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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 reller symmetrischer Matrizen vorgestellt.

# Contents

# 1 Introduction

{chapter:intr

This thesis presents a modification of the *Rayleigh Quotient Iteration* that improves convergence to a target eigenpair under the assumption that a good approximation of the eigenvector but possibly not the eigenvalue is available. In this chapter we introduce an example from physics that has this property. We also collect all the definitions and results from linear algebra that will be needed later. Finally, we describe the objectives of this thesis.

## 1.1 Objectives and structure of this thesis

Rewrite

We have now established all the necessary results from linear algebra that are crucial to understanding the remaining of the thesis. We have also introduced the most basic iterative methods for solving the the eigenvalue problem (1.1) numerically.

In the next Chapter we study the Rayleigh Quotient and the above mentioned Rayleigh Quotient Iteration. Among others, we give a proof for the local cubic convergence of RQI and show that RQI converges for almost all starting vectors.

In the third chapter we introduce a novel shift-and-invert method that overcomes some of the disadvantages of classic RQI. We provide a wide variety of numerical examples that are carefully studied and analysed.

## 1.2 Motivation

The following example introduces a physical problem that requires the solution of an eigenvalue problem. Of course there are numerous problems in almost all of the natural sciences but also in finance and other social sciences (see, for example, ).

References for eigenvalue problems

{ex:modelprob

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

## 1.3 Results from 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.

### 1.3.1 The Symmetric Eigenvalue Problem

{sec:symmetri

In Example 1.1 a problem of the form

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

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 $\mathbf{A} \in \mathbb{C}^{n\times n}$ be a matrix. 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

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

{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 called the *spectrum* and is denoted by $\sigma(\mathbf{A})$.

Too often “is called”

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 of appropriate size. That is, $\lambda$ is an eigenvalue of $\mathbf{A}$ if and only if the matrix $\mathbf{A} - \lambda\mathbf{I}$ is singular. It follows, that the eigenvalues of $\mathbf{A}$ are the roots of the *characteristic polynomial*

$$\chi_{\mathbf{A}}(t) \coloneqq \chi(t) \coloneqq \det(\mathbf{A} - t\mathbf{I})\,.$$

This fact, however, cannot be used to calculate eigenvalues numerically since the computation of the coefficients of the polynomial is not stable [3, p. 37]. And even if it were, it is well-known that even small perturbations in the coefficients of $\chi_{\mathbf{A}}(t)$ can lead to devastating errors in the roots. In other words, finding the roots of a polynomial is an ill-conditioned task [cf. 18, 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 [6]. Below

we present essential facts from linear algebra preparing us for discussing such iterative methods in Section 1.3.2.

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., $\mathbf{A} = \mathbf{A}^* := \overline{\mathbf{A}}^\intercal$, 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 1.3.** *Let $\mathbf{A} = \mathbf{A}^* \in \mathbb{C}^{n\times n}$ be a Hermitian matrix. Denote by $\lambda_1, \lambda_2, \ldots, \lambda_n$ the eigenvalues[1] of $\mathbf{A}$ with associated eigenvectors $\mathbf{v}_1, \ldots, \mathbf{v}_n$.*

*(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 $\lambda_1^{-1}, \ldots, \lambda_n^{-1}$ with eigenvectors $\mathbf{v}_1, \ldots, \mathbf{v}_n$.*

*(iv) Let $\mu \in \mathbb{R}$ an arbitrary scalar. Then the eigenvalues of $\mathbf{A} - \mu\mathbf{I}$ are $\lambda_i - \mu$ with eigenvectors $\mathbf{v}_1, \ldots, \mathbf{v}_n$.*

*Proof.* The proofs for (i) and (ii) can be found in most standard linear algebra literature (see for example [4, 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

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

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

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

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

[1] Of course, the eigenvalues need not be distinct. But since the eigenvalues of $\mathbf{A}$ are the roots of the $n$-degree polynomial $\det(\mathbf{A} - t\mathbf{I})$, 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. e., $(\lambda - \mu, \mathbf{v})$ 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 $\lambda_1, \ldots, \lambda_n$ and $\mathbf{v}_1, \ldots, \mathbf{v}_n$, respectively. We assume that the eigenvalues are normalised w. r. t. the Euclidean norm, i. e.,

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

Note, that due to Proposition 1.3 (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

$$|\lambda_1| \leqslant |\lambda_2| \leqslant \ldots \leqslant |\lambda_n|\,.$$

The eigenvalues $\lambda_1$ and $\lambda_n$ are called *extreme* eigenvalues. The remaining eigenvalues $\lambda_2, \ldots, \lambda_{n-1}$ are called *interior* eigenvalues. Sometimes we will make the assumption that $\mathbf{A}$ is positive definite, i. e., that

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

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

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

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 $j = 1, \ldots, n$.

### 1.3.2 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.

#### Power method

The power method is based on generating the sequence $\mathbf{A}^k\mathbf{x}^{(0)}$ where $\mathbf{x}^{(0)}$ is a non-zero unit vector. Of course, $\mathbf{A}^k$ does not have to be computed explicitly since

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

When combined with some sort of normalisation step we arrive at Algorithm 1.4. There we normalise by ensuring that the largest component of the current approximation is equal to one as proposed in [16]. It is of course also possible to normalise w. r. t. the Euclidean norm [14, p. 75]. The sequence $\mathbf{x}^{(k)}$ converges to the eigenvector associated with the eigenvalue $\lambda_n$ (under the assumptions that $\lambda_n$ is semi-simple and that $\mathbf{x}^{(0)}$ is not orthogonal to $\mathbf{v}_n$, cf. [16, Theorem 4.1, p. 86]). The proof of the theorem also shows that the sequence $\alpha^{(k)}$ converges to the eigenvalue $\lambda_n$ and that the method converges linearly with convergence factor

Define semi-simple

$$\rho = \frac{|\lambda_{n-1}|}{|\lambda_n|}\,. \tag{1.2}$$ {eq:convergen

Thus, the method can be very slow if the distance between the eigenvalues $\lambda_n$ and $\lambda_{n-1}$ is very small.

**Algorithm 1.4:** 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:metho

Besides the possible slow convergence rate, the power method only allows to compute the extreme eigenvalue and associated eigenvector. In many applications, however, one

already has a good approximation of an eigenvalue and wants to compute the eigenvector it belongs to. The following method overcomes both of these drawpacks (at least partly).

### (Shifted) Inverse Iteration

The *inverse iteration* is the power method applied to $\mathbf{A}^{-1}$ (provided that $\mathbf{A}$ is non-singular). Due to Proposition 1.3 (iii) this will produce a sequence of vectors $\mathbf{v}_k$ converging to the eigenvector associated to the smallest eigenvalue $\lambda_1$. Combining this idea with Proposition 1.3 (iv) produces the *shifted inverse iteration*.[2] There, the iterates are defined by

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

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 $\mathbf{LU}$ decomposition of $\mathbf{A} - \sigma\mathbf{I}$ and solve the system

$$(\mathbf{A} - \sigma\mathbf{I})\mathbf{v}_k = \mathbf{v}_{k-1}$$

for $\mathbf{v}_k$ reducing the complexity from $\mathcal{O}(n^3)$ to $\mathcal{O}(n^2)$ at each step. We summarise the results in Algorithm 1.5 (there, we normalise w. r. t. the Euclidean norm such that at every step $\left\|\mathbf{v}^{(k)}\right\| = 1$ holds).

**Algorithm 1.5:** 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** $k = 1, 2, \ldots$ *until convergence* **do**
  Solve $(\mathbf{A} - \sigma\mathbf{I})\tilde{\mathbf{x}}^{(k)} = \mathbf{x}^{(k-1)}$ for $\tilde{\mathbf{x}}^{(k)}$
  $\mathbf{x}^{(k)} \leftarrow \tilde{\mathbf{x}}^{(k)} / \left\|\tilde{\mathbf{x}}^{(k)}\right\|$

{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

[2] Note that some authors call this the inverse iteration and do not make a distinction of a shift being used or not.

$(\mathbf{A} - \sigma\mathbf{I})^{-1}$ is $1/(\mu_1 - \sigma)$ and (1.2) suggests that the convergence factor is

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

Hence, the method can be very fast if the shift $\sigma$ is very close to the desired eigenvalue $\mu_1$. Therefore, the method is often used to compute an eigenvector of $\mathbf{A}$ if a good approximation of the corresponding eigenvalue is already available.

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

**Example 1.6.** Consider the matrix

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

Example of Power method and inverse iteration

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 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. [3, 5, 17].

# 2 Classic Rayleigh Quotient Iteration

{chapter:rqi}

In this chapter we thouroughly introduce the Rayleigh Quotient Iteration (or RQI, for short) and present important results regarding its analyis. 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 that will directly lead us the main part of the thesis, discussed in the next chapter.

## 2.1 The Rayleigh Quotient

Recall the general problem: Given approximations of an eigenvector of a symmetric matrix $\mathbf{A} = \mathbf{A}^\intercal \in \mathbb{R}^{n\times n}$ we want to compute the exact eigenvector and associated eigenvalue. In Section 1.3.2 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.

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

$$R_{\mathbf{A}} : \mathbb{C}^n \setminus \{\mathbf{0}\} \to \mathbb{C}, \qquad \mathbf{x} \mapsto \frac{\mathbf{x}^*\mathbf{A}\mathbf{x}}{\mathbf{x}^*\mathbf{x}}$$

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

Note that for real matrices, we have

$$R_{\mathbf{A}} : \mathbb{R}^n \setminus \{\mathbf{0}\} \to \mathbb{R}, \qquad \mathbf{x} \mapsto \frac{\mathbf{x}^\intercal\mathbf{A}\mathbf{x}}{\mathbf{x}^\intercal\mathbf{x}}$$

We begin by discussing some basic facts.

{lem:rq:prope

**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) For an eigenpair* $(\lambda, \mathbf{v})$ *of* $\mathbf{A}$ *we have* $R_{\mathbf{A}}(\mathbf{v}) = \lambda$.

*(ii)* $R_{\beta\mathbf{A}}(\alpha\mathbf{x}) = \beta R_{\mathbf{A}}(\mathbf{x})$ *(Homogenity)*

*(iii)* $R_{\mathbf{A}-\alpha\mathbf{I}}(\mathbf{x}) = R_{\mathbf{A}}(\mathbf{x}) - \alpha$ *(Translation invariance)*

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

$$R_{\mathbf{A}}(\mathbf{x}) = \frac{\langle \mathbf{x}, \mathbf{A}\mathbf{x}\rangle}{\langle \mathbf{x}, \mathbf{x}\rangle}, \tag{2.1}$$ {eq: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

$$R_{\mathbf{A}}(\mathbf{v}) = \frac{\langle \mathbf{v}, \mathbf{A}\mathbf{v}\rangle}{\langle \mathbf{v}, \mathbf{v}\rangle} = \frac{\langle \mathbf{v}, \lambda\mathbf{v}\rangle}{\langle \mathbf{v}, \mathbf{v}\rangle} = \lambda\frac{\langle \mathbf{v}, \mathbf{v}\rangle}{\langle \mathbf{v}, \mathbf{v}\rangle} = \lambda\,.$$

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

$$R_{\beta\mathbf{A}}(\alpha\mathbf{x}) = \frac{\langle \alpha\mathbf{x}, \beta\mathbf{A}(\alpha\mathbf{x})\rangle}{\langle \alpha\mathbf{x}, \alpha\mathbf{x}\rangle} = \beta\frac{\overline{\alpha}\alpha\langle \mathbf{x}, \mathbf{A}\mathbf{x}\rangle}{\overline{\alpha}\alpha\langle \mathbf{x}, \mathbf{x}\rangle} = \beta R_{\mathbf{A}}(\mathbf{x})\,.$$

(iii)
$$R_{\mathbf{A}-\alpha\mathbf{I}}(\mathbf{x}) = \frac{\mathbf{x}^*(\mathbf{A}-\alpha\mathbf{I})\mathbf{x}}{\mathbf{x}^*\mathbf{x}} = \frac{\mathbf{x}^*\mathbf{A}\mathbf{x} - \alpha\mathbf{x}^*\mathbf{x}}{\mathbf{x}^*\mathbf{x}} = R_{\mathbf{A}}(\mathbf{x}) - \alpha\,.$$

□

Altough 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

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

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. [2, 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

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

To see how good of an approximation the Rayleigh Quotient is we first need the notion of an *angle* between to vectors. This definition will be also used later when analysing the convergence of RQI.

**Definition 2.3** (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 identites are convenient

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

## 2.2 History and recent developments

In this section we provide an overview of the historic developments of Rayleigh Quotient Iteration. We also discuss recent contributions that are relevant to this thesis.

### 2.2.1 Chronology of Rayleigh Quotient iteration

We start by giving an overview on different algorithms that strongly resemble what we now call Rayleigh Quotient iteration. This section starts with the first mentioning of the Rayleigh quotient and ends with the paper the first defines Rayleigh quotient iteration as it is given in Algorithm **??**. This overview is mainly based on [17].

**1894 — Lord Rayleigh** In the second edition of his book titled "The Theory of Sound" John William Strutt, 3rd Baron Rayleigh [15, p. 110], proposed the following iteration for imporoving an approximate eigenvector $\mathbf{x}^{(0)}$:

$$\text{Solve} \quad (\mathbf{A} - \mathrm{R}_{\mathbf{A}}(\mathbf{x}^{(i)})\mathbf{I})\,\mathbf{x}^{(i+1)} = \mathbf{e}_1\,, \tag{2.2}$$

{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*

$$\mathbf{A}\mathbf{v} = \lambda\mathbf{M}\mathbf{v} \tag{2.3}$$

{eq:general:e

and so in his text, the iteration reads

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

**1949 — Kohn** In a letter to the editor Walter Kohn [7] suggest the following iteration

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

where $\mathbf{e}_k$ is *any* of the natural coordinate vectors. Without a rigorous proof Kohn argues that $\mathrm{R}_{\mathbf{A}}(\mathbf{x}^{(i)})$ 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 (2.2), Kohn does not mention Lord Rayleigh's method and it is not known whether or not he was aware of it.

Define notion of (linear, quadratic, cubic) convergence

**1951 — Crandall** In a text communicated to the Royal society of London Crandall [1] suggests

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

{eq:unnormali

Actually, Crandall also considered the generalised eigenproblem (2.3) but again for our 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 $\mathbf{x}^{(i)} \longrightarrow \mathbf{v}_k$ for some

Full name

$k = 1, \ldots, n$. From (2.4) we have

$$\boldsymbol{A}\mathbf{v}_k - R_{\boldsymbol{A}}(\mathbf{v}_k)\mathbf{v}_k = \mathbf{v}_k \qquad \Leftrightarrow \qquad \boldsymbol{A}\mathbf{v}_k = (1 + R_{\boldsymbol{A}}(\mathbf{v}_k))\mathbf{v}_k\,,$$

i. e., $\mathbf{v}_k$ is an eigenvector of $\boldsymbol{A}$ with corresponding eigenvalue $1 + R_{\boldsymbol{A}}(\mathbf{v}_k)$. Since we know that for any eigenvector, the value of $R_{\boldsymbol{A}}(\mathbf{v}_k)$ is the eigenvalue it belongs to we have

$$R_{\boldsymbol{A}}(\mathbf{v}_k) = 1 + R_{\boldsymbol{A}}(\mathbf{v}_k)$$

which is a contradiction.

**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 Cbaracterist Roots and Vectors. I-VI" [8–13]. 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

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

He rigorously establishes a *quadratic* convergence rate for the sequence $\{R_{\boldsymbol{A}}(\mathbf{x}^{(i)})\}$. He then refers to a paper of Wielandt [19] and his *fractional* or *broken iteration* (German: *gebrochene Iteration*). Inspired by Wielandt's method he proposes the following iteration

$$\text{Solve} \quad (\boldsymbol{A} - R_{\boldsymbol{A}}(\mathbf{x}^{(i)})\mathbf{I})\mathbf{x}^{(i+1)} = \mathbf{x}^{(i)}\,, \tag{2.5}$$ {eq: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 $\sigma_i \coloneqq R_{\boldsymbol{A}}(\mathbf{x}^{(i)})$, i. e.,

$$\frac{\sigma_{i+1} - \lambda}{(\sigma_i - \lambda)^3} \longrightarrow \gamma \quad \text{as } i \to \infty\,, \tag{2.6}$$ {eq:rqi:cubic

where $\lambda$ is an eigenvalue of $\boldsymbol{A}$ 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 (2.5) is the same algorithm previously proposed by Crandall given in Equation (2.4). Ostrowski, however, was not aware of Crandall's method. 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." [8, p. 241].[1]

In the beginning of the second paper [9] Ostrowski discusses this in more detail. 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. 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 [10] 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.

Read Ostrowski's other papers

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.

### 2.2.2 Further developments and recent contributions

## 2.3 Convergence of RQI

[1] 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 (2.5) and the asymptotic formula (46) he references is given in (2.6).

# 3 Complex Rayleigh Quotient Iteration

In this chapter we introduce *Complex Rayleigh Quotient Iteration* (CRQI[1]). This is a novel shift and invert type algorithm similar to classic RQI that overcomes some of its disadvantages.
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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 $\mathbf{v}_1, \ldots, \mathbf{v}_n$ 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 $\alpha_1, \ldots, \alpha_n \in \mathbb{R}$. Suppose now, that $\mathbf{u}$ is a good approximation for one of the eigenvectors, say for $\mathbf{v}_k$. Then

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

Due to the pairwise orthogonality of the eigenvectors this implies

$$\mathbf{u}^\mathsf{T}\mathbf{v}_j \approx \begin{cases} 1 & \text{if } j = k\,, \\ 0 & \text{if } j \neq k\,. \end{cases} \tag{3.1}$$ {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

Rewrite

[1] 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*.

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.

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

$$\tilde{\mathbf{A}} \coloneqq \mathbf{A} - \gamma \mathrm{i}(\mathbf{I} - \mathbf{u}\mathbf{u}^{\mathsf{T}}) \tag{3.2}$$ {eq:a:tilde}

instead of $\mathbf{A}$, where $\gamma > 0$ is positive real number and $\mathrm{i}$ denotes the imaginary unit. To get an intuition on why we choose this matrix, we first note that the matrix $\mathbf{I} - \mathbf{u}\mathbf{u}^{\mathsf{T}}$, 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

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

Look up projection formulas, search references and correct dervia-tion

Therefore, a vector $\mathbf{x}$ that is almost parallel to $\mathbf{u}$ will bareley "see" the imaginary part $\gamma \mathrm{i}(\mathbf{I} - \mathbf{u}\mathbf{u}^{\mathsf{T}})$ 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

$$\tilde{\mathbf{A}}\mathbf{x} = \mathbf{A}\mathbf{x} - \gamma \mathrm{i}\mathbf{x} - \mathbf{u} \underbrace{\mathbf{u}^{\mathsf{T}}\mathbf{x}}_{\approx 0} \approx (\mathbf{A} - \gamma \mathrm{i}\mathbf{I})\mathbf{x}. \tag{3.3}$$ {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 $\lambda_j - \gamma \mathrm{i}$ due to (3.3). The eigenvalue corresponding to $\mathbf{v}_k$ would then be approximately equal to $\lambda_k$ since $\tilde{\mathbf{A}}\mathbf{v}_k \approx \mathbf{A}\mathbf{v}_k = \lambda_k \mathbf{v}_k$.

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* $\tilde{\mathbf{A}}^{(0)} \coloneqq \mathbf{A} - \gamma i(\mathbf{I} - \mathbf{v}_k\mathbf{v}_k^T)$ *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* $\lambda_k(\tilde{\mathbf{A}}^{(0)}) = \lambda_k$.

Introduce eigenvalue notation in chapter 1

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

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

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

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

□

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

$$\tilde{\mathbf{A}}^{(1)} \coloneqq \gamma i(\mathbf{u}\mathbf{u}^T - \mathbf{v}_k\mathbf{v}_k^T)\,.$$

Weyl's perturbation inequality then gives the bound

$$\max_{k=1}^{n} |\lambda_k(\tilde{\mathbf{A}}) - \lambda_k(\tilde{\mathbf{A}^0})| \leqslant \left\|\tilde{\mathbf{A}}^{(1)}\right\|. \tag{3.4}$$

{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., ,*

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

# A Implementation of the Numerical Algorithms

{AppendixA}

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

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