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Using Complex Shifts in Rayleigh Quotient Iteration to Compute Close Eigenvalues

Bachelor Thesis

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Erklärung

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Heidelberg, den 21. Mai 2020

(Nils Frieß)

Abstract Rayleigh Quotient Iteration (RQI) is an algorithm to compute an approximate eigenvector and corresponding eigenvalue of a real symmetric matrix. It is well-known that RQI exhibits local cubic convergence but the behaviour of the method is sometimes erratic. Even when started with accurate approximations of an eigenvalue, the algorithm might converge to a different eigenpair than the desired one and this becomes worse when the eigenvalues around the target are closely spaced. In this thesis we propose a modification of RQI that ensures convergence to the desired eigenpair provided that the angle between the initial vector and the target eigenvector is sufficiently small. Numerical examples suggest that “sufficiently small” means approximately below 45° —independent of the spacing of the eigenvalues.

Zusammenfassung Die Rayleigh-Quotient-Iteration (RQI) ist ein Algorithmus um einen Eigenvektor und zugehörigen Eigenwert einer reellen, symmetrischen Matrix zu berechnen. Es ist bekannt, dass RQI lokal kubisch konvergiert, jedoch ist das Verhalten der Methode bisweilen unberechenbar. Selbst wenn RQI mit guten Approximationen eines Eigenvektors ausgeführt wird, ist nicht sichergestellt, dass das berechnete Eigenpaar das gewünschte ist. Dieses Verhalten tritt besonders dann auf, wenn die Eigenwerte um den gesuchten Eigenwert einen sehr geringen Abstand zu diesem Eigenwert haben. In dieser Arbeit schlagen wir eine Abwandlung von RQI vor, die sicherstellt, dass die Methode das gewünschten Eigenpaar berechnet, vorausgesetzt der Winkel zwischen Anfangsvektor und dem Ziel-Eigenvektor ist hinreichend klein. Numerische Beispiele weisen darauf hin, dass „hinreichend klein“ bedeutet, dass der Winkel ungefähr kleiner als 45° ist – unabhängig vom Abstand der Eigenwerte.

Contents

List of Algorithms	ii
List of Figures	iii
1 Introduction	1
1.1 The Symmetric Eigenvalue Problem	2
1.2 Iterative Methods for Eigenvalue Problems	6
2 Classic Rayleigh Quotient Iteration	13
2.1 The Rayleigh Quotient	13
2.2 History and Recent Developments	18
2.2.1 Chronology of Rayleigh Quotient Iteration	18
2.2.2 Further Developments and Recent Contributions	22
2.3 Convergence Analysis	25
2.4 Conclusions	34
3 Complex Rayleigh Quotient Iteration	35
3.1 Motivation	36
3.2 Numerical Experiments	44
4 Concluding Remarks	57
A Proofs	59
B Additional Plots and Tables	63
Bibliography	80

List of Algorithms

1.6	Power method	8
1.7	Shifted inverse iteration	10
2.4	Rayleigh Quotient Iteration	16
3.4	Complex Rayleigh Quotient Iteration (first version)	40
3.6	Complex Rayleigh Quotient Iteration	43

List of Figures

3.1	Spectrum of the original problem and the perturbed problem	38
3.2	Residuals for different choices of $\gamma^{(k)}$	48
3.3	RQI and CRQI with varying initial shifts	51
3.4	Effect of the initial error angle	54
3.5	Number of iterations for different angles for a random matrix .	56
B.1	Residuals for the [1, 2, 1] matrix	64
B.2	Residuals for the Wilkinson matrix \mathbf{W}^+	65
B.3	Residuals for the Martin-Wilkinson matrix \mathbf{MW}	66
B.4	Residuals for the Laplace matrix	67
B.5	Effect of real shift for [1, 2, 1] matrix	69
B.6	Effect of real shift for the Wilkinson matrix \mathbf{W}^+	70
B.7	Effect of real shift for the Martin-Wilkinson matrix \mathbf{MW} . . .	71
B.8	Effect of real shift for the Laplace matrix	72
B.9	Effect of the initial error angle for the matrix [1, 2, 1]	73
B.10	Effect of the initial error angle for the Wilkinson matrix \mathbf{W}^+ .	74
B.11	Effect of the initial error angle for the Martin-Wilkinson matrix \mathbf{MW}	75
B.12	Number of iterations for different angles for the [1, 2, 1] matrix	76
B.13	Number of iterations for different angles for the Wilkinson matrix \mathbf{W}^+	77
B.14	Number of iterations for different angles for the Martin-Wilkinson matrix \mathbf{MW}	78
B.15	Number of iterations for different angles for the Laplace matrix	79

1 Introduction

In this thesis we propose 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) designed to overcome some of the drawbacks of RQI. It is well-known that RQI is often unpredictable in the sense that even when executed with accurate eigenvector approximations it does not necessarily yield the correct eigenpair. This problem becomes worse in cases where the distance between the wanted eigenvalue and its neighbours is very small. In our new method we perturb the original problem in such a way that the spacing between the target eigenvalue and the other eigenvalues is increased and apply RQI to this perturbed problem. Obviously, this approach alone would lead to incorrect results. Therefore, the perturbation is successively decreased until we finally arrive at the original problem and we hope that by that time the current eigenvalue approximation has become sufficiently close to the correct result so that RQI succeeds. For this approach to work, a sufficiently good eigenvector approximation is needed and our numerical experiments suggest that “sufficiently good” means that the angle between the initial approximation and the target eigenvector is below 45° —independent of the spacing of the eigenvalues. Although the method converges not as fast as RQI, often merely three or four additional iterations are required compared to RQI.

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. Since our new algorithm is strongly related to RQI, the second chapter is devoted to a detailed study of the Rayleigh Quotient and RQI. Among others, we give a proof of 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 for various test problems to better understand its behaviour and to illustrate the good properties mentioned above.

The aim of this thesis is not to carry out a mathematical analysis of the method but rather to discuss various numerical examples that illustrate different behavioural aspects of the algorithm. We leave a detailed analysis of the method based on our observations for future work.

1.1 The Symmetric Eigenvalue Problem

Eigenvalues and eigenvectors of matrices play an important role in many branches of science and engineering. A typical example from physics is the computation of the natural frequencies of a structure, i.e., frequencies at which the structure is prone to vibrate. To determine these frequencies, an eigenvalue problem needs to be solved. Often, the actual problem is given for a differential operator and the matrix eigenvalue problem arises when the operator is discretized. To accurately approximate the operator, the matrix needs to be large but when discretized with, for example, a finite difference or finite element approach it is usually sparse. In a number of applications the resulting matrix is real and symmetric and the task of finding eigenvalues and eigenvectors is then referred to as the *symmetric eigenvalue problem*. For completeness, we collect some facts from linear algebra on eigenvalues and eigenvectors for the general complex case.

Definition 1.1. Let $\mathbf{A} \in \mathbb{C}^{n \times n}$. A scalar $\lambda \in \mathbb{C}$ is called an *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 $\mathbf{Av} - \lambda\mathbf{v} = \mathbf{0}$ or $(\mathbf{A} - \lambda\mathbf{I})\mathbf{v} = \mathbf{0}$, where \mathbf{I} is the identity matrix. This equation has a solution if and only if the matrix $\mathbf{A} - \lambda\mathbf{I}$ is singular since by definition \mathbf{v} must not be the zero vector. 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 [10, p. 37]. Second, it is well-known that even small perturbations in the coefficients of $\chi_{\mathbf{A}}(t)$ can lead to large errors in the calculation of the roots [35, p. 190]. Thus, other methods are necessary to solve (1.1), which has given 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 [14]. Below we present essential facts from linear algebra preparing us for a discussion of 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*

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

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 symmetry and 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 almost exclusively consider problems of the form (1.1).

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.

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

(i) *All eigenvalues of \mathbf{A} are real.*

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 .

- (ii) There exists an orthonormal basis of \mathbb{C}^n consisting of eigenvectors of \mathbf{A} . If \mathbf{A} is a real symmetric matrix, then the eigenvectors form an orthonormal basis of \mathbb{R}^n .
- (iii) If \mathbf{A} is non-singular, then 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. Then 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, [12, 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

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

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

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

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.

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

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

For the error angle $\phi^{(k)} = \angle(\mathbf{x}^{(k)}, \mathbf{z})$ to be zero it suffices that the vectors are scalar multiples of each other. For the error norm $\|\mathbf{x}^{(k)} - \mathbf{z}\|$ to be zero they must also have the same norm. Since for eigenvectors only their direction is important, the angle is often a more natural measure for convergence and unnecessary normalisations can be avoided in the analysis.

Power method

The *power method* or *Von Mises iteration* 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 analysis, see [31, pp. 85–87].

Algorithm 1.6: Power method

Input: Nonzero unit vector $\mathbf{x}^{(0)}$
for $k = 1, 2, \dots$ *until convergence do*

$$\left[\begin{array}{l} \alpha^{(k)} \leftarrow \max |\mathbf{A}\mathbf{x}^{(k-1)}| \\ \mathbf{x}^{(k)} \leftarrow \alpha^{(k)-1} \mathbf{A}\mathbf{x}^{(k-1)} \end{array} \right]$$

In addition to 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. In this situation, the following method can be used.

(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. The most expensive step of this procedure is obviously the computation of the inverse at each step. Fortunately, this computation is not necessary since instead of explicitly computing the inverse, before the loop we can compute the LU decomposition of $\mathbf{A} - \sigma\mathbf{I}$ and solve the system $(\mathbf{A} - \sigma\mathbf{I})\mathbf{x}^{(k)} = \mathbf{x}^{(k-1)}$ 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

²Note that we did not specify the “until convergence” criterion in either 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 \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 $\tilde{\mathbf{x}}^{(k)}$
 | $\mathbf{x}^{(k)} \leftarrow \tilde{\mathbf{x}}^{(k)}/\|\tilde{\mathbf{x}}^{(k)}\|$

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 a shift that is very close to an eigenvalue produces a very ill-conditioned linear system, and one might expect inverse iteration to fail in this case. Despite this seemingly obvious problem, in practice it was observed that the method produces good approximations. According to Parlett [26, pp. 84f.], 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 in a backwards-stable way. For a detailed analysis of this problem, see [37, pp. 621–630], [26, pp. 68–71] and [28]. 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. There are different techniques to obtain approximations of the corresponding eigenvalue. One of these methods, which

leads to the *Rayleigh Quotient Iteration*, is discussed in detail in the next chapter. For further discussion on the variants and developments of these so called *shift-and-invert* methods see, e. g., the historic survey [13] or Sections 2 and 3 of [34].

As mentioned above, we want to find the eigenvalues and eigenvectors of a real symmetric matrix \mathbf{A} . There is a wide variety of other algorithms, both direct and iterative, that are suitable for this problem. Some of them also compute only a single eigenvector (and/or eigenvalue) as the algorithms from above do, some compute the complete spectrum and full set eigenvectors while some compute only a fixed number of the eigenvalues and corresponding eigenvectors. We make the following additional assumptions about the problem:

- (A1) The matrix \mathbf{A} is large and sparse.
- (A2) A good approximation of the wanted eigenvector is available.
- (A3) The wanted eigenvalue lies in the interior of the spectrum.
- (A4) The eigenvalues around the wanted eigenvalue are closely spaced.

The first assumption prohibits us from using an algorithm that computes the full eigendecomposition and rules out direct methods. Due to the second assumption we seek a method that makes use of the approximation in the sense that fewer iterations are required the more accurate the given approximation is. Assumption (A3) seems to pose no real constraint at first sight. However, many of the different eigenvalue algorithms are only capable of finding a few eigenvalues at either end of the spectrum or they are at least considerably faster/more likely to succeed in these cases. As we will see later, RQI is a suitable choice if we omit the last assumption, i. e., for problems with well-separated eigenvalues. Since our novel method is based on RQI it is also suited for problems that fulfil the first three assumptions. Obviously,

1 Introduction

it is also adequate for problems with closely spaced eigenvalues since it is precisely designed for such problems.

Apart from Rayleigh Quotient Iteration and our new method we do not discuss any other algorithms. For further discussion on the variants and developments of the different eigenvalue methods we refer to the historic survey [10] and the references therein which include the classic monographs by Saad [31] (that is concerned with large scale problems) and by Parlett [26] (that considers the symmetric eigenvalue problem).

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 most appealing property of RQI, namely the (local) cubic convergence. We also provide an overview on the history of RQI and discuss some more recent contributions. Various numerical experiments that illustrate the different properties will be given in the next chapter where we compare RQI with our new method. In this chapter we only look at very few numerical examples.

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} .³

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 $\mathbf{A} \in \mathbb{C}^{n \times n}$.*

³Other 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 (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

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

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

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

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. [8, 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” [26, p. 77]. We postpone the proof of this statement until Section 2.3 where 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 normal⁴ matrix \mathbf{A} with corresponding eigenvalue λ . Then*

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

This result is often paraphrased as “the Rayleigh Quotient is a *quadratically accurate* estimate of an eigenvalue” (see, for example, [35, p. 204]). If \mathbf{A} is

⁴A 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.

non-normal, the Rayleigh Quotient is still an estimate of order one, i.e.,

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

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. We summarise the results in Algorithm 2.4.

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

Note, that in the computation of the Rayleigh Quotient the division by $(\mathbf{x}^{(k)})^* \mathbf{x}^{(k)}$ can be omitted. The vector is already normalised at the previous step so that the denominator of the Rayleigh Quotient is equal to one.

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

$$\|\mathbf{r}^{(k)}\| = \|\mathbf{A}\mathbf{x}^{(k)} - \mu^{(k)}\mathbf{x}^{(k)}\| < \text{tol}, \quad (2.2)$$

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, 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 [31, 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. [31, p. 59]) states that there exists an eigenvalue λ of \mathbf{A} such that

$$|\lambda - \mu^{(k)}| \leq \|\mathbf{r}^{(k)}\|. \quad (2.3)$$

Thus, if the stopping criterion is fulfilled, we have $|\lambda - \mu^{(k)}| < \text{tol}$. For the eigenvector one can show [31, 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.,

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

Thus, if the wanted eigenvalues and its neighbours are very close, δ is large and the eigenvector might not be accurate. Due to the cubic convergence of RQI (which we will discuss below) instead of stopping the iteration as soon as the criterion in (2.2) is fulfilled, we simply run another iteration. Often, the residual norm will then already be close to working accuracy and the

eigenvector is sufficiently accurate. If more information about the spectrum is available, one could also adjust the stopping criterion accordingly.

2.2 History and Recent Developments

In this section we give an overview on the history 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 [34].

1894 — Lord Rayleigh In the second edition of his book titled “The Theory of Sound” John William Strutt, 3rd Baron Rayleigh [29, p. 110], proposed the following iteration for improving an approximate eigenvector $\mathbf{x}^{(0)}$:

$$\text{Solve } (\mathbf{A} - \mathcal{R}_{\mathbf{A}}(\mathbf{x}^{(k)})\mathbf{I})\mathbf{x}^{(k+1)} = \mathbf{e}_1, \quad (2.4)$$

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

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

1949 — Kohn In a letter to the editor Walter Kohn [15] suggests the following iteration

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

where \mathbf{e}_m is *any* of the natural coordinate vectors. Without a rigorous proof Kohn argues that $\mathcal{R}_{\mathbf{A}}(\mathbf{x}^{(k)})$ 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 (2.4), 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

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

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. Crandall establishes cubic convergence of the sequence of vector iterates and the approximate eigenvalue sequence $\mathcal{R}_{\mathbf{A}}(\mathbf{x}^{(k)})$. His analysis is based on the assumption that the sequence of vectors $\mathbf{x}^{(k)}$ does converge. To see why the assumption is wrong, we assume the contrary, i. e., suppose that the sequence converges to an eigenvector, say \mathbf{v}_j . From (2.5) we have

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

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

it belongs to, this implies

$$\mathcal{R}_A(\mathbf{v}_j) = 1 + \mathcal{R}_A(\mathbf{v}_j),$$

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 [34, 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” [18–23]. 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

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

He rigorously establishes a *quadratic* convergence rate for the sequence of Rayleigh Quotients $\mathcal{R}_A(\mathbf{x}^{(i)})$. He then refers to a paper of Wielandt [36] 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 (2.6) by the solution from the previous step

$$(\mathbf{A} - \mathcal{R}_A(\mathbf{x}^{(i)})\mathbf{I})\mathbf{x}^{(i+1)} = \mathbf{x}^{(i)}, \quad (2.7)$$

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

$\mu_i := \mathcal{R}_A(\mathbf{x}^{(i)})$, i.e.,

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

where λ is an eigenvalue of 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 (2.7) 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 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.” [18, p. 241].⁵

In the beginning of the second paper [19] Ostrowski discusses this in more detail and remarks that Crandall proved 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 [20] 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

⁵Here, 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 (2.7) and the asymptotic formula (46) he references is given in (2.8).

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 [27] showed that RQI applied to symmetric matrices converges for almost all starting vectors and in 1974 Parlett [25] generalised the result to the case when \mathbf{A} is normal. A slightly more concise version of the proof has been again published in Parlett's book [26].

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 [24, 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 results in the eigenpair $(1, \mathbf{e}_1)$ although the Rayleigh Quotient of the initial shift is

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

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

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

The corresponding 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 makes 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 [18] 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, and 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 computable criteria that ensure that the iterates and thus the computed eigenvalue stay within a given interval; only the number of eigenvalues contained in the interval needs to be known.

Szyld [33] 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).

Recently, Rommes [30] derived sharper bounds for local convergence neighbourhoods. He compares RQI with 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.

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 $\mathbf{x}^{(0)}$ ’ [26, p. 82] and it looks as if this statement still holds true today. Pantazis and Szyld [24] 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 [33] 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 [32] and Notay in [17]. 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

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

is sought that satisfies

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

where $\tau^{(k)}$ is a tolerance that might change at each step. In [32] the authors also show 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 [7]. There, it is also studied how different preconditioners for the linear system can be used to improve the outer convergence of inexact RQI. 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 [18] but over time a number of different, simpler proofs were presented. The one we give below follows closely the one given by Demmel [6, pp. 215 f.].

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 $(\mathbf{x}^{(k)})_i$ 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 [26, p. 77].

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 RQI⁶ to $\hat{\mathbf{x}} := \mathbf{Q}^\top \mathbf{x}$ and $\hat{\mathbf{y}} := \mathbf{Q}^\top \mathbf{y}$. Then

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

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

$$\begin{aligned} \hat{\mathbf{y}}^{(k+1)} &= \mathbf{Q}^\top (\mathbf{A} - \mu^{(k)} \mathbf{I})^{-1} \mathbf{Q} \hat{\mathbf{x}}^{(k)} \\ &= (\mathbf{Q}^\top \mathbf{A} \mathbf{Q} - \mu^{(k)} \mathbf{I})^{-1} \hat{\mathbf{x}}^{(k)} = (\Lambda - \mu^{(k)} \mathbf{I})^{-1} \hat{\mathbf{x}}^{(k)} , \end{aligned}$$

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 Λ and $\hat{\mathbf{x}}^{(0)}$. Thus, we assume that $\mathbf{A} = \Lambda$ is already diagonal which in particular implies that the eigenvectors of \mathbf{A} are \mathbf{e}_i , the natural coordinate vectors.

Proof of Theorem 2.6. Suppose without loss of generality that $\mathbf{x}^{(k)}$ 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 k we can write $\mathbf{x}^{(k)} = \mathbf{e}_1 + \mathbf{d}^{(k)}$ with $\|\mathbf{d}^{(k)}\| = \epsilon \ll 1$. To show cubic convergence, we have to verify that

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

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

⁶Recall the notation from Algorithm 2.4 where $\mathbf{y} = \mathbf{y}^{(k)}$ denotes the unnormalised k th iterate and $\mathbf{x} = \mathbf{x}^{(k)}$ denotes the same iterate after normalisation.

Since the vectors are normalised at each step we have

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

where $d_1^{(k)}$ denotes the first component of the vector $\mathbf{d}^{(k)}$. Rewriting gives $d_1^{(k)} = -\epsilon^2/2$ and using the symmetry⁷ of Λ we obtain

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

where

$$\eta := -2\mathbf{e}_1^\top \Lambda \mathbf{d}^{(k)} - (\mathbf{d}^{(k)})^\top \Lambda \mathbf{d}^{(k)} = \lambda_1 \epsilon^2 - (\mathbf{d}^{(k)})^\top \Lambda \mathbf{d}^{(k)}.$$

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

$$|\eta| \leq |\lambda_1| \epsilon^2 + \|\Lambda\| \|\mathbf{d}^{(k)}\|^2 \leq |\lambda_{\max}| \epsilon^2 + \|\Lambda\| \epsilon^2 = 2\|\Lambda\| \epsilon^2 \quad (2.9)$$

⁷For a symmetric matrix $\mathbf{B} = \mathbf{B}^\top$ holds

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

and we see that $\mu^{(k)} = \lambda_1 - \eta = \lambda_1 + \mathcal{O}(\epsilon^2)$ (note that this proves Lemma 2.3, the quadratic accuracy of the Rayleigh Quotient). We obtain

$$\begin{aligned}
 \mathbf{y}^{(k+1)} &= (\Lambda - \mu^{(k)})^{-1} \mathbf{x}^{(k)} \\
 &= \left(\frac{x_1^{(k)}}{\lambda_1 - \mu^{(k)}}, \frac{x_2^{(k)}}{\lambda_2 - \mu^{(k)}}, \dots, \frac{x_n^{(k)}}{\lambda_n - \mu^{(k)}} \right)^T \\
 &= \left(\frac{1 + d_1^{(k)}}{\lambda_1 - \mu^{(k)}}, \frac{d_2^{(k)}}{\lambda_2 - \mu^{(k)}}, \dots, \frac{d_n^{(k)}}{\lambda_n - \mu^{(k)}} \right)^T \\
 &= \left(\frac{1 - \frac{\epsilon^2}{2}}{\eta}, \frac{d_2^{(k)}}{\lambda_2 - \lambda_1 + \eta}, \dots, \frac{d_n^{(k)}}{\lambda_n - \lambda_1 + \eta} \right)^T \\
 &= \frac{1 - \frac{\epsilon^2}{2}}{\eta} \left(1, \frac{d_2^{(k)} \eta}{(1 - \frac{\epsilon^2}{2})(\lambda_2 - \lambda_1 + \eta)}, \dots, \frac{d_n^{(k)} \eta}{(1 - \frac{\epsilon^2}{2})(\lambda_n - \lambda_1 + \eta)} \right)^T \\
 &=: \frac{1 - \frac{\epsilon^2}{2}}{\eta} (\mathbf{e}_1 + \hat{\mathbf{d}}^{(k+1)}),
 \end{aligned}$$

where in the first step we used that the inverse of a diagonal matrix consists of the inverse of the entries on the diagonal. The next step holds since $\mathbf{x}^{(k)} = \mathbf{e}_1 + \mathbf{d}^{(k)}$ by assumption. After that we use that we can write $\mu^{(k)} = \lambda_1 - \eta$ and $d_1^{(k)} = -\epsilon^2/2$. If we denote again by δ the gap between λ_1 and the rest of the spectrum, i. e.,

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

we can bound the denominators of $\hat{\mathbf{d}}^{(k+1)}$ using $|\lambda_j - \lambda_1 + \eta| \geq \delta - |\eta|$, and in conjunction with (2.9) we get

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

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

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

we see that also $\|\mathbf{d}^{(k+1)}\| = \mathcal{O}(\epsilon^3)$, 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 [26, 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 greater detail, cubic convergence of RQI is proved 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 [35, p. 208] or [3, pp. 89f.].

To conclude this section 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 [26, p. 85], is due to Kahan [27]. 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 $(k + 1)$ st iterate of RQI by

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

for some β which implies

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

and thus

$$\|(\mathbf{A} - \mu^{(k)} \mathbf{I}) \mathbf{x}^{(k+1)}\| = |(\mathbf{x}^{(k)})^* (\mathbf{A} - \mu^{(k)} \mathbf{I}) \mathbf{x}^{(k+1)}|. \quad (2.10)$$

Proof of Lemma 2.7.

$$\begin{aligned} \|\mathbf{r}^{(k+1)}\| &= \|(\mathbf{A} - \mu^{(k+1)} \mathbf{I}) \mathbf{x}^{(k+1)}\| \\ &\leq \|(\mathbf{A} - \mu^{(k)} \mathbf{I}) \mathbf{x}^{(k+1)}\| \quad (\mu^{(k+1)} \text{ minimises the residual norm}) \\ &= |(\mathbf{x}^{(k)})^* (\mathbf{A} - \mu^{(k)} \mathbf{I}) \mathbf{x}^{(k+1)}| \quad (\text{by (2.10)}) \\ &\leq \|(\mathbf{x}^{(k)})^* (\mathbf{A} - \mu^{(k)} \mathbf{I})\| \|\mathbf{x}^{(k+1)}\| \quad (\text{by the Cauchy-Schwarz inequality}) \\ &= \|(\mathbf{x}^{(k)})^* (\mathbf{A} - \mu^{(k)} \mathbf{I})\| \quad (\mathbf{x}^{(k+1)} \text{ is a unit vector}) \\ &= \|(\mathbf{A} - \mu^{(k)} \mathbf{I}) \mathbf{x}^{(k)}\| \quad (\mathbf{A} \text{ is symmetric}) \\ &= \|\mathbf{r}^{(k)}\|. \end{aligned}$$

□

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 $\mathbf{v}_{pq}^\pm = (\mathbf{v}_p \pm \mathbf{v}_q)/\sqrt{2}$ and λ_p, 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 [26]. We begin by observing that the monotonicity of the residuals implies

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

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 Parlett concludes 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 \mathbf{A} to its square \mathbf{A}^2 . Therefore, as mentioned above, we do not discuss this part of the proof here.

Example 2.9. To illustrate the situation in the second part of the theorem consider RQI applied to the diagonal matrix $\mathbf{A} = \text{diag}(1, 2, 4)$ with initial vector

$$\mathbf{x}^{(0)} = \begin{pmatrix} \frac{1}{\sqrt{2}} & \frac{1}{\sqrt{2}} & 0 \end{pmatrix}^\top.$$

It is easy to check that this results in $\mu^{(k)} = 1.5$ and

$$\mathbf{x}^{(2k)} = \begin{pmatrix} \frac{1}{\sqrt{2}} & \frac{1}{\sqrt{2}} & 0 \end{pmatrix}^\top \quad \text{and} \quad \mathbf{x}^{(2k+1)} = \begin{pmatrix} -\frac{1}{\sqrt{2}} & \frac{1}{\sqrt{2}} & 0 \end{pmatrix}^\top$$

for $k = 0, 1, 2, \dots$. The instability mentioned in the theorem essentially prevents the method from failing in practice since roundoff errors will inevitably introduce perturbations of the vector iterate. However, this can drastically increase the number of steps before the cubic convergence takes place. In this particular example, when executed in Matlab [16] the method requires 36 steps in total.

Parlett states in [26, p. 61] and in [25, 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 2.10. *The set of unit vectors for which RQI does not converge to an eigenvector is a set of measure zero.*

2.4 Conclusions

In this chapter we have seen that RQI possesses some very favourable properties. It is practically impossible to make RQI fail to converge to any eigenpair and convergence is locally cubic. However, we have also discussed that in some cases it seems to be difficult, if not impossible, to predict which eigenpair the method will converge to. As we will see in the next chapter, for problems with closely spaced eigenvalues even very accurate eigenvector approximations can lead to the wrong result. While virtually every publication that discusses RQI mentions its appealing properties, almost all of them do also mention this erratic behaviour. For instance, the papers [2, 5] and [24] refer to the “unpredictability” of RQI. In Parlett’s book [26] it is posed as an exercise to find a 3×3 example that shows this behaviour. Beattie and Fox [2] and Dax [5] even claim that this might be one of the reasons why RQI is not as widely used (another reason being its high cost).

The main purpose of our novel method is to alter RQI in such a way that this problem is overcome. Although this cannot be done without loosing some of the beneficial properties of RQI, the observations from the numerical experiments in the next chapter are very promising. The algorithm does generally require more iterations but is much more predictable; once the error angle between the initial vector and the target eigenvector is sufficiently small, it will always yield the correct result.

3 Complex Rayleigh Quotient Iteration

In this chapter we introduce the *Complex Rayleigh Quotient Iteration* (CRQI⁸). 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.

The idea of the method can be outlined as follows. Using the eigenvector approximation, the original problem is perturbed such that the distance between the desired eigenvalue and the remaining eigenvalues is increased. In particular, we make use of the fact that the eigenvalues are all real and “raise” them into the complex plane. By making use of the orthogonality of the eigenvectors we are able to keep the target eigenvalue near the real line and push the remaining eigenvalues into the complex plane. RQI is then applied to this perturbed problem. Of course, this approach alone would yield incorrect results. We therefore decrease the perturbation successively until we finally arrive at the original problem and we hope by that time the current eigenvalue approximation is sufficiently close to the wanted eigenvalue so that RQI succeeds.

After discussing this idea in more detail we provide various numerical experiments. The outcome of the examples is very promising; in particular we will see that the method seems to compute the correct result provided that

⁸We 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*.

the angle between the eigenvector approximation and the target eigenvector is below 45° —independent of the spacing of the eigenvalues.

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

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

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 see in Section 3.2 that classic RQI seems to barely make use of the information incorporated in the initial vector. The main goal 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 system will lead to wrong solutions and so we will decrease this perturbation successively until we arrive at the unperturbed problem and hope that by the time we reach the original problem, the shift is sufficiently close to the target eigenvalue.

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 eigenvalues is increased (since the close spacing of the spectrum is what makes computing the correct eigenvalue so hard in the first place). This is done by incorporating the approximation \mathbf{u} of the target eigenvector \mathbf{v}_k into the perturbed matrix. Let

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

where $\gamma > 0$ is positive real number and i denotes the imaginary unit. Note that the matrix $\mathbf{I} - \mathbf{u}\mathbf{u}^T$ 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 $i\gamma(\mathbf{I} - \mathbf{u}\mathbf{u}^T)$ 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

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

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 . Since the latter is the subspace spanned by the remaining eigenvectors, 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 $\lambda_j - i\gamma$. The eigenvalue correspond-

ing to \mathbf{v}_k would then be approximately equal to λ_k since $\tilde{\mathbf{A}}\mathbf{v}_k \approx \mathbf{A}\mathbf{v}_k = \lambda_k\mathbf{v}_k$. In the figure below we plotted the spectrum of \mathbf{A} together with the spectrum of the perturbed matrix $\tilde{\mathbf{A}}$ for $\gamma = 1$. In this example we had $\mathbf{u}^\top \mathbf{v}_k \approx 0.83568$, where \mathbf{v}_k is the target eigenvector. The wanted eigenvalue stays near the real line while the rest of the spectrum gets “pushed down” into the complex plane.⁹

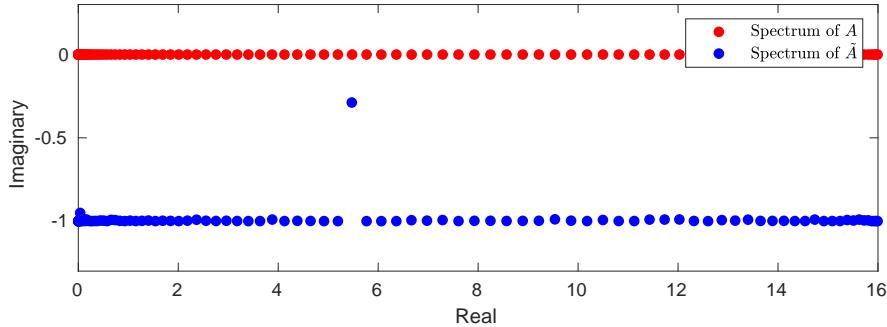


Figure 3.1: Spectrum of the original problem and the perturbed problem

To make this intuition more quantitative, we decompose $\tilde{\mathbf{A}}$ into the sum $\tilde{\mathbf{A}} = \tilde{\mathbf{A}}_{(0)} + \tilde{\mathbf{A}}_{(1)}$, where

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

and

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

and first analyse the individual summands. The proofs for the following results can be found in the Appendix.

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

⁹The matrix \mathbf{A} we used here is a 200×200 Martin-Wilkinson matrix which is defined in the next section.

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.

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 give an estimate of the eigenvalues of $\tilde{\mathbf{A}}$.

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

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

To see why this estimate 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

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

For $j = k$ the middle part is small 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 possible 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 Section 3.2. We summarise the idea of CRQI in Algorithm 3.4. Note that this is not the full algorithm but only the inner loop. Since we will shortly change the algorithm slightly, we postpone the complete definition until later.

Algorithm 3.4: Complex Rayleigh Quotient Iteration (first version)

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

$$\left| \begin{array}{l} \text{Solve } (\mathbf{A} - i\gamma^{(k)} (\mathbf{I} - \mathbf{x}^{(k)}(\mathbf{x}^{(k)})^*) - \mu^{(k)} \mathbf{I}) \tilde{\mathbf{x}}^{(k+1)} = \mathbf{x}^{(k)} \\ \mathbf{x}^{(k+1)} \leftarrow \tilde{\mathbf{x}}^{(k+1)} / \|\tilde{\mathbf{x}}^{(k+1)}\| \\ \mu^{(k+1)} \leftarrow (\mathbf{x}^{(k+1)})^* \mathbf{A} \mathbf{x}^{(k+1)} \\ \gamma^{(k+1)} \leftarrow \|(\mathbf{A} - \mu^{(k+1)} \mathbf{I}) \mathbf{x}^{(k+1)}\| \end{array} \right.$$

As $\gamma^{(k)} \rightarrow 0$ then linear system that is solved at each step becomes the same system as in classic RQI. The remaining steps are essentially the same except that every transpose (e.g. in the computation of the Rayleigh Quotient) has to be replaced by a complex conjugate transpose since the vectors might now contain a non-zero imaginary part.

Obviously, we cannot expect this method to possess the same convergence properties as classic RQI. The matrix $\tilde{\mathbf{A}}$ is neither real symmetric nor Hermitian but *complex symmetric*. As we will see in the next section, 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 posses only few,

if any, zero entries. Although this might seem like a serious disadvantage it will shortly be resolved. We will see that it is not necessary to perturb the matrix by $-i\gamma(\mathbf{I} - \mathbf{u}\mathbf{u}^\top)$ but that it suffices to subtract from \mathbf{A} the diagonal matrix $i\gamma\mathbf{I}$. The way that we introduced the method 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. We begin with the following auxiliary result.

Lemma 3.5. *Define the matrices*

$$\mathbf{B} := \mathbf{A} - \mu\mathbf{I} - i\gamma\mathbf{I}$$

and

$$\mathbf{C} := \mathbf{A} - i\gamma(\mathbf{I} - \mathbf{u}\mathbf{u}^*) - \mu\mathbf{I},$$

where $\mu, \gamma > 0$ are positive real numbers. Then $\mathbf{B}^{-1}\mathbf{u}$ is a scalar multiple of $\mathbf{C}^{-1}\mathbf{u}$.

Proof. Let $\hat{\mathbf{A}} := \mathbf{A} - \mu\mathbf{I}$ and rewrite \mathbf{B} and \mathbf{C} as

$$\mathbf{B} = \hat{\mathbf{A}} - i\gamma\mathbf{I} \quad \text{and} \quad \mathbf{C} = \hat{\mathbf{A}} - i\gamma(\mathbf{I} - \mathbf{u}\mathbf{u}^*),$$

respectively. Now observe that $\mathbf{C} = \mathbf{B} + i\gamma\mathbf{u}\mathbf{u}^*$. Using the Sherman-Morrison formula (see, for example, [11, p. 50]) and letting $\alpha := 1 + i\gamma\mathbf{u}^*\mathbf{B}^{-1}\mathbf{u} \in \mathbb{C}$ we obtain

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

Thus, the vector $\mathbf{C}^{-1}\mathbf{u}$ is a scalar multiple of $\mathbf{B}^{-1}\mathbf{u}$. \square

This result shows that it suffices to perturb the matrix by the diagonal matrix $\gamma^{(k)}i\mathbf{I}$ instead of $i\gamma^{(k)}(\mathbf{I} - \mathbf{x}^{(k)}(\mathbf{x}^{(k)})^*)$. Consider the linear system from Algorithm 3.4. The lemma states that there exists a scalar $\alpha \in C$ such that solving this system is equivalent to solving

$$\alpha (\mathbf{A} - i\gamma^{(k)}\mathbf{I} - \mu^{(k)}\mathbf{I}) \mathbf{x}^{(k+1)} = \mathbf{x}^{(k)}. \quad (3.8)$$

Hence, the solution of (3.8) *without* the factor α is a scalar multiple of the result obtained by solving the linear from Algorithm 3.4. Since the result gets normalised immediately after, both solutions will result in the same vector that is used in the next iteration. The Rayleigh Quotient that is computed using this vector consequently is the same in either of the variants.

Thus, it does indeed suffice to perturb the matrix only by the diagonal matrix $-i\gamma^{(k)}\mathbf{I}$. We can collect the real shift $\mu^{(k)}$ and the imaginary shift $\gamma^{(k)}i$ into a complex-valued shift

$$\sigma^{(k)} := \mu^{(k)} + i\gamma^{(k)}$$

and can now fully define Complex Rayleigh Quotient Iteration as it is given in Algorithm 3.6.

The last three steps after the loop remove the imaginary part that might be “left” in the vector approximation ($\text{Re}(\cdot)$ extracts the real part of a complex vector). Since we again use a stopping criterion based on the norm of the residual, the same error bounds we discussed earlier in Chapter 2 hold and thus the vector iterates could still contain a small imaginary part. This does also imply that the final residual norm $\|\mathbf{Ax} - \mu\mathbf{x}\|$ might be slightly larger than the residual norm computed in the last iteration. In practice, however, we observed that the final residual norm is still of the same order as the norm of the residual computed in the last iteration.

Algorithm 3.6: Complex Rayleigh Quotient Iteration

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

begin

```

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

```

Note, that although the step where the linear system is solved looks almost identical to the respective step in classic RQI, this algorithm is still different. The shift $\sigma^{(k)}$ is not the Rayleigh Quotient of the vector iterate $\mathbf{x}^{(k)}$ as is the case in classic RQI. One could try to interpret the method as classic RQI applied to the matrix $\mathbf{A} - i\gamma^{(k)} \mathbf{I}$ but this is also not true since this matrix changes from one step to the next. Hence, we cannot expect that CRQI possesses the same appealing convergence properties as classic RQI. However, numerical examples suggest that convergence is still fast and often merely three or four additional steps are required compared to classic RQI. Moreover, we did not encounter an example where CRQI failed to converge to any eigenpair.

This concludes the motivation part of this section. As mentioned in the beginning of this thesis, our aim is not to provide a detailed mathematical analysis of the method. Instead, we discuss various numerical examples to demonstrate that the idea introduced above works.

3.2 Numerical Experiments

The purpose of this section is twofold. First, we study various numerical examples to understand the behaviour of CRQI and demonstrate the good properties we already mentioned at the beginning of the chapter. Second, we illustrate the erratic behaviour of classic RQI that we mentioned several times before. This is not done separately but by running the same experiments for both methods and comparing the results throughout. All experiments were executed in Matlab 9 [16]. The criterion for convergence is $\|\mathbf{r}^{(k)}\| = \|\mathbf{Ax}^{(k)} - \mu^{(k)}\mathbf{x}^{(k)}\| < 10^{-9}$. The source codes for both classic and complex RQI can be found in the Appendix. Note, that the 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 3.6 the initial shifts are always initialised to the Rayleigh Quotient of the initial vector and the initial residual, respectively. This will become useful when investigating how the initial shift influences the outcome of the method.

All of the experiments were carried out for different matrices that are common for assessing eigenvalue algorithms. In particular, they have been used to evaluate shift-and-invert type algorithms and algorithms related to classic RQI, see, e. g. [5] and the references therein. They are described below. Recall that we are particularly interested in problems with closely spaced eigenvalues and, except for the first two examples, all of the test matrices will lead to such problems. Since in three of the test problems the spacing even becomes closer the larger the matrix gets, we will also study the algorithm's behaviour under increasing matrix size.

Random matrices These matrices are pseudo-randomly generated using the Matlab command “sprandsym”. Apart from being sparse and symmetric, they have no special structure or properties.

The matrix [1, 2, 1] This matrix is a tridiagonal matrix with all diagonal elements set to 2 and all off-diagonal elements set to 1. The eigenvalues of this matrix are all distinct and their exact values are known to be

$$\lambda_k = 4 \sin^2 \left(\frac{\pi k}{2(n+1)} \right)$$

where n denotes the order (i. e., the number of rows) of the matrix [37, pp. 299–307]. Thus, for every n , the eigenvalues lie in the interval $[0, 4]$ and so consequently their spacing gets smaller the larger the matrix gets.

Wilkinson's matrix \mathbf{W}^+ This tridiagonal matrix was extensively studied by Wilkinson in [37], hence its name. It is of order $n = 2p + 1$ for some $p \in \mathbb{N}$. The i -th diagonal entry is set to $|p + 1 - i|$ and all off-diagonal entries are set to 1. For instance, for $p = 2$ this yields the 5×5 matrix

$$\mathbf{W}_5^+ = \begin{bmatrix} 2 & 1 & & & \\ 1 & 1 & 1 & & \\ & 1 & 0 & 1 & \\ & & 1 & 1 & 1 \\ & & & 1 & 2 \end{bmatrix}.$$

The spectrum consists of pairs of nearly, but not exactly, equal eigenvalues. For example, the two largest eigenvalues of \mathbf{W}_{21}^+ agree to 15 significant decimals [37, pp. 300–309].

The Martin-Wilkinson matrix MW If we denote by a_{ij} the j -th entry of the i -th row of MW , this matrix is defined by

$$\begin{aligned} a_{ii} &= 6 && \text{for } i = 2, \dots, n-1 \quad \text{but } a_{11} = a_{nn} = 5, \\ a_{i,i-1} = a_{i-1,i} &= -4 && \text{for } i = 2, \dots, n, \\ a_{i,i-2} = a_{i-2,i} &= 1 && \text{for } i = 2, \dots, n. \end{aligned}$$

The eigenvalues are known to be [9, p. 39]

$$\lambda_k = 16 \sin^4 \left(\frac{k\pi}{2(n+1)} \right)$$

and thus, independent of n , the eigenvalues lie in the interval $[0, 16]$. Hence, the eigenvalues become increasingly close the larger the size of the matrix.

The Laplace matrix L This matrix arises, for instance, when discretizing the Laplace operator using a five-point stencil in the finite difference method (see, for example, [6, pp. 270–272]). Let m be an integer and define the $m \times m$ matrix

$$\mathbf{T} = \begin{bmatrix} 4 & -1 & & & \\ -1 & 4 & -1 & & \\ & \ddots & \ddots & \ddots & \\ & & -1 & 4 & -1 \\ & & & -1 & 4 \end{bmatrix}.$$

The Laplace matrix is a block tridiagonal matrix of order $n = m^2$ defined as

$$\mathbf{L} = \begin{bmatrix} \mathbf{T} & -\mathbf{I} & & \\ -\mathbf{I} & \mathbf{T} & -\mathbf{I} & \\ & \ddots & \ddots & \ddots \\ & & -\mathbf{I} & \mathbf{T} & -\mathbf{I} \\ & & & -\mathbf{I} & \mathbf{T} \end{bmatrix}$$

where \mathbf{I} is the $m \times m$ identity matrix. Again, the eigenvalues can be computed analytically and all lie in an interval that is independent of the matrix's size; in this case they are all contained in the interval $[0, 8]$.

Below we give some numerical examples that highlight different behavioural aspects of the algorithm. Plots and/or tables that illustrate our findings are given for each of the test matrices. They are either included directly within the example or can be found in Appendix B. Those included in this section are the ones we found most meaningful for the particular example.

Recall that we assume that a good approximation of the wanted eigenvector is available. To simulate this, the full set of eigenvectors is computed using built-in Matlab routines. These vectors are then collected as columns of a 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 (in this case this would be \mathbf{v}_{50}) and random (smaller) contributions in the directions of the other eigenvectors.

Example 3.7. The first example demonstrates how difference choices for the imaginary shift $i\gamma^{(k)}$ affect the convergence speed. We run three different

3 Complex Rayleigh Quotient Iteration

variants of CRQI: The first uses $\gamma^{(k)} = \|\mathbf{r}^{(k)}\|$, which is the same as in Algorithm 3.6 above. The second uses the square of the residual norm, the third approach is explained below. A plot of the residuals norm and the iteration number for all three approaches together with the results using classic RQI¹⁰ is given in Figure 3.2.

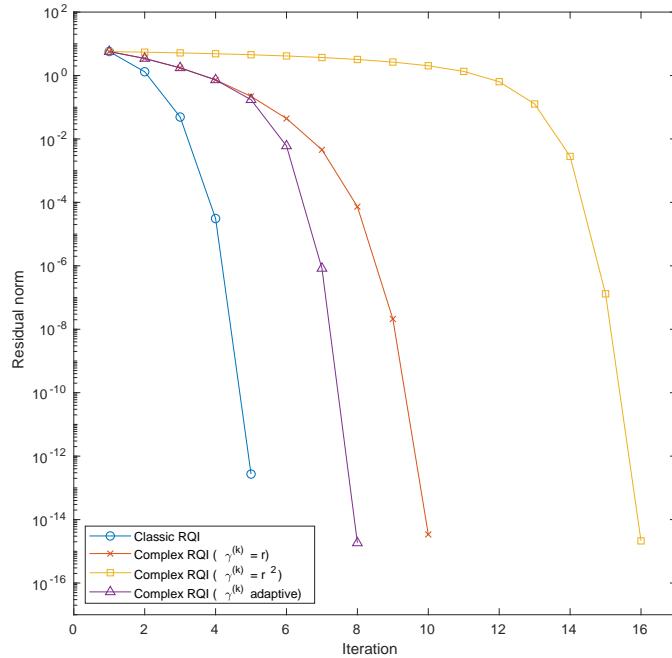


Figure 3.2: Plot of residuals of Classic RQI, Complex RQI with $\gamma^{(k)} = \|\mathbf{r}^{(k)}\|$, Complex RQI with $\gamma^{(k)} = \|\mathbf{r}^{(k)}\|^2$ and Complex RQI with the imaginary shift chosen adaptively (see text) using a 1000×1000 random matrix. The last variant seems to combine the advantages of the second and third alternatives.

We observe that in the initial phase of the iteration, the second variant (squared residual norm) seems to be slower than the first. Although it might not be clearly observable in the figure, further investigation of other examples

¹⁰Classic RQI is merely included for speed comparison. In most of the examples it failed to converge to the correct eigenvalue.

suggested that during the final steps of the iterations the second version was faster than the first (see also Figures B.1 to B.4 in the Appendix). Consequently, by combining both approaches and thus changing the shift adaptively we expect faster convergence. The results are also plotted in Figure 3.2 (labelled with “ $\gamma^{(k)}$ adaptive”) and are in accordance with the expectation. In this particular case, the shift was changed according to

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

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; this observation is analysed in more detail in Example 3.10. 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 often failed to converge to the target eigenpair.

The plots also show that the convergence rate of CRQI (using the adaptive choice of imaginary shifts) seems to be similar to that of classic RQI and that it is the preasymptotic stage which comprises more steps. Table B.1 shows the results of classic RQI and CRQI, again using the adaptive choice of imaginary shifts (for this example we slightly increased the residual tolerance to 10^{-12}). In the first four iterations of CRQI only one digit of the eigenvalue approximation is correct. After this preasymptotic stage, the method converges within three steps.

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 that convergence often hardly depends on the initial vector but rather on the initial shift. This is why especially for problems with closely spaced eigenvalues RQI fails to compute the right eigenpair. CRQI seems to be more robust to changes in the initial shift.

Example 3.8. 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 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 numbers were slightly adapted for the other test matrices). The results using random matrices are plotted in Figure 3.3. The initial vector was set to a weighted combination of the exact eigenvectors as described above. In the first two examples the contribution in the target direction was small while in the third example it was bigger. The last example shows the result using a vector that does not approximate any particular eigenvector. In this figure and the following ones, we denote by N the matrix's order and by α the angle between the initial vector and the target eigenvector.

We 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 accurate approximations of an eigenvector. 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 within the spectrum (see also the results using the other test

3 Complex Rayleigh Quotient Iteration

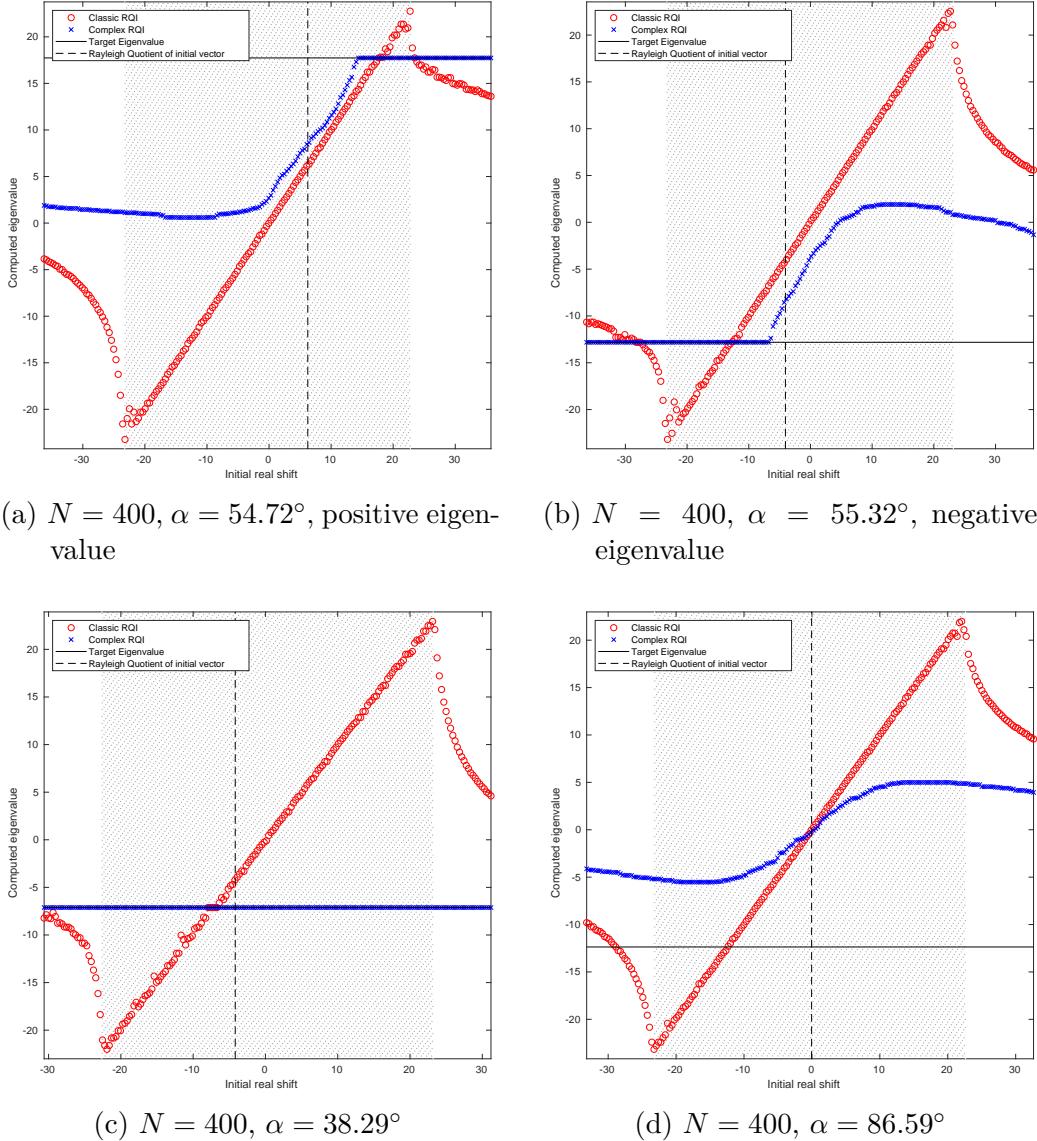


Figure 3.3: Plot of initial real shift against the computed eigenvalue using classic RQI and CRQI for a random matrix. The dotted area encloses the initial shifts that lie in the spectrum of \mathbf{A} . The dashed line is located at the Rayleigh Quotient of the initial vector.

matrices given in Figures B.5 to B.8). If it is below the centre of the spectrum the behaviour is as in Figure 3.3(a) and for eigenvalues above the centre the results are similar to those in Figure 3.3(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.

If one does not have any a priori knowledge about the distribution of the eigenvalues it seems best to use the algorithm as defined above, i. e., to use the Rayleigh Quotient as the initial shift. Even in cases where the outcome of the method varied with changing initial shift, using the Rayleigh Quotient usually produced the correct result, see for instance the first two examples of Figure B.8. Thus, in all of the remaining examples, CRQI is run with the initial real shift set to the Rayleigh Quotient of the initial vector.

This example also revealed another property of CRQI. It seems that the method is in some sense more stable if the target eigenvalue lies near the centre of the spectrum. If we consider the examples where the initial vector was chosen completely random, i. e., is not an approximation of any of the eigenvectors, we see that the computed eigenvalues are not spread along the entire spectrum but are distributed inside a sub interval of $[\lambda_{\min}, \lambda_{\max}]$ (see Figures 3.3(d) and B.5(d)). Furthermore, the method seems to be less stable if the target eigenvalue is located near either end of the spectrum in the sense that it is more sensitive to changes in the initial real shift. This instability is depicted, for example, in Figures B.5(a) and B.5(c). In the first plot, the target eigenvalue lies near the right end of the spectrum, while in the other example it lies near the centre. The angles between the initial vectors and the target eigenvectors are about the same size but the second variant leads to the correct result, independent of the initial real shift. This observation will be confirmed in the next examples. There we will see that sometimes a much more accurate eigenvector approximation is required for CRQI to succeed if the corresponding eigenvalue is close to either of the ends of the spectrum.

We have introduced CRQI as an improvement of classic RQI in the sense that good approximations of an eigenvector should lead to convergence to this very eigenvector. In the following examples we examine how good of an approximation the initial vector needs to be. This is achieved by studying the relationship between the angle that the initial vector makes with the target eigenvector and the outcome of the method. To that end, artificial approximations of the wanted eigenvector are created as explained above where the contribution in the target direction is successively increased throughout the experiment. We will see that

- (a) classic RQI indeed suffers from the problem that good approximations of an eigenvector do not necessarily lead to convergence to this very eigenvector and that
- (b) complex RQI seems to take much more advantage of the information in the initial vector.

Example 3.9. In Figure 3.4 we plotted the angle between the initial vector and the wanted eigenvector and the computed eigenvalue for classic RQI and CRQI. This particular example shows the results for a Laplace matrix of different sizes; the results for the remaining test problems are given in Figures B.9 to B.11 in the Appendix.

We see that complex RQI seems to converge to the right eigenvector once the angle between the initial vector and the target is sufficiently small. Classic RQI, on the other hand, still often converges to the wrong eigenpair for very small angles. The figure suggests that “sufficiently small” means approximately below $\pi/4$, or 45° . In some test cases where the target eigenvalue was very close to either end of the spectrum a much smaller angle was required for CRQI to succeed. If the eigenvalue is located in the interior of the spectrum, however, it seemed almost impossible to make CRQI fail for angles below $\pi/4$. This substantiates the observation from the previous example that CRQI

3 Complex Rayleigh Quotient Iteration

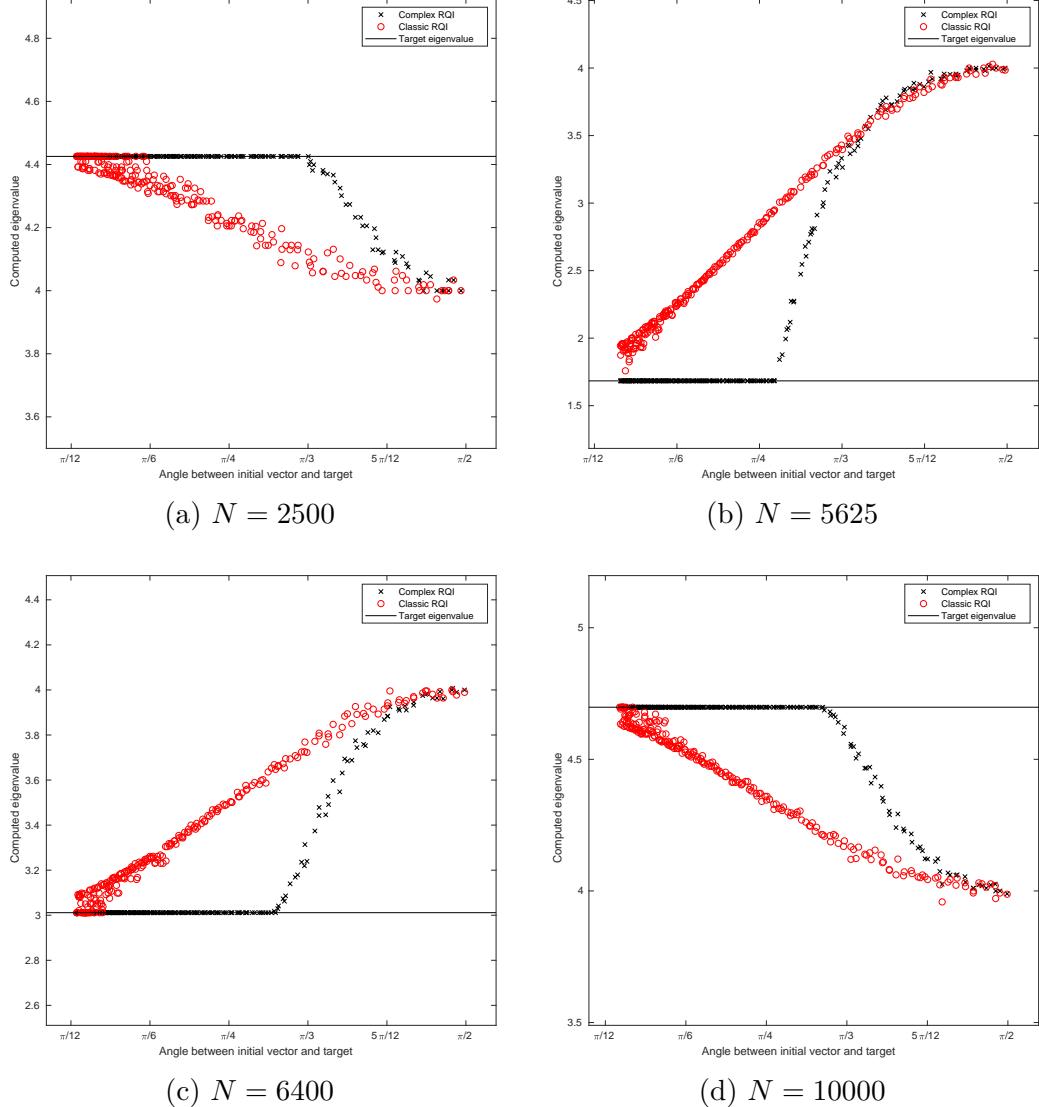


Figure 3.4: Plot of the computed eigenvalue against the angle between the initial vector and the target eigenvector for the Laplace matrix. While classic RQI even fails for very small angles, CRQI produces the correct result as soon as the angle is sufficiently small, which in these examples means approximately below $\pi/4$.

seems to be more robust when the eigenvalue is located near the centre of the spectrum. More importantly, the observations seem to be independent of the size of the matrix and thus, independent of the spacing of the eigenvalues.

In essence, this example showed that the idea from the previous section does indeed yield the desired behaviour. The method seems to make more use of the information incorporated in the initial eigenvector guess. This is precisely the purpose of the modification of classic RQI as it was introduced in the previous section.

In the first example of this section we briefly looked at how many iterations CRQI requires compared to classic RQI. This is now studied in more detail. As we will see shortly, CRQI requires fewer iterations the more accurate an eigenvector the initial vector is and classic RQI seems to not possess this property.

Example 3.10. In Figure 3.5 we plotted the number of iterations against the initial error angle for classic RQI and complex RQI, respectively. We also indicated whether or not the computed eigenvalue was the correct one (indicated by a circle) or not (indicated by a cross). The results using classic RQI are slightly shifted upwards so that the results can be better distinguished.

We can clearly see that the number of iterations of CRQI indeed decreases as the initial error angle gets smaller once the angle is approximately below 45° . For very small angles CRQI often requires merely one additional step and sometimes both method even finish within the same number of iterations.

In some cases classic RQI requires a higher number of iterations even for small angles while still computing the wrong result. This again portrays another aspect of the erratic behaviour of classic RQI. For the test problems where the spacing between the eigenvalues is very small, classic RQI often produced very few correct results while CRQI showed the same behaviour as described above, independent of the matrix's size and hence the distance between the eigenvalues.

3 Complex Rayleigh Quotient Iteration

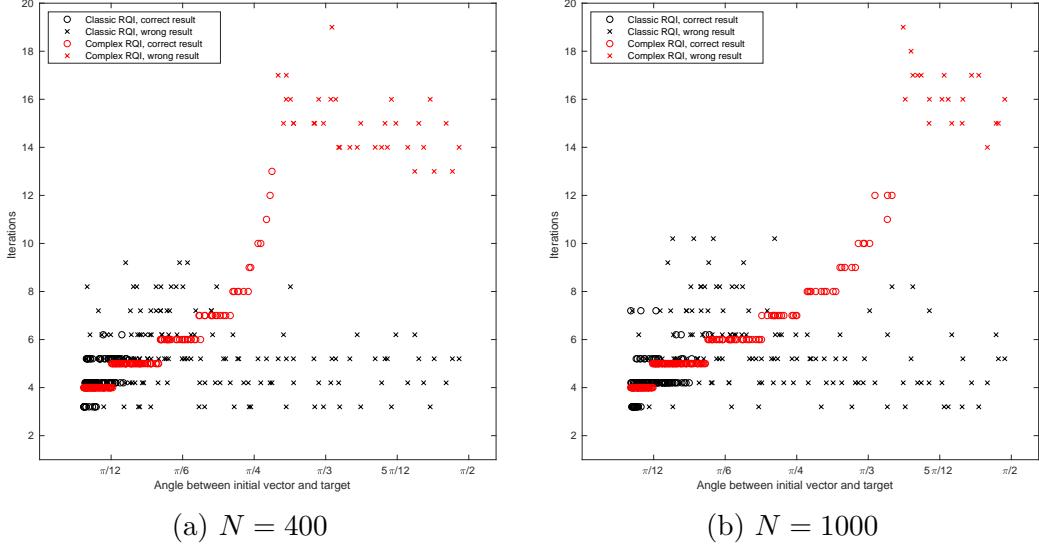


Figure 3.5: Plot of the number of iterations of classic RQI and complex RQI for a random matrix.

We have also included some plots that illustrate the fact that a smaller angle is required in cases where the target eigenvalue is very close to either end of the spectrum which we already mentioned above, see Figures B.12(d) and B.14(b) in the Appendix. In these cases the behaviour is still the same as in the other examples in the sense that the number of iterations is decreasing as the initial error angles becomes smaller. However, the initial error angle required for the method to succeed at all needs to be lower.

We conclude this chapter with a summary of the findings.

4 Concluding Remarks

Appendices

A Proofs

Proof of Lemma 3.1. First consider $j \neq k$. Using the orthogonality of the eigenvectors we have $\mathbf{v}_k^\top \mathbf{v}_j = 0$ and thus

$$\begin{aligned} (\mathbf{A} - i\gamma(\mathbf{I} - \mathbf{v}_k \mathbf{v}_k^\top)) \mathbf{v}_j &= \mathbf{A} \mathbf{v}_j - i\gamma \mathbf{v}_j + i\gamma \mathbf{v}_k \mathbf{v}_k^\top \mathbf{v}_j \\ &= \lambda_j \mathbf{v}_j - i\gamma \mathbf{v}_j \\ &= (\lambda_j - i\gamma) \mathbf{v}_j. \end{aligned}$$

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

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

□

Proof of Lemma 3.2. Since

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

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{E} 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. Since only two eigenvalues of \mathbf{E} are non-zero, the trace is the sum of these eigenvalues, i. e.,

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

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 and the fact that both vectors are assumed to be normalised, we get

$$\text{tr}(\mathbf{E}) = \|\mathbf{u}\|^2 - \|\mathbf{v}_k\|^2 = 0,$$

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

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

Therefore,

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

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. \square

Proof of Proposition 3.3. For this proof we treat $\tilde{\mathbf{A}}_{(1)}$ as a perturbation of $\tilde{\mathbf{A}}_{(0)}$ and use a classic result from perturbation theory¹¹ which states that the eigenvalues of $\tilde{\mathbf{A}} = \tilde{\mathbf{A}}_{(0)} + \tilde{\mathbf{A}}_{(1)}$ satisfy

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

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

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

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

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

for $j \neq k$ and

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

¹¹This result can be found, for example, in [37, pp. 66–69] or [11, p. 323].

for $j = k$ and thus

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

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

B Additional Plots and Tables

In this chapter we include some additional plots for the examples of Section 3.2. We fix the following notation: N denotes the order of the test matrix that was used in the respective example, i. e., the size of the matrix is $N \times N$. The (acute) angle between the target eigenvector and the initial vector that was used in the algorithm is denoted by α (the angle is always given in degrees).

B Additional Plots and Tables

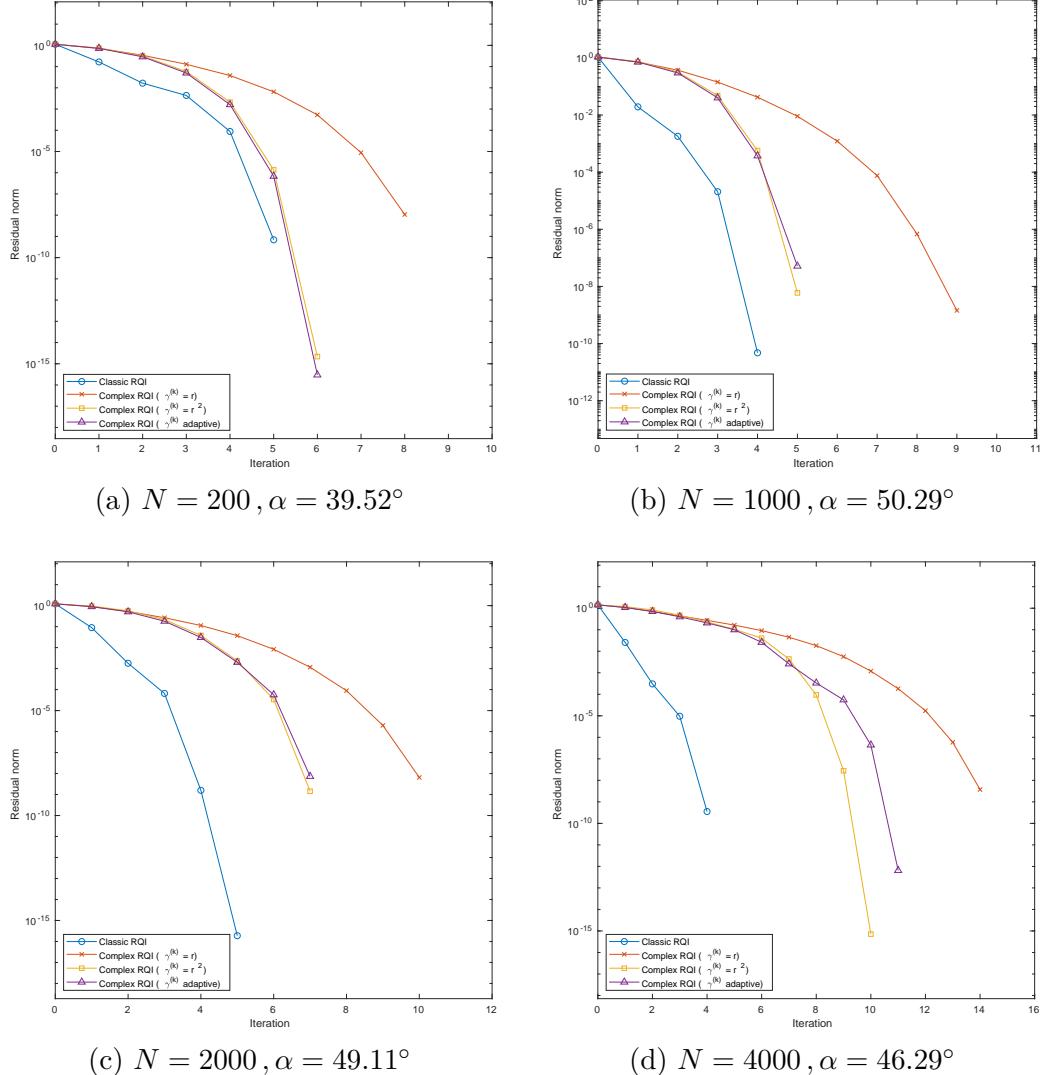


Figure B.1: Plot of the residual for different choices of imaginary shifts for the $[1, 2, 1]$ matrix.

B Additional Plots and Tables

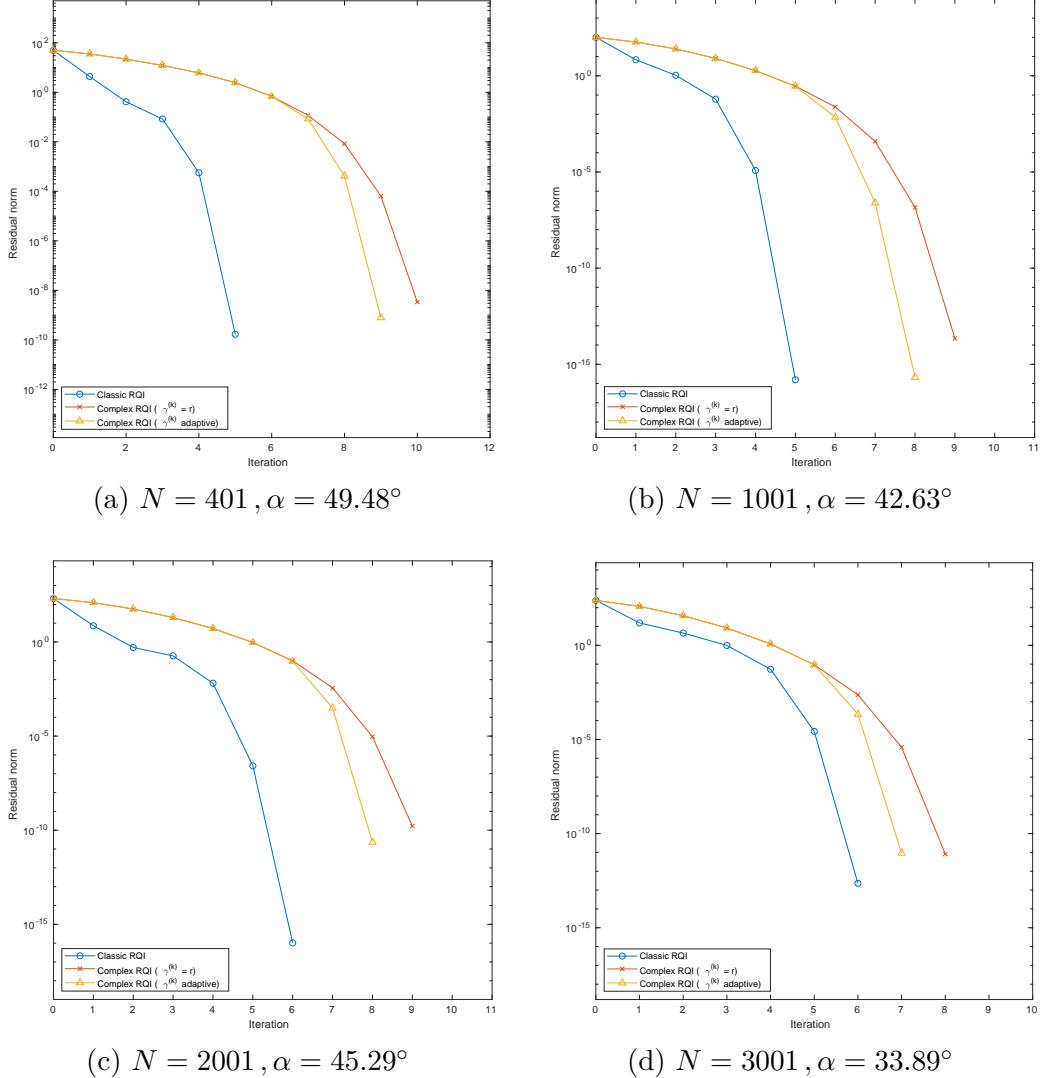


Figure B.2: Plot of the residual for different choices of imaginary shifts for the Wilkinson matrix \mathbf{W}^+ . The results using the squares residual norm as the imaginary shift are not included since in all cases the number of iterations was too high.

B Additional Plots and Tables

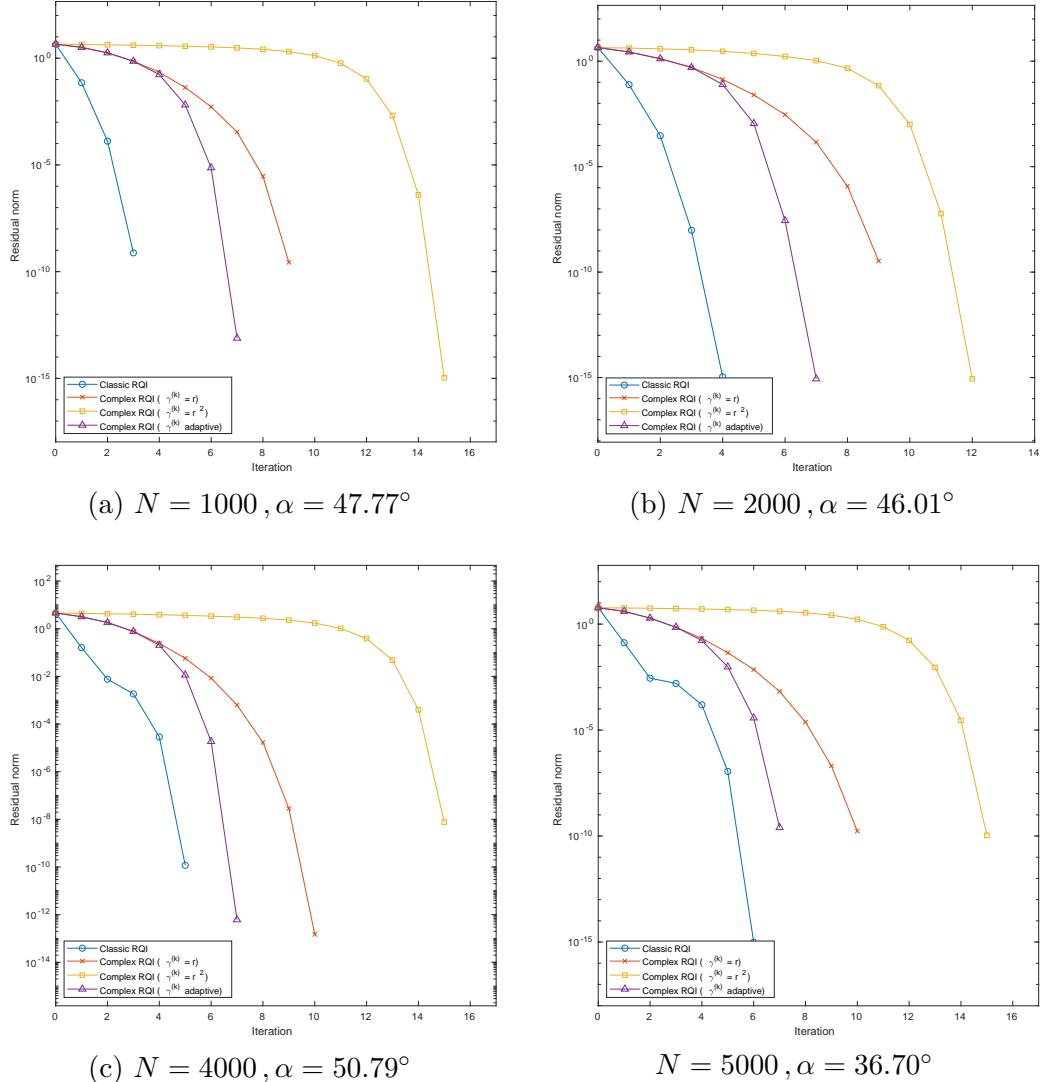


Figure B.3: Plot of the residual for different choices of imaginary shifts for the Martin-Wilkinson matrix $\mathbf{M}\mathbf{W}$.

B Additional Plots and Tables

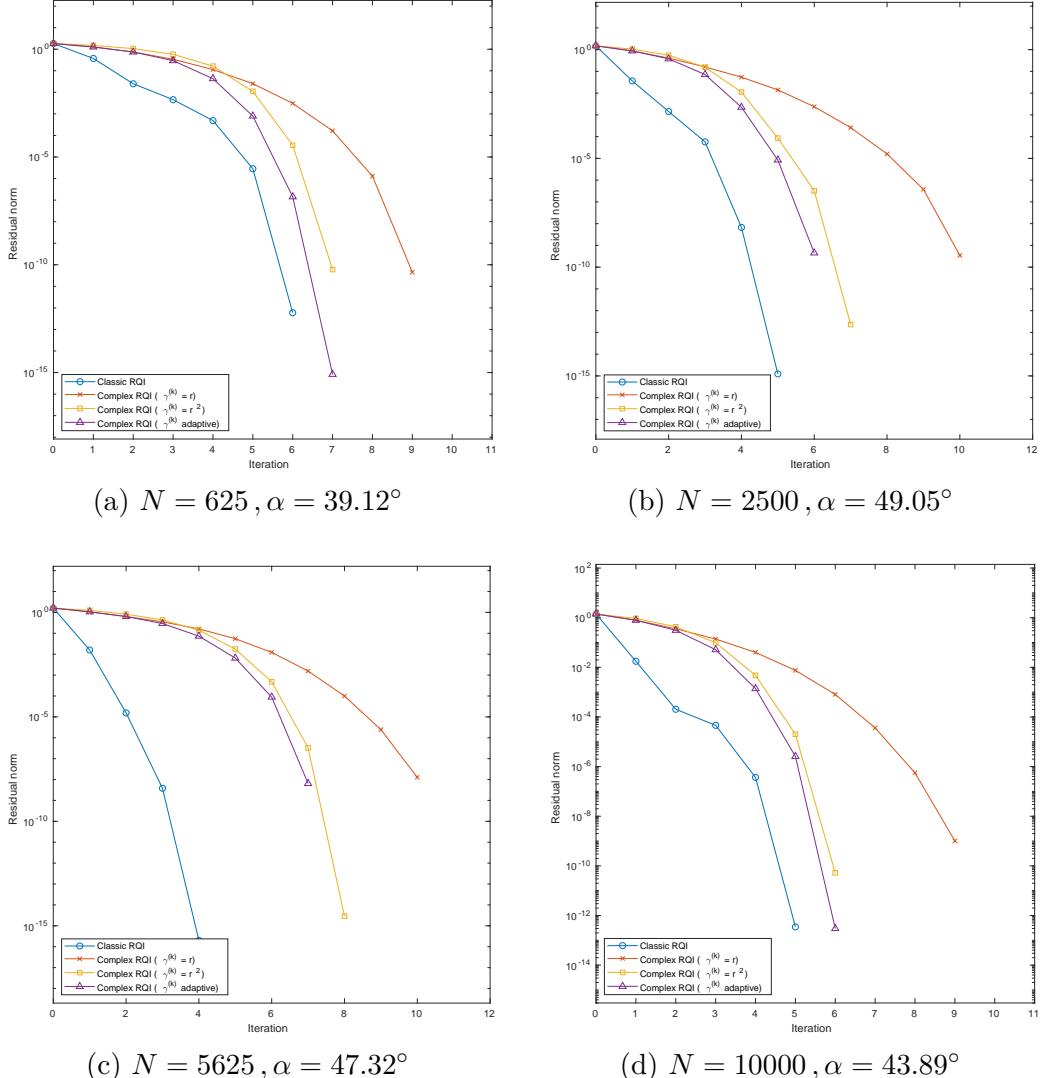


Figure B.4: Plot of the residual for different choices of imaginary shifts for the Laplace matrix.

It.	Classic RQI		Complex RQI		
	Residual norm	Eigenvalue approx.	Residual norm	Eigenvalue approx.	
68	0	4.988771234471549	<u>-1.356761316880883</u>	4.988771234471549	<u>-1.356761316880883</u>
	1	0.299574076827218	<u>-1.670940785795473</u>	2.643902978677971	<u>-1.548973644619087</u>
	2	0.016273891784549	<u>-1.712599523046921</u>	1.031117447928710	<u>-1.648235887691692</u>
	3	0.000050858811562	<u>-1.713396087264200</u>	0.280137375907241	<u>-1.699935574796257</u>
	4	0.000000000004228	<u>-1.713396099691558</u>	0.017265270986613	<u>-1.713304367059983</u>
	5	conv.		0.000018910192652	<u>-1.713396100366165</u>
	6			0.000000000000041	<u>-1.713396099691559</u>

Table B.1: Residual norms and eigenvalue iterates for classic RQI and CRQI applied to a 200×200 random matrix. The correct digits of the eigenvalue approximations are underlined. Both algorithms were run with the same initial vector. The eigenvalue approximation in the first line (iteration 0) is the Rayleigh Quotient of the initial vector. Although CRQI requires more steps, it seems that it is merely the preasymptotic stage that takes more iterations; once the eigenvalue approximation is sufficiently accurate the algorithm converges within three steps.

B Additional Plots and Tables

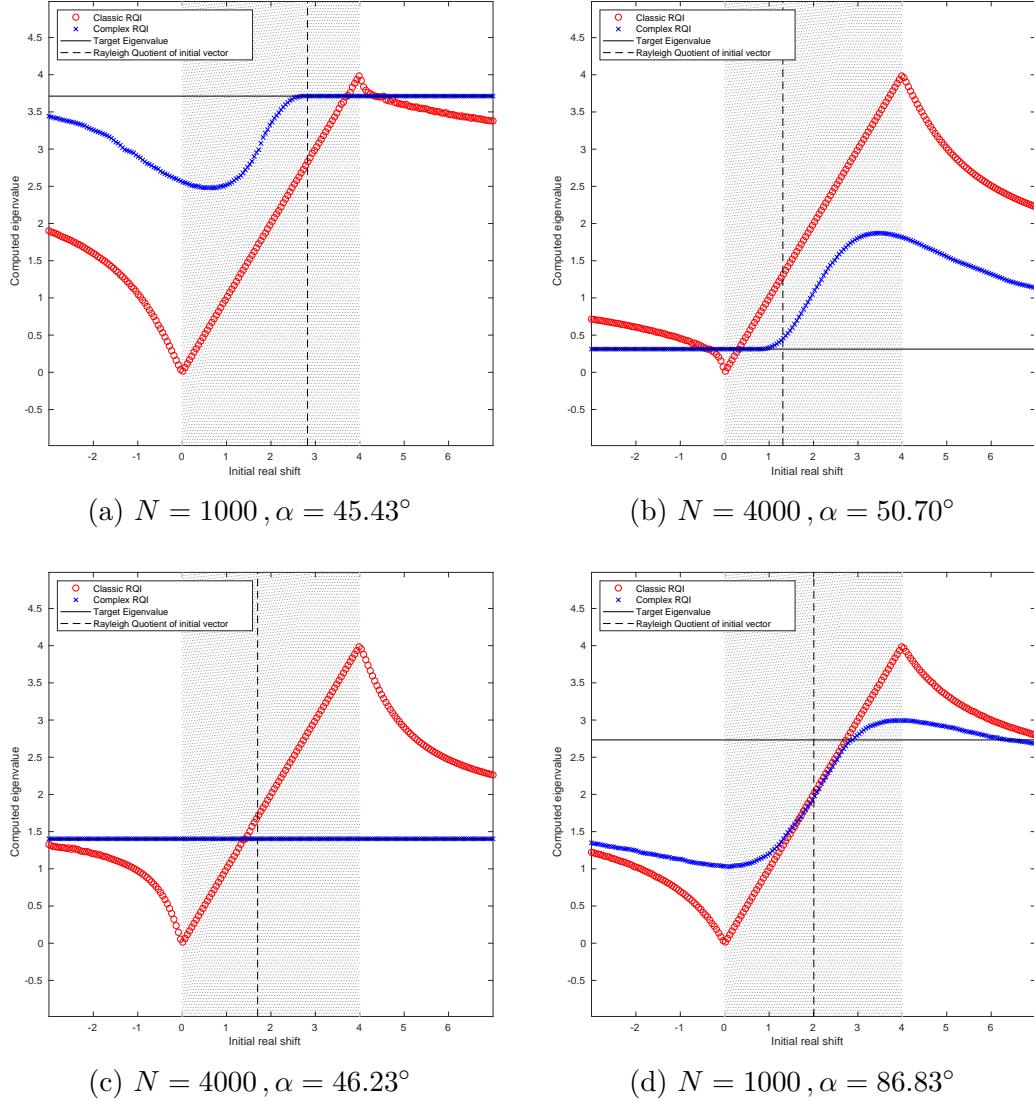


Figure B.5: Plot of the computed eigenvalue against the initial real shift for the $[1, 2, 1]$ matrix.

B Additional Plots and Tables

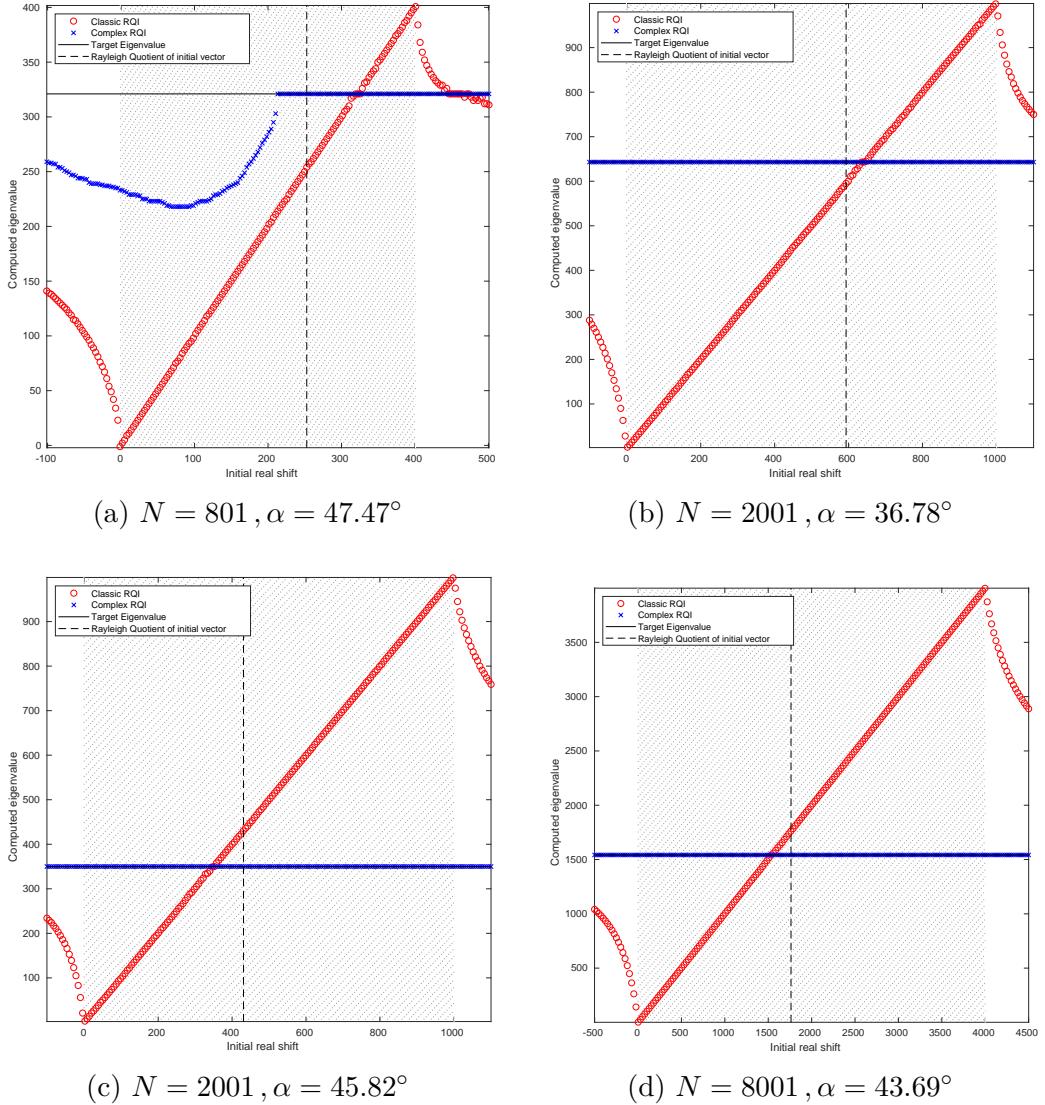


Figure B.6: Plot of the computed eigenvalue against the initial real shift for the Wilkinson matrix \mathbf{W}^+ .

B Additional Plots and Tables

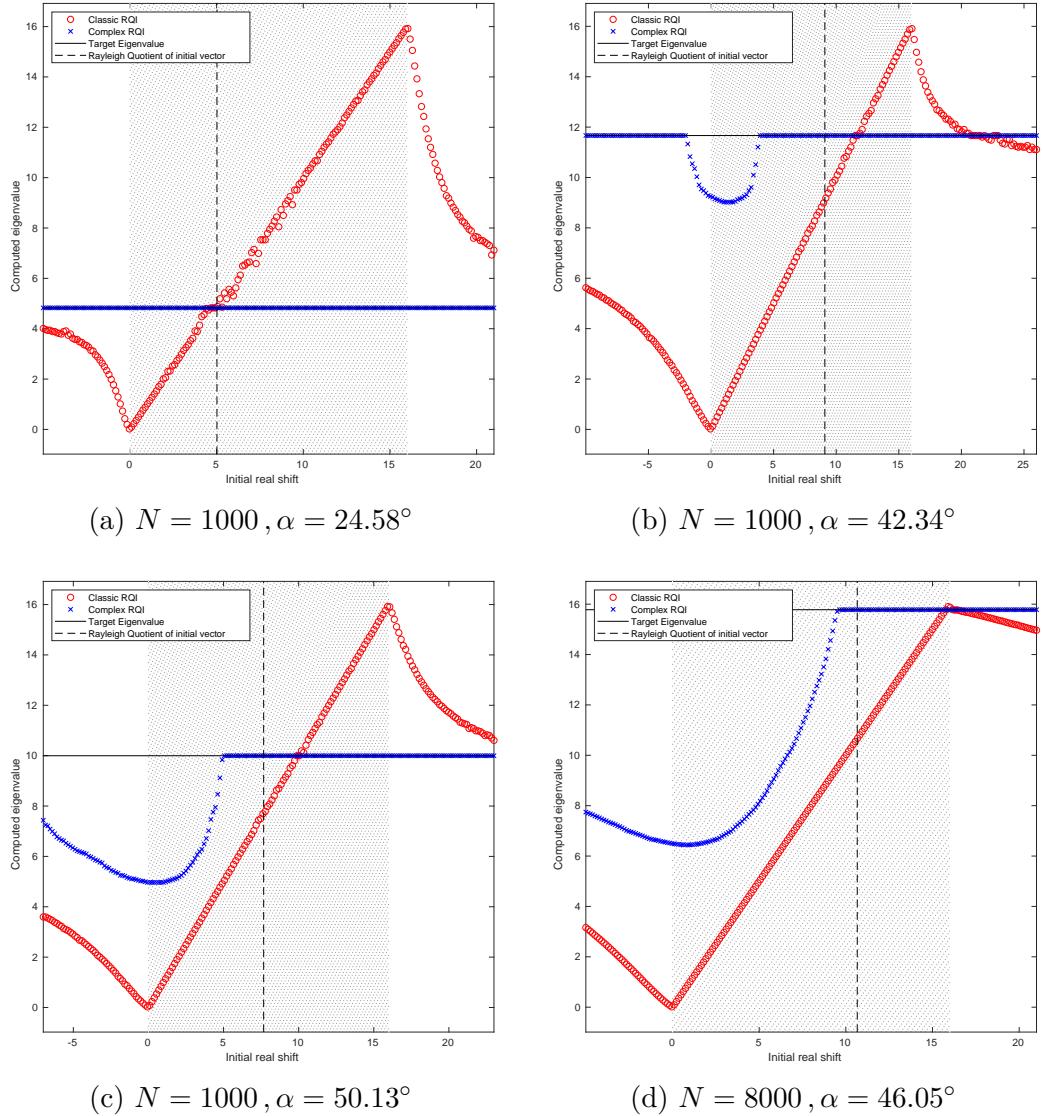


Figure B.7: Plot of the computed eigenvalue against the initial real shift for the Martin-Wilkinson matrix \mathbf{MW} .

B Additional Plots and Tables

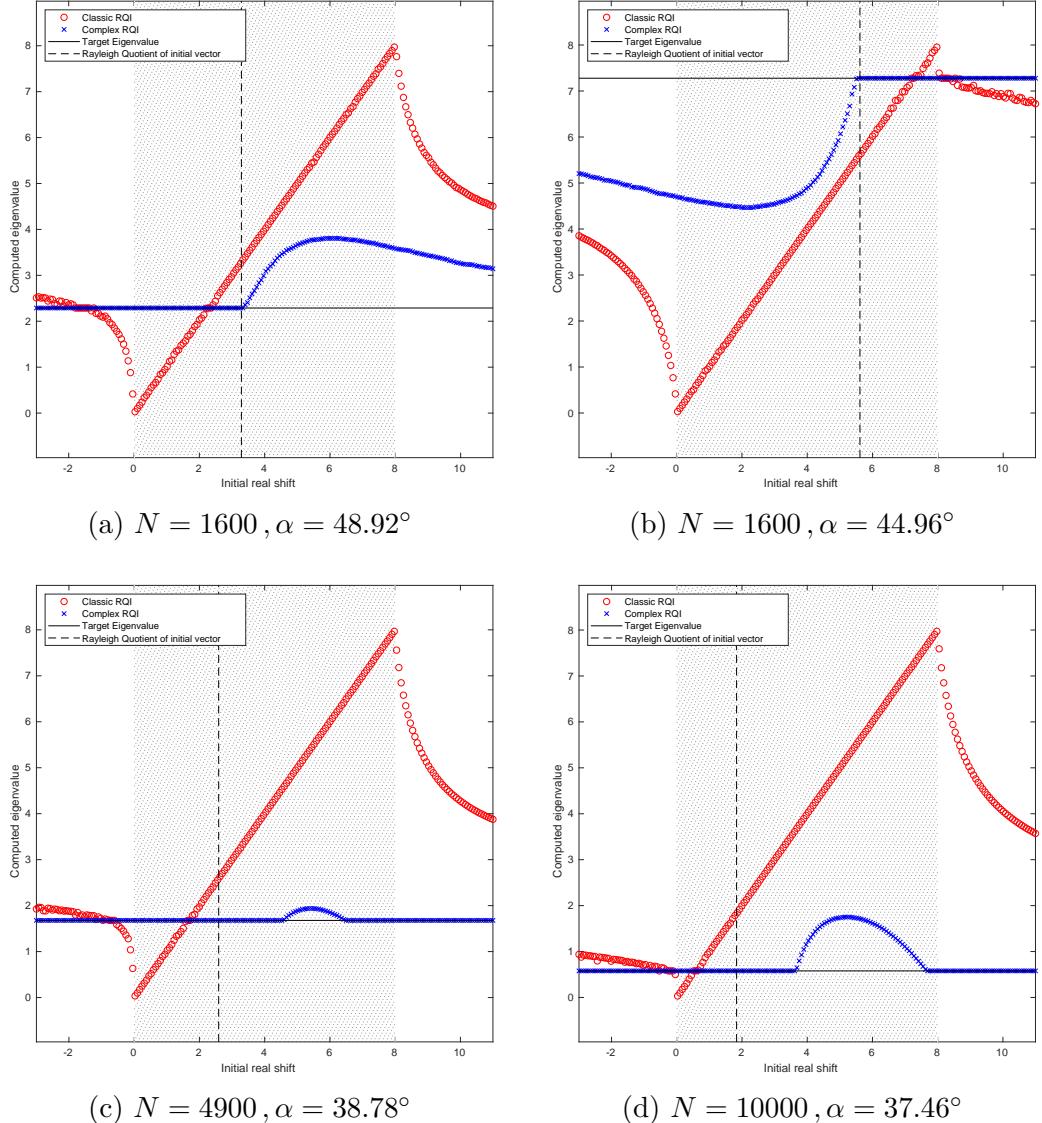


Figure B.8: Plot of the computed eigenvalue against the initial real shift for the Laplace matrix.

B Additional Plots and Tables

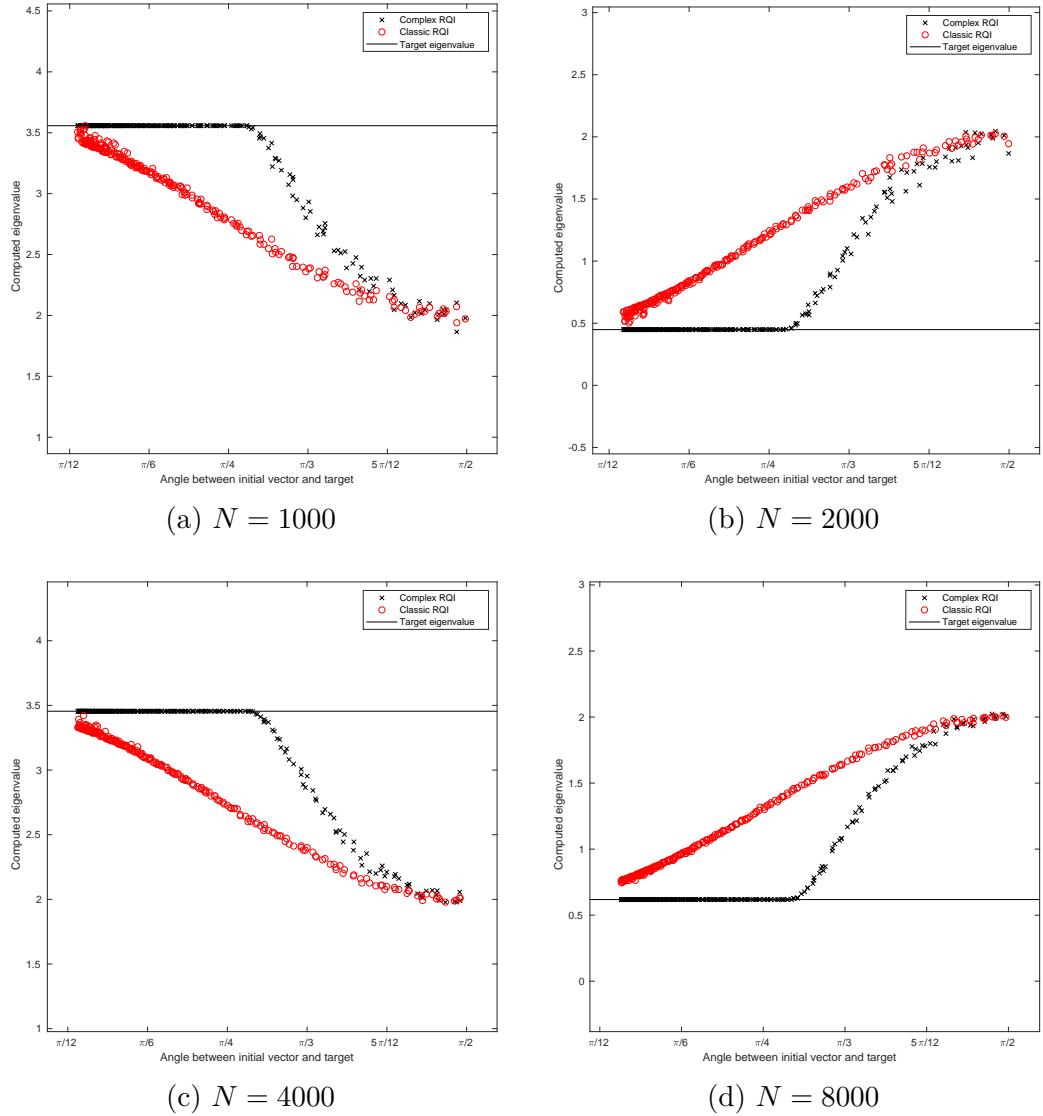


Figure B.9: Plot of the computed eigenvalue against the angle between the initial vector and the target eigenvector for the matrix $[1, 2, 1]$.

B Additional Plots and Tables

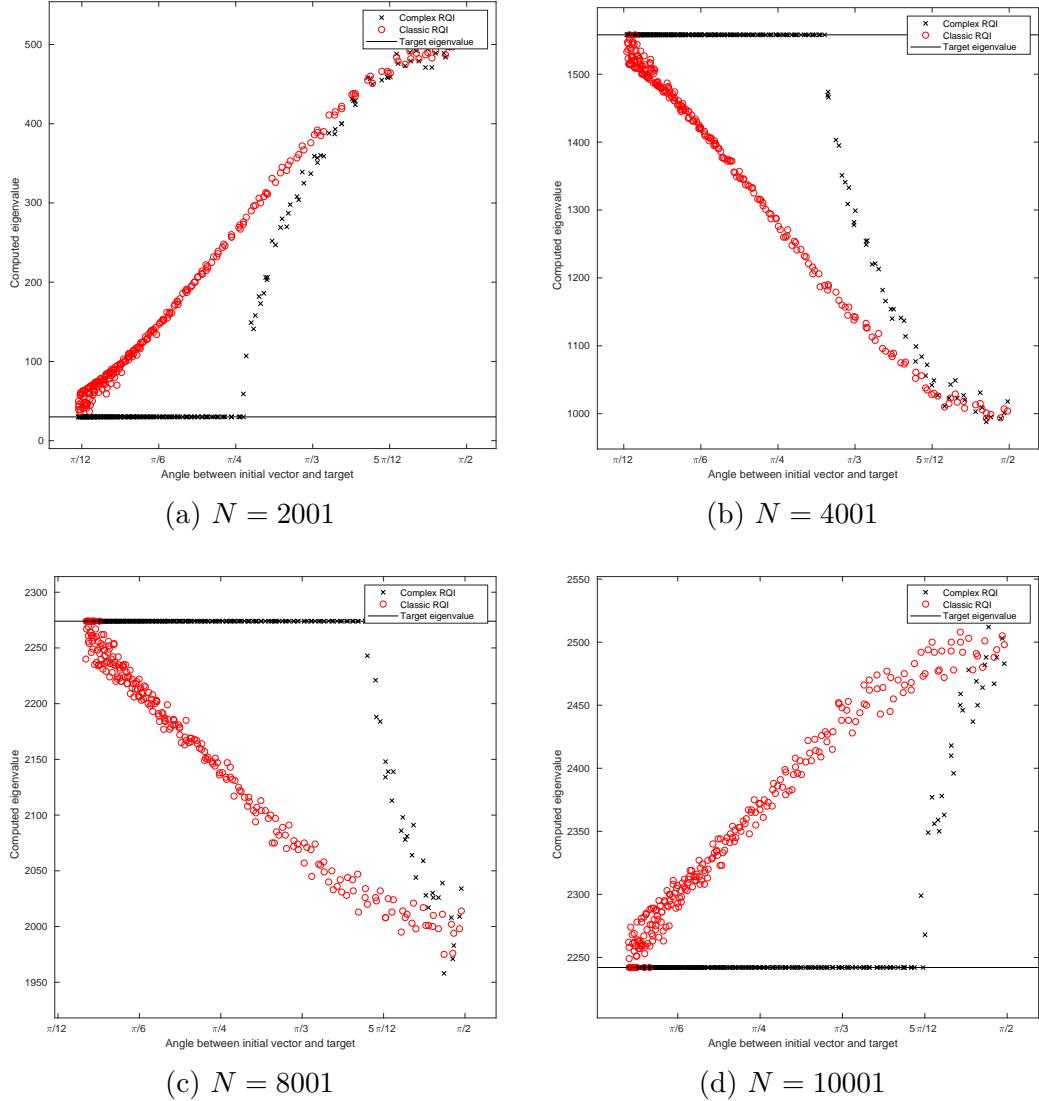


Figure B.10: Plot of the computed eigenvalue against the angle between the initial vector and the target eigenvector for the Wilkinson matrix \mathbf{W}^+ .

B Additional Plots and Tables

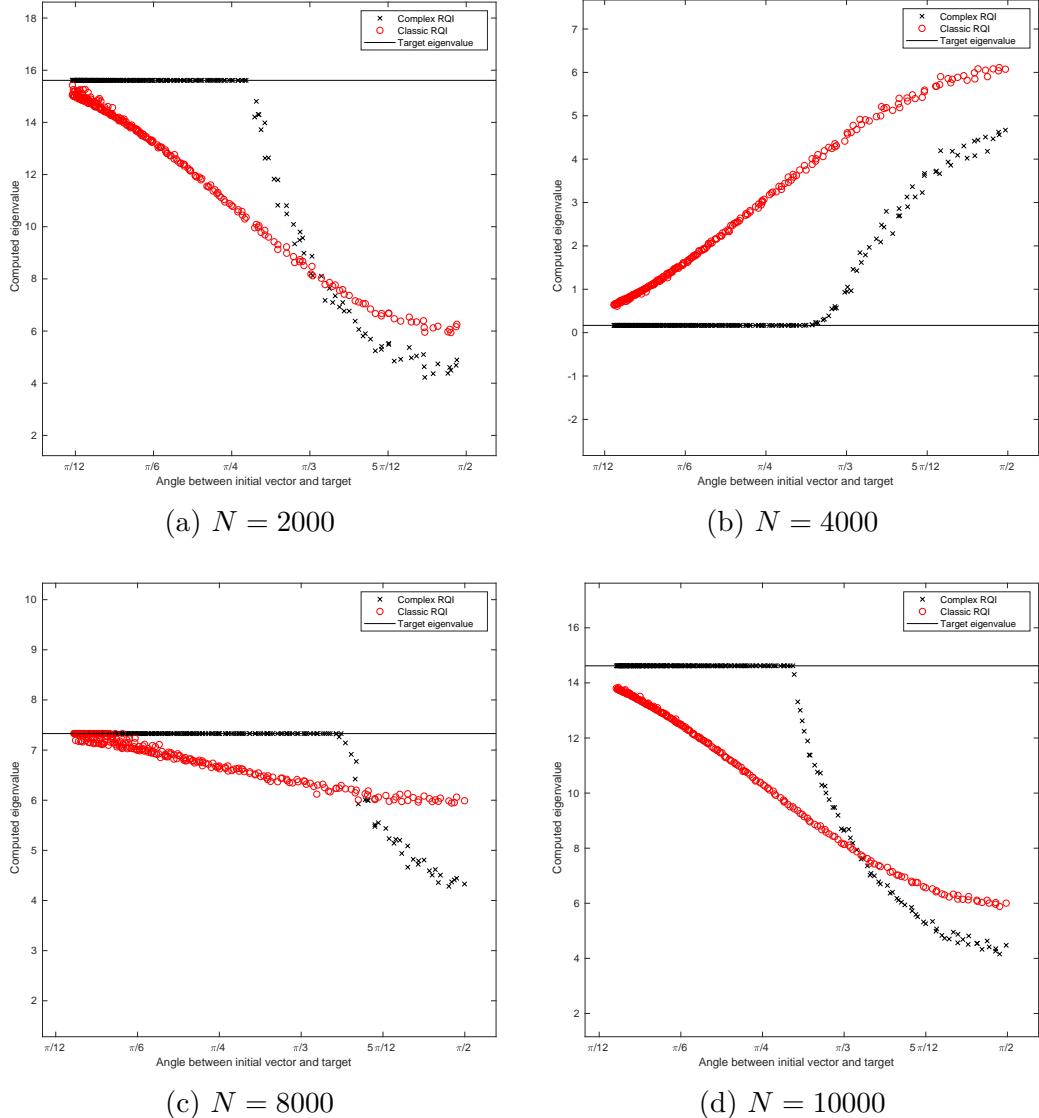


Figure B.11: Plot of the computed eigenvalue against the angle between the initial vector and the target eigenvector for the Martin-Wilkinson matrix MW .

B Additional Plots and Tables

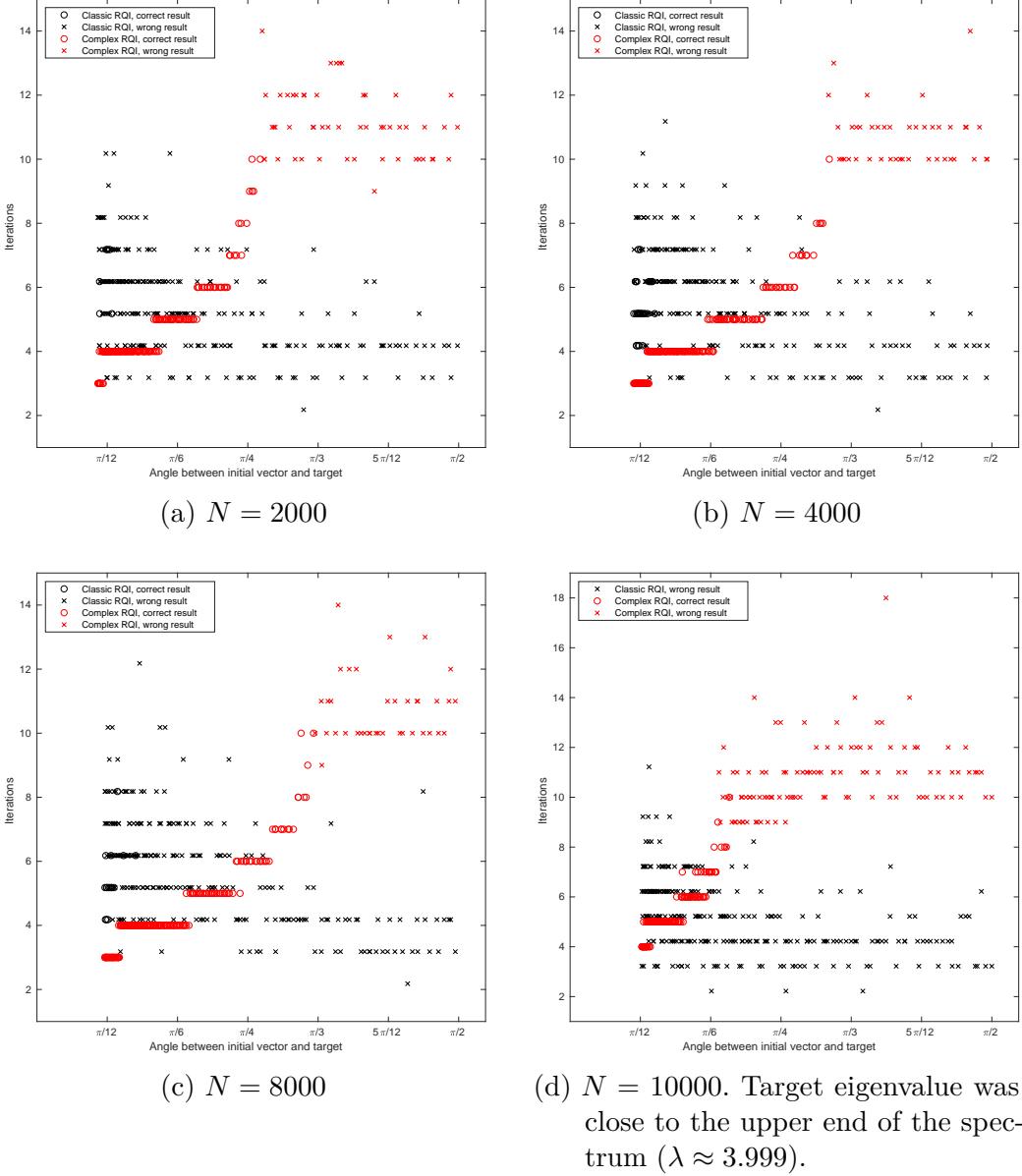


Figure B.12: Plot of the number of iterations of classic RQI and complex RQI for the $[1, 2, 1]$ matrix.

B Additional Plots and Tables

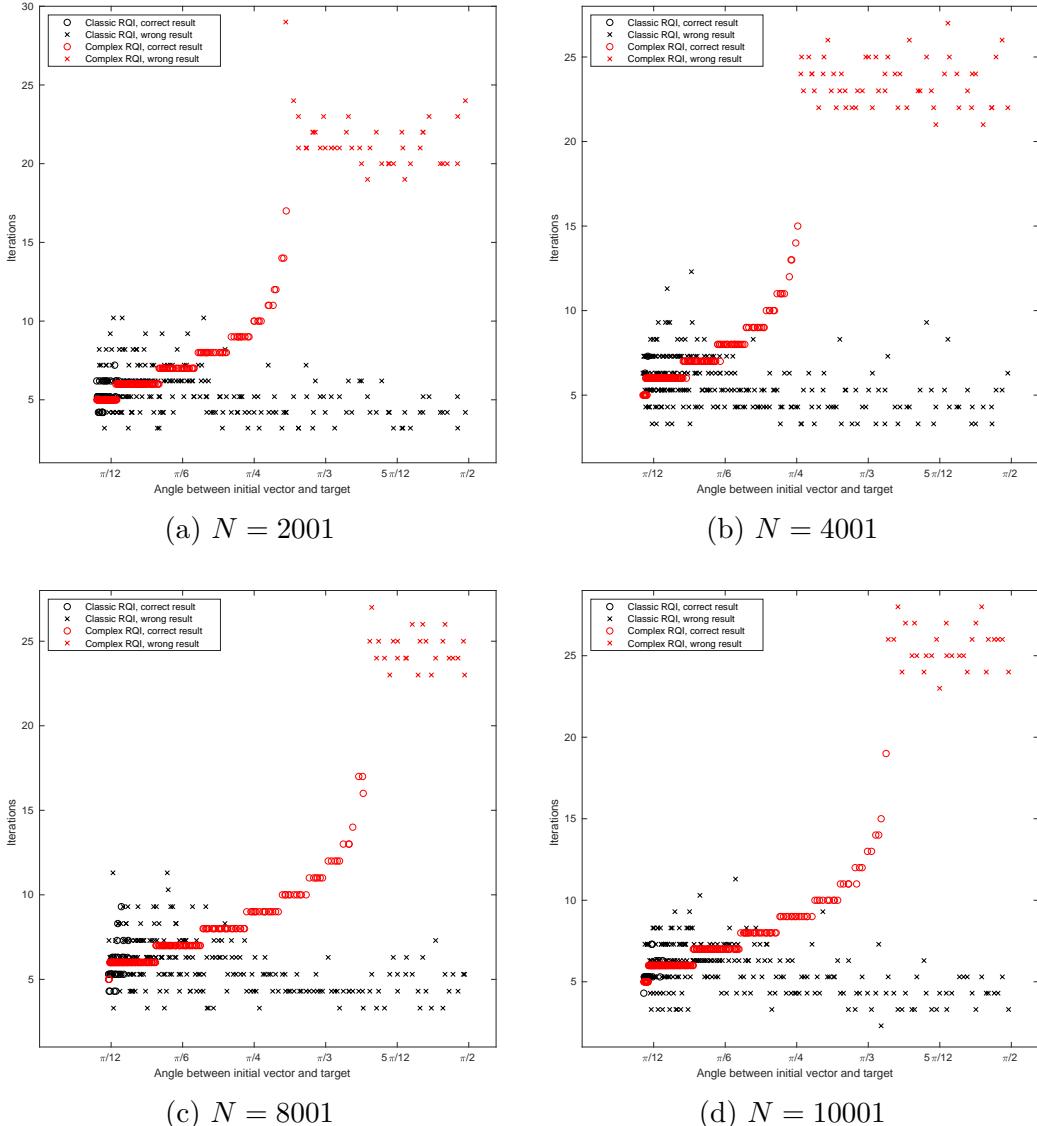


Figure B.13: Plot of the number of iterations of classic RQI and complex RQI for the Wilkinson matrix \mathbf{W}^+ .

B Additional Plots and Tables

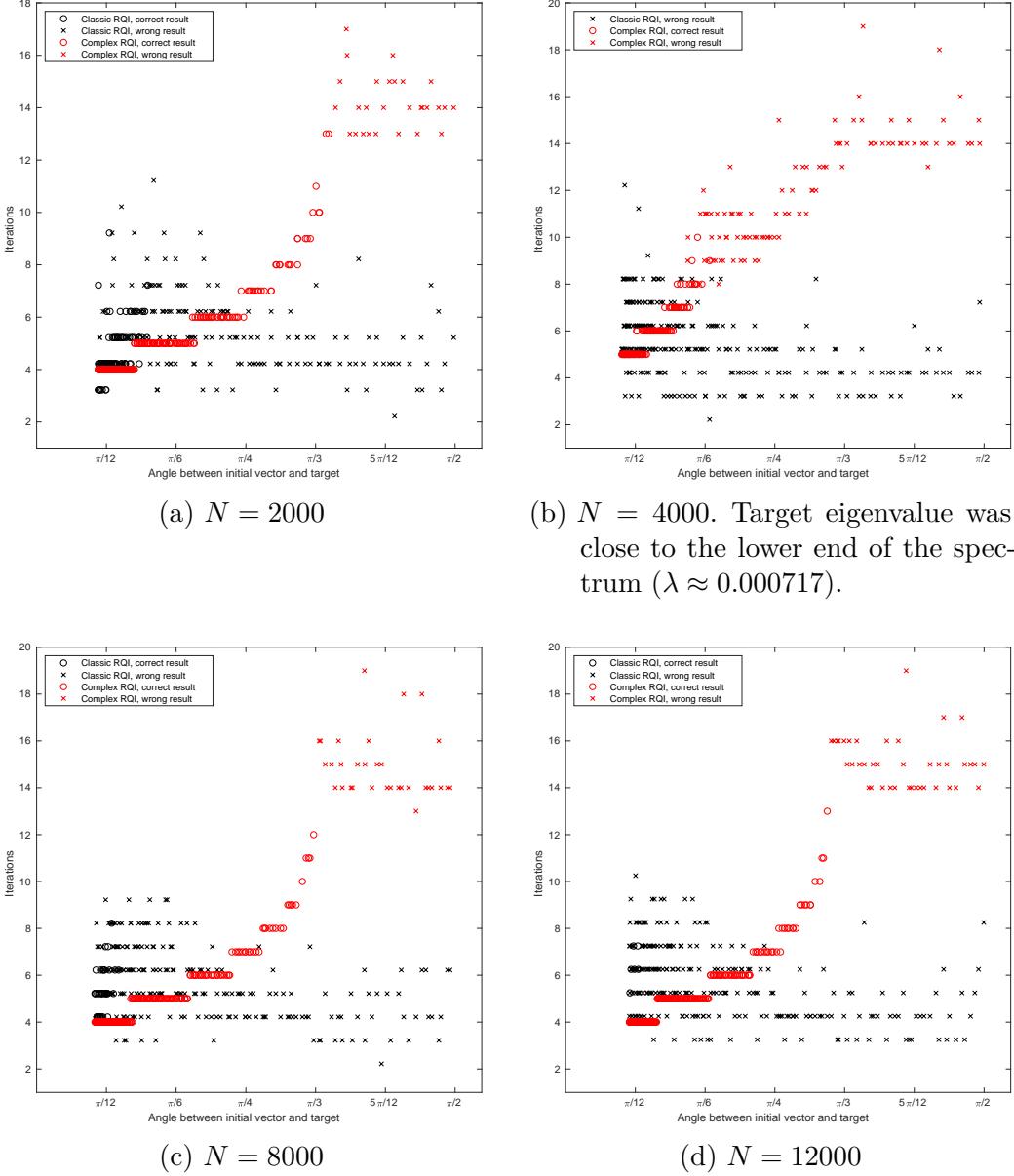


Figure B.14: Plot of the number of iterations of classic RQI and complex RQI for the Martin-Wilkinson matrix MW .

B Additional Plots and Tables

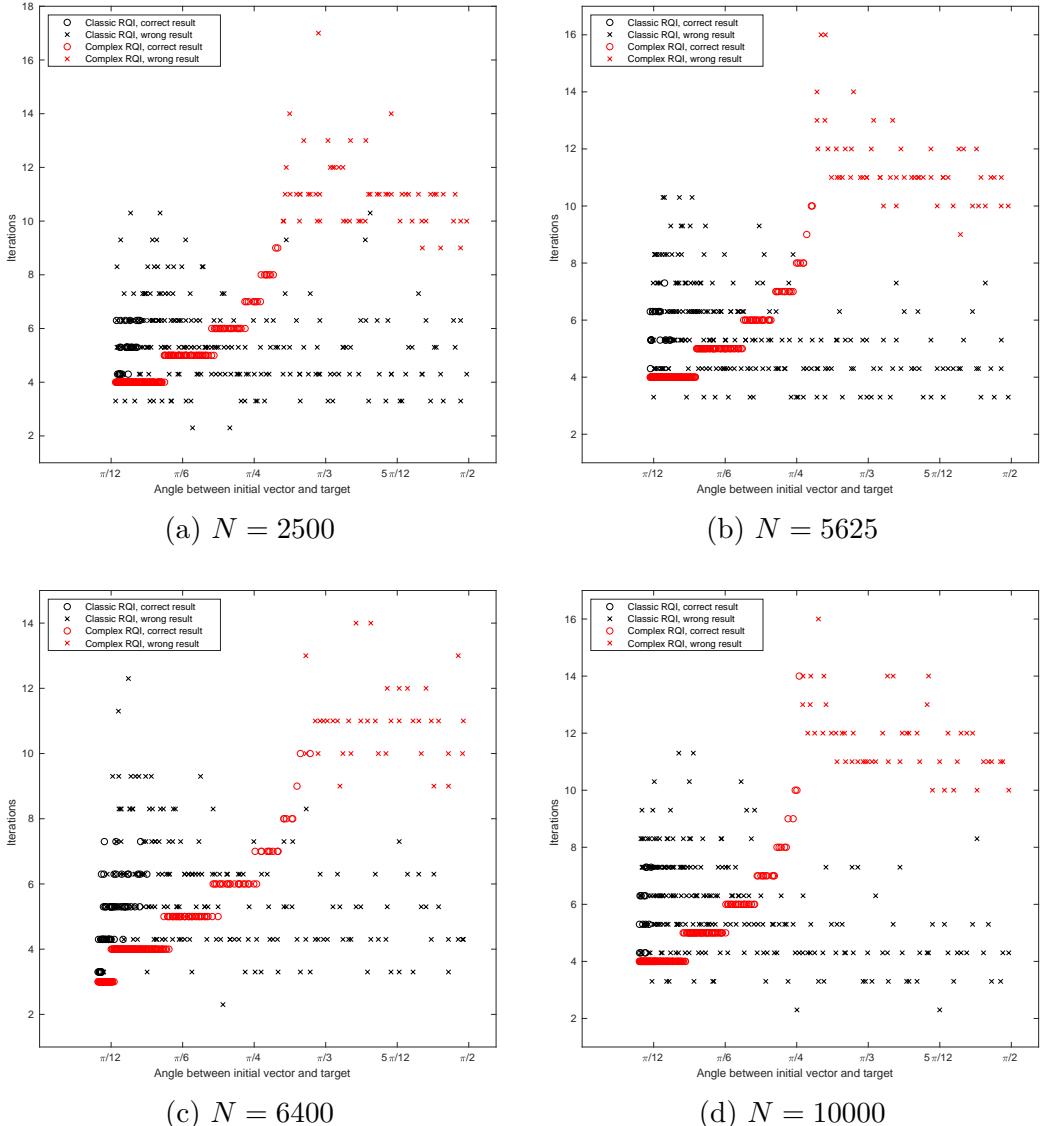


Figure B.15: Plot of the number of iterations of classic RQI and complex RQI for the Laplace matrix.

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