathbf{x}) \mathbf{v} = \mathbf{x} - (\mathbf{v}\mathbf{v}^\top) \mathbf{x} = (\mathbf{I} - \mathbf{v}\mathbf{v}^\top) \mathbf{x}.$$

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

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

Now recall that  $\mathbf{u}$  is assumed to be a good approximation of an eigenvector  $\mathbf{v}_k$  of  $\mathbf{A}$ . This also implies that the orthogonal subspace of the span of  $\mathbf{u}$  approximates the orthogonal subspace spanned by  $\mathbf{v}_k$ . However, the latter is the space spanned by the remaining eigenvectors of  $\mathbf{A}$ , since the eigenvectors are pairwise orthogonal. 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  $\lambda_j - \gamma i$  due to (3.3). The eigenvalue corresponding to  $\mathbf{v}_k$  would then be approximately equal to  $\lambda_k$  since  $\tilde{\mathbf{A}}\mathbf{v}_k \approx \mathbf{A}\mathbf{v}_k = \lambda_k \mathbf{v}_k$ .

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derivation

To make this intuition more quantitative, we first need the following result where we replace  $\mathbf{u}$  by the exact target eigenvector  $\mathbf{v}_k$ .

{lem:eigs:ati}

**Lemma 3.1.** *The matrix  $\tilde{\mathbf{A}}^{(0)} := \mathbf{A} - \gamma i(\mathbf{I} - \mathbf{v}_k \mathbf{v}_k^\top)$  has the same eigenvectors as  $\mathbf{A}$  with corresponding eigenvalues  $\lambda_j(\tilde{\mathbf{A}}^{(0)}) = \lambda_j - \gamma i$  for  $j \neq k$  and  $\lambda_k(\tilde{\mathbf{A}}^{(0)}) = \lambda_k$ .*

*Proof.* First consider  $j \neq k$ . We have

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

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

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

□

We now decompose  $\tilde{\mathbf{A}}$  into the sum  $\tilde{\mathbf{A}} = \tilde{\mathbf{A}}^{(0)} + \tilde{\mathbf{A}}^{(1)}$ , where  $\tilde{\mathbf{A}}^{(0)}$  is defined in Lemma 3.1 and  $\tilde{\mathbf{A}}^{(1)}$  is given by

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

Weyl's perturbation inequality then gives the bound

$$\max_{k=1}^n |\lambda_k(\tilde{\mathbf{A}}) - \lambda_k(\tilde{\mathbf{A}}^{(0)})| \leq \|\tilde{\mathbf{A}}^{(1)}\|. \quad (3.4) \quad \text{\{eq:weyl\}}$$

To compute the norm on the right hand side of (3.4) we make use of the following well-known facts from linear algebra.

**Proposition 3.2.** *Let  $\mathbf{A} \in \mathbb{R}^{n \times n}$  be a real symmetric matrix. Then*

- (a) *The sum of the eigenvalues of  $\mathbf{A}$  is equal to the trace of  $\mathbf{A}$  that is defined as the sum of its diagonal entries, i. e., ,*

$$\sum_{j=1}^n \lambda_j(\mathbf{A}) = \sum_{k=1}^n \mathbf{A}_{kk}.$$

Introduce  
eigen-  
value  
notation  
in  
chapter 1

# Appendices

# A Proofs

{AppendixProo

*Proof of Lemma 2.3.* This proof is due to Börm [1, p. 70].

Let  $\alpha \in \mathbb{C}$ . By using Lemma 2.2 (ii) we obtain

$$\begin{aligned}
 |\mathcal{R}_A(\mathbf{x}) - \lambda| &= |\mathcal{R}_{A-\lambda I}(\mathbf{x})| \\
 &= \left| \frac{\langle \mathbf{x}, (A - \lambda I)\mathbf{x} \rangle}{\langle \mathbf{x}, \mathbf{x} \rangle} \right| \\
 &= \frac{|\langle \mathbf{x}, (A - \lambda I)(\mathbf{x} - \alpha \mathbf{v}) \rangle|}{\|\mathbf{x}\|^2} \\
 &= \frac{|\langle (A - \lambda I)^* \mathbf{x}, \mathbf{x} - \alpha \mathbf{v} \rangle|}{\|\mathbf{x}\|^2} \\
 &= \frac{|\langle (A - \lambda I)^*(\mathbf{x} - \alpha \mathbf{v}), \mathbf{x} - \alpha \mathbf{v} \rangle|}{\|\mathbf{x}\|^2} \\
 &= \frac{|\langle \mathbf{x} - \alpha \mathbf{v}, (A - \lambda I)(\mathbf{x} - \alpha \mathbf{v}) \rangle|}{\|\mathbf{x}\|^2} \\
 &\leq \frac{\|\mathbf{x} - \alpha \mathbf{v}\| \|A - \lambda I\| \|\mathbf{x} - \alpha \mathbf{v}\|}{\|\mathbf{x}\|^2} \\
 &= \|A - \lambda I\| \left( \frac{\|\mathbf{x} - \alpha \mathbf{v}\|}{\|\mathbf{x}\|} \right)^2
 \end{aligned}$$

□

Finish  
proof  
(maybe  
in ap-  
pendix?)

## B Implementation of the Numerical Algorithms

{AppendixAlgo

### B.1 Generating random uniformly-distributed vectors on the $n$ -dimensional unit sphere

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