Bachelorarbeit

Constrained Optimisation of Rational Functions for Accelerating Subspace Iteration

Konrad A. S. Kollnig

Aachen, den 21. August 2017

Erstprüfer: Prof. Paolo Bientinesi, Ph.D.
Zweitprüfer: Prof. Georg May, Ph.D.
Betreuer: Jan Winkelmann, M.Sc.
Danksagungen

Meine Zeit am HPAC-Lehrstuhl habe ich sehr genossen. Die Vernetzung in alle Welt stellte eine Bereicherung mit neuen Eindrücken für mich dar. Dies war neben meiner Arbeit an dieser Ausarbeitung eine willkommene Abwechslung, um den Blick über den Tellerrand dieses Dokuments hinaus zu wagen.

Mein Dank gilt in erster Linie meinem Betreuer, Jan Winkelmann. Von ihm stammt das Gros der hier ausgearbeiteten Ideen. Ohne seine fortwährende Unterstützung wäre diese Arbeit nicht möglich gewesen. Mit größter Sorgfalt stand er mir Antwort auf alle meine Fragen gleich welcher Stunde.

Großer Dank gilt auch Prof. Paolo Bientinesi, dem Leiter des HPAC-Lehrstuhls. Seine Expertise war ein wertvolles Quell an Wissen. Geschätzt habe ich die Genauigkeit, mit der er die notwendigen Arbeitsschritte zu jeder Zeit herausstellen konnte.

Erklärung

Hiermit versichere ich, dass ich die vorliegende Arbeit selbständig verfasst, und keine anderen als die angegebenen Quellen und Hilfsmittel verwendet, sowie Zitate kenntlich gemacht habe.

Aachen, den 21. August 2017

______________________________
Konrad A. S. Kollnig
Acknowledgements

My time at the HPAC group has been a pleasure. I have enjoyed the international atmosphere and the exchange with researchers from all over the world. Besides my work on my thesis, this has been an enriching glimpse over the rim of the tea cup.

Foremost, I thank my supervisor, Jan Winkelmann. The majority of ideas discussed in this thesis are his achievement. Without his ongoing support, the creating of this document would have not been possible. Paying attention to the detail, he answered my questions even late at night.

Furthermore, I thank Prof. Paolo Bientinesi, the head of HPAC. His expertise was a valuable source of knowledge. He could tell accurately, what to focus on during the work on this document.
Abstract

Earlier this decade, the so-called FEAST algorithm was released for computing the eigenvalues of a matrix in a given interval. Previously, rational filter functions have been examined as a parameter of FEAST. In this thesis, we expand on existing work with the following contributions: (i) Obtaining well-performing rational filter functions via standard minimisation algorithms, (ii) Obtaining constrained rational filter functions efficiently, and (iii) Improving existing rational filter functions algorithmically. Using our new rational filter functions, FEAST requires up to one quarter fewer iterations on average compared to state-of-art rational filter functions.
## Contents

1. Introduction
   1.1. Rational filter functions for FEAST ......................... 1
   1.2. Contributions ................................................ 3
   1.3. Structure .................................................... 3
   1.4. Preliminaries ............................................... 4

2. FEAST algorithm, subspace iteration with rational filter functions 5
   2.1. Problem ...................................................... 5
   2.2. Algorithm ................................................... 6
   2.3. Convergence rate ............................................ 9

3. Existing rational filter functions 11
   3.1. Gauss-Legendre ............................................... 11
   3.2. Zolotarev ................................................... 13
   3.3. SLiSe ....................................................... 14

4. Embedding into standard minimisation algorithms 19
   4.1. Loss function ............................................... 20
   4.2. Transformation to real arguments ............................ 20
   4.3. BFGS minimisation algorithm ............................... 22
   4.4. Performance of BFGS ....................................... 23

5. Constrained rational filter functions 25
   5.1. Box-constraints ............................................. 26
      5.1.1. Problem ............................................... 26
      5.1.2. Solution ............................................... 27
      5.1.3. Performance ........................................... 28
   5.2. Shape constraints .......................................... 29
   5.3. Probabilistic rational filter functions ................... 32
Introduction

1.1. Rational filter functions for FEAST

Eigenvalue problems are a fundamental subject of computational linear algebra. The FEAST algorithm solves a particular case of eigenvalue problems, i.e. HERMITIAN interior eigenvalue problems [1]. By construction, FEAST offers a natural support for parallelism to make use of state-of-art computer architectures. Recent discussion of the underlying parameters of FEAST has led to significant improvements in performance [2]–[6]. To achieve better performance, we examine rational filter functions (RFFs), a parameter\(^1\) of FEAST, in this thesis.

An RFF is a rational function, defined as

\[
r^{\beta,w}(x) := \sum_{i=1}^{m} \frac{\beta_i}{x - w_i} + \frac{\overline{\beta_i}}{x - \overline{w_i}} - \frac{\beta_i}{x + w_i} - \frac{\overline{\beta_i}}{x + \overline{w_i}}, \quad \text{for } x \in \mathbb{R},
\]

where \(\beta \in \mathbb{C}^m, w \in (\mathbb{C} \setminus \mathbb{R})^m\), for some \(m \in \mathbb{N}\).

The problem is finding appropriate RFFs \(r^{\beta,w}\), that perform well in FEAST for a variety of eigenvalue problems. This is essential for good average performance of FEAST.

\(^1\)Other rational functions are accepted as well, but we want to build upon the currently used RFFs.
1. Introduction

Recently, Winkelmann and Di Napoli have introduced a new approach, called SLiSe minimisation, to obtain well-performing RFFs [5]. This approach aims at improving existing state-of-art RFFs, such as Gauss-Legendre [1] or Zolotarev [2], by solving non-linear minimisation problems. Non-linear means, that a minimisation problem cannot be solved directly. In other words, non-linear problems are computationally difficult to solve.

An integral parameter of SLiSe are weight functions, i.e. non-negative step functions. By weight functions, arbitrary degrees of freedom are offered in SLiSe minimisation to reflect and overcome the diversity of eigenvalue problems. It has been discussed, that the choice of weight function is crucial for obtaining well-performing RFFs via SLiSe. However, by a judicious selection of weight functions, a variety of RFFs $r_{\beta,w}$ have been computed via SLiSe minimisation, outperforming the state-of-art RFFs used in FEAST [5].

In summary, two aspects of SLiSe are of utmost importance: Solving the computationally difficult SLiSe minimisation problems efficiently and choosing suitable weight functions in SLiSe. This currently results in the following drawbacks.

1. Incompatibility with standard minimisation algorithms. The non-linear SLiSe minimisation problems require complex variables. This approach is problematic, as standard minimisation algorithms are incompatible with complex variables. Standard minimisation algorithms potentially yield better RFFs, while decreasing the time required for solving the non-linear minimisation problems.

2. Impracticable performance of box-constraints. To improve the performance of RFFs in FEAST, Winkelmann and Di Napoli suggested the usage of box-constraints in SLiSe minimisation [5]. While they demonstrated the potential of this method, the performance of their implementation is not yet suitable for practice.

3. Choice of suitable weight functions. The choice of suitable weight functions as part of SLiSe is fundamental for computing well-performing RFFs. In the past, weight functions have been chosen empirically. If we had a criterion for estimating the performance of weight functions, we could algorithmically compare a multitude of weight functions to obtain better RFFs via SLiSe minimisation.

Our contributions solve these three issues of SLiSe. We present them in the following.
1.2. Contributions

In this thesis, we solve the three issues of SLiSe introduced previously.

1. **Embedding into standard minimisation algorithms.** We perform the embedding of SLiSe into standard minimisation algorithms in Chapter 4. As a prominent example of a minimisation algorithm, we study the BFGS algorithm, which provides a good performance in our case.

2. **Improving the performance of box-constraints.** We have improved the performance of solving the box-constrained SLiSe minimisation by the L-BFGS-B algorithm. Compared to previous approaches, our approach works well for different SLiSe minimisation problems, requires fewer iterations in general and yields better RFFs. We outline our approach and further improvements of RFFs in Chapter 5.

3. **Algorithmic choice of weight functions.** We propose a method to obtain well-performing weight functions for SLiSe algorithmically instead of empirically. This has enabled us to compute better SLiSe RFFs. Our procedure and an analysis are presented in Chapter 6. All our resulting RFFs can be found in Appendix A. They can be used in FEAST directly. Our new weight functions to improve SLiSe are denoted in Appendix B.

1.3. Structure

In Chapters 2 – 3, we revise the required background briefly: In Chapter 2, we introduce the FEAST algorithm. Notably, we focus on the convergence rate of FEAST in Section 2.3. Reducing this convergence rate is our aim in this thesis. In Chapter 3, we introduce existing RFFs for further improvement in the following chapters.

In Chapters 4 – 6, we present our contributions: In Chapter 4, we embed SLiSe into standard minimisation algorithms. In Chapter 5, we examine constraints on RFFs. In Chapter 6, we obtain new weight functions for SLiSe algorithmically.

In Appendix A, all the discussed RFFs can be found. In Appendix B, all the considered weight functions are denoted. In Appendix C, the BFGS minimisation algorithm is discussed extensively. In Appendix D, we provide proofs of mentioned theoretical details.
1. Introduction

1.4. Preliminaries

The following notation will be used throughout this thesis:

- We denote the natural numbers excluding 0 as $\mathbb{N}$.

- The complex numbers are defined as

  $$\mathbb{C} := \{ a + b \cdot i \mid a, b \in \mathbb{R} \},$$

  where the symbol $i$ is called the imaginary unit. For any complex number $z = a + b \cdot i$, $a, b \in \mathbb{R}$, we call $\Re(z) := a$ the real part of $z$ and $\Im(z) := b$ the imaginary part of $z$. Furthermore, we define the complex conjugate as $\overline{z} := a - b \cdot i$ and the absolute value as $|z| := \sqrt{a^2 + b^2}$.

- For a given matrix $A$, we denote the conjugate transpose of $A$ as $A^H = A^T$. The conjugate of a matrix is defined as the conjugate of its elements.

- For a set $M$ and a function $f : M \to \mathbb{R}$, the notation

  $$\arg\min_{x \in M} f(x)$$

  indicates, that we want to find an $x \in M$ that $f$ attains its minimum for. This is called the minimisation problem or optimisation problem of $f$.

- When we first introduce new terminology, we use italics. We explain terminology when first used.

- When we refer to equations, we use braces: “The BFGS update is given by (C.12).”

- For a given function $f : A \to B$, we denote the image of $f$ as

  $$\text{Im}(f) := \{ f(x) \mid x \in A \} \subseteq B.$$


“Dieser Erfolg ist wesentlich durch den Umstand bedingt, daß ich nicht, wie es bisher geschah, in erster Linie auf den Beweis für die Existenz der Eigenwerte ausgehe.”

“This success is mainly determined by the circumstance, that I do not, as happened previously, focus on the proof of the existence of eigenvalues in the first place.”

— D. Hilbert, Grundzüge einer allgemeinen Theorie der linaren Integralrechnungen

# FEAST, subspace iteration with RFFs

To study the FEAST algorithm, we first examine in Section 2.1 the problem it solves, i.e. the Hermitian interior eigenvalue problem. For further improvement, we introduce the FEAST algorithm in Section 2.2. In Section 2.3, we discuss the convergence rate of FEAST. This is what existing rational filter functions try to reduce for a variety of eigenvalue problems and what we will further dissect in this thesis.

## 2.1. Problem

For the rest of this thesis, we assume a Hermitian matrix $A = A^H \in \mathbb{C}^{n \times n}$, for some $n \in \mathbb{N}$. The Hermitian eigenvalue problem is then identified by the equation

$$Av = \lambda v,$$

(2.1)

for coefficients $\lambda \in \mathbb{C}$ and associated vectors $v \in \mathbb{C}^n \setminus \{0\}$ and some $n \in \mathbb{N}$.

We will call a solution $(\lambda, v)$ to this problem an eigenpair of $A$. The coefficient $\lambda$ is known as an eigenvalue of $A$, the vector $v$ as an eigenvector of $A$. It can be shown that a matrix $A$ has only finitely many different eigenvalues. Thus, it is possible to compute the eigenvalues for a given matrix $A$. It is sufficient to compute one corresponding eigenvector each.
In this thesis, we study the **Hermitian interior** eigenvalue problem (HIEP). Interior means, that the eigenvalues lie in a bounded interval: For a given proper interval \((a, b)\), the HIEP is computing the eigenpairs \((\lambda, v)\) of \(A\) such that \(\lambda \in (a, b)\), where \(a, b \in \mathbb{R}\) fixed. We will refer to such an interval as the **search interval** of the HIEP. We focus on search intervals where \(\lambda_{\text{min}} \leq a, b \leq \lambda_{\text{max}}\), where \(\lambda_{\text{min}}\) denotes the minimum and \(\lambda_{\text{max}}\) the maximum eigenvalue of \(A\). It can be shown that all the eigenvalues of a Hermitian matrix are real-valued. This justifies searching for eigenvalues in a particular real search interval only.

Note that any HIEP can be reduced to a canonical form as follows. The search interval of a HIEP can be phrased as \((m - r, m + r)\), where \(m \in \mathbb{R}\) denotes the midpoint and \(r \in (0, \infty)\) the radius of the given search interval. We then solve the HIEP for the Hermitian matrix \(A'\) given by

\[
A' := (A - m \cdot I) / r
\]

instead of \(A\) with search interval \((-1, 1)\), where \(I\) denotes the matching identity matrix. This is shifting and scaling of the eigenvalues of \(A\) in \((m - r, m + r)\) to \((-1, 1)\). The eigenvectors of both the matrices \(A\) and \(A'\) remain unchanged. We will refer to a HIEP with search interval \((-1, 1)\) as **Canonical HIEP** (CHIEP). In the following, it is sufficient to focus on CHIEPs only.

### 2.2. Algorithm

To introduce the FEAST algorithm for solving CHIEPs\(^2\), we proceed as follows: First, we discuss the inputs of the algorithm. Then, we express the algorithm in terms of pseudo-code and point out the most important details for our analysis. Afterwards, we discuss implementation details for further understanding.

In addition to a Hermitian matrix, the FEAST algorithm requires two main inputs: a rational filter function and an upper bound on the number of eigenvalues in the search interval. These inputs are introduced in the following.

1. **Rational filter function.** For our analysis, the most important input of FEAST is the rational filter function (RFF). An RFF can be used by FEAST to transform

---

\(^2\)FEAST can also solve **generalised HIEPs**. We will only study the standard case. However, this entire document holds for the generalised case as well.
2.2. Algorithm

a **CHIEP** to a *reduced* (unbounded) eigenvalue problem. Reduced means that this eigenvalue problem contains fewer eigenvalues than the original matrix $A$. An **RFF** is defined as

$$r^{β,w} := r(x) := \sum_{i=1}^{m} \frac{β_i}{x - w_i} + \frac{\overline{β_i}}{x - \overline{w_i}} - \frac{β_i}{x + w_i} - \frac{\overline{β_i}}{x + \overline{w_i}},$$  \hspace{1cm} (2.3)

for some $β \in \mathbb{C}^m$, $w \in (\mathbb{C} \setminus \mathbb{R})^m$ and $m \in \mathbb{N}$.

By assuming $w$ to be non-real, we assure that any **RFF** is well-defined. The **RFF** is said to have *degree* $4m$. The values $\pm w_i$, $\pm \overline{w_i}$ are called *poles* of $r$.

An **RFF** appears to map to complex values. However, from its definition, we note that $r(x) = \overline{r(x)}$, for all $x \in \mathbb{R}$. There exists no $z \in \mathbb{C} \setminus \mathbb{R}$ with $z = \pi$. So, an **RFF** is indeed *real-valued*. Furthermore, from its definition, we have $r(x) = r(-x)$, for all $x \in \mathbb{R}$. This means that **RFFs** are *symmetric with respect to the y-axis*. These two properties are important, as shown in the analysis of the convergence rate in the following Section 2.3. More properties were proved in [5].

In the **FEAST** algorithm, an **RFF** is interpreted as a *matrix function*. This is induced by a given **RFF** $r$ as per

$$r(A) = \sum_{i=1}^{m} \beta_i (A - w_i I)^{-1} + \overline{\beta_i} (A - \overline{w_i} I)^{-1} - \beta_i (A + w_i I)^{-1} - \overline{\beta_i} (A + \overline{w_i} I)^{-1},$$  \hspace{1cm} (2.4)

where $I$ denotes the matching identity matrix.

This matrix function is only evaluated when multiplied with another vector $v \in \mathbb{C}^n \setminus \{0\}$. Then, by computing the product $r(A)v$, $4m$ linear systems of the form

$$\alpha(A - zI)^{-1}v,$$  \hspace{1cm} (2.5)

have to be solved, where $α \in \mathbb{C}$ and $z \in \mathbb{C} \setminus \mathbb{R}$.

The synergy of **FEAST** and **RFF** is important for the algorithm to function. However, for this thesis, this is out of scope, because we focus on the performance **RFFs** in **FEAST**. This performance is solely determined by the convergence rate, discussed in the following section. For more details on the usage of **RFFs** in **FEAST**, see [4].

2. **Upper bound on eigenvalue number**. As an additional input, **FEAST** requires an upper bound $N \in \mathbb{N}$ on the number of eigenvalues in $(-1, 1)$, the search interval
2. **FEAST algorithm, subspace iteration with rational filter functions**

The algorithm requires knowledge on how many (interior) eigenpairs to search for. There exists an efficient technique to compute such an upper bound \( N \) as part of the **FEAST** algorithm, see [3]. Thus, in practice, no such prior knowledge of the **CHIEP** is required.

The core of the **FEAST** algorithm is given as follows. It can also be called *subspace iteration with rational filter functions*, as it generalises the well-known *subspace iteration* algorithm using RFFs. For more details, confer [7, ch. 5].

**Algorithm 1** (Subspace iteration with rational filter functions [1], [2], [7], [8]).

**Input:** Hermitian matrix \( A \in \mathbb{C}^{n \times n} \), an upper bound \( N \in \mathbb{N} \) on the number of eigenvalues of \( A \) in \((-1, 1)\) and an RFF \( r \).

**Output:** All eigenpairs \((\lambda, v)\) of \( A \), where \( \lambda \in (-1, 1) \).

1: \( \text{function RFFSubspaceIteration}(A, N, r) \)
2: \( V \leftarrow \text{Random}(\mathbb{C}^{n \times N}) \) \Comment{Initial eigenvector approximation.}
3: \( \text{repeat} \)
4: \( X \leftarrow r(A)V \)
5: \( Q \leftarrow \text{Orthogonalise}(X) \)
6: \( B \leftarrow Q^H A Q \)
7: \( (\Lambda, Y) \leftarrow \text{Solve}(BY = BA) \) \Comment{Reduced eigenvalue problem.}
8: \( V \leftarrow QY \)
9: \( \text{until converged} \)
10: \( \text{return SoughtEigenpairs}(V, \Lambda) \)

Note, that in line 7, we solve a reduced (unbounded) eigenvalue problem of finding \( N \) eigenvalues of \( B = Q^H A Q \in \mathbb{C}^{N \times N} \), where \( N \) denotes the upper bound on the number of eigenvalues of \( A \) in \((-1, 1)\). This can yield an enormously improved performance opposed to computing all the eigenvalues of \( A \in \mathbb{C}^{n \times n} \), if \( N \) is much smaller than \( n \), the size of \( A \).

There are two important notes to make on the implementation of this algorithm, for further understanding of Algorithm 1:

1. **Orthogonalisation.** In line 5, we compute a matrix \( Q \in \mathbb{C}^{n \times N} \) with orthogonal columns, i.e. for two different columns \( q_i, q_j \) of \( Q \), we have \( q_i^T q_j = 0 \). To achieve this, the well-known QR algorithm can be used. A central feature of **FEAST** is the absence of this orthogonalisation step, see [1], [2]. This yields an improved performance, as the QR algorithm is not efficient for large-scale orthogonalisation problems.

2. **Convergence criterion.** For the convergence criterion in line 9, there are different approaches feasible. A common approach is monitoring the sum of absolute values of
the computed eigenvalue approximations in $\Lambda = \text{diag}(\lambda_1, \ldots, \lambda_k)$ lying in the search interval $(-1, 1)$. This sum is known as \textit{eigentrace}. Thus, we have
\[
eigentrace(\Lambda) = \sum_{\lambda_i \in (-1,1)} |\lambda_i|.
\]
(2.6)

In each iteration, the algorithm computes the \textit{relative change} of the eigentrace compared to the previous iteration. The algorithm terminates when a user-selected tolerance is reached by the relative change. In the original publication of \textsc{FEAST} [1], a tolerance of $10^{-13}$ was proposed. More sophisticated approaches are possible, confer [4].

2.3. Convergence rate

In this thesis, we want to improve \textsc{FEAST} by reducing its \textit{convergence rate} for a variety of HIEPs. In the following, we introduce this convergence rate. This result was shown in [8].

Assume, the eigenvalues in the search interval $(-1, 1)$ of $A$ were given by $\lambda_1, \ldots, \lambda_k$, and all the eigenvalues of $A$ by $\lambda_1, \ldots, \lambda_k, \ldots, \lambda_n$, for some $k \in \mathbb{N}$. Then, the convergence rate of the \textsc{FEAST} algorithm is
\[
\max_{1 \leq i \leq k} \left| \frac{r(\lambda_{N+1})}{r(\lambda_i)} \right|,
\]
(2.7)
assuming the eigenvalues of $A$ can be ordered such that
\[
|r(\lambda_1)| \geq \cdots \geq |r(\lambda_k)| \geq \cdots |r(\lambda_N)| \geq |r(\lambda_{N+1})| \geq \cdots,
\]
(2.8)
where $N$ denotes the upper bound on the eigenvalues of $A$ in $(-1, 1)$ as in Algorithm 1.

The \textsc{FEAST} algorithm converges faster, if this convergence rate is smaller. So, we want to reduce this convergence rate for various \textsc{Hermitian} matrices $A$ and eigenvalue distributions in this thesis.

The convergence rate explains, why we assumed \textsc{RFF}s to be both real-valued and symmetric with respect to the $y$-axis in their definition. The former is a consequence of the eigenvalues of a \textsc{Hermitian} matrix being real. The latter is a consequence of an \textsc{RFF} trying to reduce the convergence rate of \textsc{FEAST}. If the underlying \textsc{CHIEP} is not known, no assumption can be made on the distribution of the eigenvalues. So, we assume, that eigenvalues not in the
search interval lie equally-likely on either side of the search interval \((-1, 1)\).

Note that assumption (2.8) can always be assured by an appropriate choice of the RFF \(r\). If the RFF has a larger absolute function value for values inside the search interval than outside\(^3\), assumption (2.8) always holds. For instance, consider the function given by

\[
r(x) = \begin{cases} 
1, & \text{if } x \in (-1, 1), \\
0, & \text{otherwise.}
\end{cases}
\] (2.9)

For this function, assumption (2.8) is satisfied for any distribution of eigenvalues of \(A\). More importantly, we note that this function induces the minimum convergence rate (2.7). It equals zero for any Hermitian matrix \(A\).

Equation (2.9) is equivalent to the definition of the *indicator function* on \((-1, 1)\), herein denoted as \(\mathbb{1}_{(-1,1)}\). As we only examine the search interval \((-1, 1)\), we can safely refer to this function as *the* indicator function.

As the indicator function is discontinuous, it is impossible for a (continuous) RFF to achieve this optimal convergence rate. So, we *approximate* the indicator function by an RFF in the following.

---

\(^3\)Any function with this property is called *filter function*. We restrict out analysis to filter functions suitable for **FEAST**, i.e. rational filter functions.
Existing rational filter functions

In this chapter, we study three different approaches to approximating the indicator function by RFFs. In other words, we analyse RFFs for solving CHIEPs using FEAST efficiently. We discuss the two RFFs primarily used by FEAST, i.e. the GAUSS-LEGENDRE RFF in Section 3.1 and the ZOLOTAREV RFF in Section 3.2. In Section 3.3, we introduce the SLiSe minimisation to further improve these RFFs.

3.1. Using Gauss-Legendre quadrature

Our first approach to approximating the indicator function is exploiting the curve integral representation of the indicator function and solving the resulting integral numerically. To achieve this, consider the unit circle $\gamma(t) := e^{it}$, $t \in [0, 2\pi]$. For $x \in \mathbb{R} \setminus \{-1, 1\}$, the integral representation of the indicator function$^4$ is given by

$$
\mathbb{I}_{(-1,1)}(x) = \begin{cases} 
1, & \text{if } x \in (-1, 1), \\
0, & \text{otherwise}
\end{cases} = \frac{1}{2\pi i} \int_{\gamma} \frac{1}{\zeta - x} \, d\zeta. \tag{3.1}
$$

$^4$For completeness, this is briefly proved in Lemma D.1.
3. Existing rational filter functions

Applying the definition of a curve integral, we obtain

\[ 1_{(-1,1)}(x) = \frac{1}{2\pi i} \int_{0}^{2\pi} \frac{\gamma'(t)}{\gamma(t) - x} \, dt = \frac{1}{2\pi} \int_{0}^{2\pi} g_x(t) \, dt, \]  

if we set

\[ g_x(t) := \frac{e^{it}}{e^{it} - x}, \quad t \in [0, 2\pi]. \]  

Recall that \( \Re \) denotes the real part of a complex number. Rewriting yields

\[ 1_{(-1,1)}(x) = \frac{1}{2\pi} \Re \int_{0}^{\pi} g_x(t) + \overline{g_x(t)} \, dt. \]  

As a simplification, we define the integrand of the resulting integral (3.4) as

\[ h_x(t) := g_x(t) + \overline{g_x(t)}. \]  

With this notation, we compute the derived integral (3.4) numerically. To achieve this, the so-called Gauss-Legendre quadrature defines nodes \( y_1, \ldots, y_{2m} \in (0, \pi) \) to evaluate an integrand at and corresponding weights \( w_1, \ldots, w_{2m} \in (0, \infty) \) to adding up the resulting values yielding

\[ 1_{(-1,1)}(x) \approx \frac{1}{2\pi} \Re \sum_{k=1}^{2m} w_k h_x(y_k). \]  

By symmetries of the nodes and weights in the Gauss-Legendre quadrature, the resulting rational function is an RFF in terms of (2.3).
3.2. Zolotarev

**Definition 3.1** (Gauss-Legendre RFF). For $m \in \mathbb{N}$, we refer to the RFF given by (3.6) as *Gauss-Legendre RFF* of degree $4m$.

There exists no analytical representation of the weights and nodes of the *Gauss-Legendre* quadrature, only a numerical one [9]. Also, it is possible to define the *Gauss-Legendre RFF* on different paths rather than the unit circle. Still, the unit circle has proved to yield good results in practice. For a more extensive analysis see [2], [3].

A graphical illustration is given in Figure 3.1a. Note that the *Gauss-Legendre RFF* does not have a sharp drop about $\pm 1$, but offers a good approximation of the indicator function everywhere else. This is a problem, if the non-sought eigenvalues are close the endpoints of the search interval, as of the convergence rate of *FEAST* (2.7). In the following, we analyse an RFF that attempts to solve this issue.

### 3.2. Zolotarev, worst-case optimality

In this section, we present an approach to minimising the maximum absolute distance between the indicator function and a rational function. This can be phrased as the *minimisation problem*:

$$\arg\min_{r \in F} \max_{x \in \mathbb{R} \setminus M} |1_{(-1,1)}(x) - r(x)|,$$

for a $G \in (0, 1)$ and $M := [-G^{-1}, -G] \cup [G, G^{-1}]$. The set $F$ denotes the rational functions of type $(2m, 2m)$, for a fixed $m \in \mathbb{N}$.

Note that we choose some *gap parameter* $G \in (0, 1)$ to exclude a small interval enclosing $\pm 1$ in order to find a solution to the minimisation problem (3.7). This is necessary, because the indicator function is discontinuous at $\pm 1$ in contrast to RFFs.

Recall the convergence rate of *FEAST* as of (2.7). Intuitively, minimising the absolute difference between the indicator function and a rational function yields the optimal worst-case convergence rate, if we assume that there were no eigenvalues in the *gaps* as of $M = [-G^{-1}, -G] \cup [G, G^{-1}]$.

The solutions to (3.7) exist, can be computed numerically and yield an RFF, as shown in [2], using results of *Zolotarev* from 1877.
3. Existing rational filter functions

![Figure 3.2: Logarithmic plot of the absolute value of the two discussed RFFs, used in FEAST, for the case of 16 poles.](image)

**Definition 3.2** (Zolotarev RFF, Elliptic RFF). Let $m = 2n$ for an $n \in \mathbb{N}$. Then, we call the RFF of degree $2m$ obtained from the version used in FEAST that solves (3.7) as Zolotarev RFF of degree $2m$. This RFF is also known as Elliptic RFF.

The Zolotarev RFF is illustrated in Figure 3.1b. In contrast to the previously discussed Gauss-Legendre RFF, the Zolotarev RFF attains the same bound repeatedly. This is also depicted in Figure 3.2. Another difference is that the decline about $\pm 1$ is sharper. Still, further away from the endpoints $\pm 1$ of the search interval $(-1, 1)$, the Gauss-Legendre RFF offers a better approximation of the indicator function.

### 3.3. SLiSe minimisation problems

In the two previous sections, we have introduced two approaches to gathering RFFs: First, we rewrote the indicator function as an integral and derived a numerical solution via Gauss-Legendre quadrature. Second, we presented the Zolotarev RFF, having a bounded absolute function value on the entire real line except a minor gap. In practice, these approaches are not flexible enough and do not offer sufficient degrees of freedom to suit different HIEPs. To solve this issue, Winkelmann and Di Napoli introduced the concept of a *weighted, squared approximation* of the indicator function [5]. They refer to their concept as SLiSe. To illustrate this approach of “weighted, squared approximation”, we introduce the terms weighted, squared and approximation in the following.

1. **Implementing weighting.** In particular, the function values of an RFF about $\pm 1$ are interesting, when approximating the indicator function. This is, where the
indicator function is discontinuous. So, we would like to put more weight on values about ±1, when approximating the indicator function. To formalise the term weight, we introduce weight functions. These functions shall yield non-negative values. The larger the weight function value, the more important is this point of the real line. We will require a weight function to be symmetric with respect to the y-axis. Thus, we ensure the same weighting for both positive and negative values.

**Definition 3.3** (Weight function). A function $\mathcal{G} : \mathbb{R} \to [0, \infty)$ is called weight function, if $\mathcal{G}$ is symmetric with respect to the y-axis.

A variety of weight functions were studied by Winkelmann and Di Napoli in [5]. Some prominent examples are given in Appendix B for completeness.

2. **Measuring the weighted, squared difference.** Recall, that in the previous chapter, we have introduced, how RFFs are parametrised as per (2.3). Via integration, a weight function $\mathcal{G}$ can be used to measure the approximation of the indicator function by an RFF $r_{\beta,w}$ as per

$$f(\beta, w) := \int_{-\infty}^{\infty} \mathcal{G}(x) \left( \mathbb{1}_{(-1,1)}(x) - r_{\beta,w}(x) \right)^2 dx,$$

(3.8)

for a fixed $m \in \mathbb{N}$ and all $\beta \in \mathbb{C}^m$, $w \in (\mathbb{C} \setminus \mathbb{R})^m$.

Note that $f$ is non-negative. Function values close to 0 are supposed to indicate “well-performing” RFFs, in contrast to function values further away from 0.

The used integral measures the overall squared distance between a given RFF and the indicator function. This is fundamentally different from the concept of the Zolotarev RFF (3.7): Not the maximum absolute error of approximation is relevant, but the overall error.

In practice, we can assume, that the integral in (3.8) always exists, because it is sufficient to consider weight functions $\mathcal{G}$, that fulfil

$$\mathcal{G}(x) = 0, \quad \text{if } |x| \geq C,$$

(3.9)

for some constant $C > 0$.

We can make this assumption for two reasons: First, as a Hermitian matrix $A$ has finitely many eigenvalues, there always exists an absolutely largest eigenvalue $\lambda$. This means that values absolutely larger than $\lambda$ do not require any weight, as of
3. Existing rational filter functions

the convergence rate of FEAST (2.7). We could choose a weight function, that fulfils (3.9) for \( C := \lambda + 1 \) to assure the existence of the studied integral in (3.8). Second, any rational filter function \( x \mapsto r(x) \) converges to 0 for \( x \to \pm\infty \) by (2.3).

If the weight function \( \mathcal{G} \) is a step function, thus piece-wise constant, the function \( f \) is twice continuously differentiable, as shown by WINKELMANN and DI NAPOLI [5]. Moreover, in this case, the function \( f \) and its gradient can be computed efficiently by matrix operations and solving standard definite integrals only. For the exact computational steps, see Theorem D.4.

3. Approximation by minimising the weighted, squared difference. For a given weight function \( \mathcal{G} \), the function \( f \) measures the quality of overall approximation of the indicator function by an RFF. So, we can use \( f \) to approximate the indicator function by a “well-performing” RFF. This can be phrased as the SLiSe minimisation problem

\[
\arg\min_{\beta \in \mathbb{C}^m, w \in (\mathbb{C} \setminus \mathbb{R})^m} f(\beta, w).
\] (3.10)

In contrast to the minimisation problem yielding the Zolotarev RFFs (3.7), we do not measure the absolute difference, but rather the weighted squared difference. This is a least-squares approximation, which comes close to the intuition of the average-case of the convergence rate of FEAST (2.8): We do not minimise the absolute difference but rather the overall difference.

As per (3.8), the previous Equation (3.10) yields a non-linear minimisation problem. Non-linear means that the problem cannot be described in terms of a linear equation system. This class of problems is computationally difficult. For linear problems, there exist such solvers such as the well-known QR algorithm. For non-linear problems, iterative solvers, such as BFGS, can be employed. The performance of solving a non-linear minimisation problem depends on both the used solver and the minimisation problem itself. So, it would be desirable to gather access to a broad selection of non-linear minimisation algorithms. We accomplish this integration in the following chapter.

Integration into standard minimisation algorithms results in another benefit: Not only solutions of the minimisation problem (3.10) can be obtained more efficiently, but also modifications can be studied more rigorously for further improvement. We focus on such improvements to SLiSe in Chapter 5.
Note that neither the function value $f$ (3.8) nor a solution to the minimisation problem (3.10) are connected with a small convergence rate of FEAST as per (2.7). The quality of a solution of the minimisation problem (3.10) solely depends on the quality of the chosen weight function. However, there has not been discovered a criterion for the quality of weight functions in FEAST in the past. They have to be obtained empirically. If a solution of the minimisation problem (3.10) could be obtained efficiently, a broad selection of weight function could be tested. With our well-performing integration into standard minimisation algorithms, we present how to obtain good weight functions algorithmically in Chapter 6.
“The real problem is that programmers have spent far too much time worrying about efficiency in the wrong places and at the wrong times; premature optimization is the root of all evil (or at least most of it) in programming.”

— D. E. Knuth, 1974 Turing Award Lecture

Using standard minimisation algorithms

(a) Convex quadratic loss function.  

(b) Non-convex quadratic loss function.

Figure 4.1.: Examples of quadratic loss functions.

In the previous chapter, we have introduced a non-negative, real-valued, twice continuously differentiable function, that measures the overall approximation of the indicator function by an RFF, denoted

\[ f(\beta, w), \quad \text{for all } \beta \in \mathbb{C}^m, w \in (\mathbb{C} \setminus \mathbb{R})^m, \]

as per (3.8), for a fixed \( m \in \mathbb{N} \).

This motivated the minimisation problem (3.10) of \( f \) to gather “well-performing” RFFs
for FEAST. We now want to solve this minimisation problem numerically, using standard minimisation algorithms, such as BFGS, to obtain well-performing RFFs efficiently. For this, we study the central input of every minimisation algorithm: The function to minimise.

4.1. Loss function

Most of the standard minimisation algorithms necessitate a standard input format for the function to minimise: the loss function. This is defined as follows.

Definition 4.1 (Loss function, residual). Let $n \in \mathbb{N}$. Then, a twice continuously differentiable function $g : \mathbb{R}^n \to [0, \infty)$ is called loss function or loss function of $n$ variables. A function value of a loss function is called residual.

The term “residual” is derived from the application of loss functions in minimisation problems: If we have found a solution to a minimisation problem induced by a loss function (thus a minimiser of the loss function), the function value of the solution (the function value of the minimiser) is the remainder, the residual, in the minimisation.

Example 4.2. The previous Definition 4.1 generalises the quadratic loss function, i.e. a function $\mathbb{R}^n \to \mathbb{R}$, $x \mapsto x^T Ax$, for some fixed matrix $A \in \mathbb{R}^{n \times n}$ and $n \in \mathbb{N}$. If $A$ is positive-semidefinite, this is equivalent to $A$ being non-negative. In this case, we have a loss function in our terms. Two examples are depicted in Figure 4.1. Note that a loss function does not necessarily have a unique minimiser. This is the case for non-convex quadratic loss functions.

The example of quadratic loss function is to illustrate loss functions. In our case, we have to handle by far more complex examples of loss functions.

4.2. Transformation to real arguments

Our function $f$ almost matches the Definition 4.1 of a loss function. The only difference is that our function requires complex arguments. We perform a transformation to real arguments in this section. To illustrate our approach, consider the following example first.
4.2. Transformation to real arguments

Example 4.3. Let $g$ be the real-valued function with complex arguments, given by

$$g(z) := \Im z = \Re(z)^2 + \Im(z)^2, \quad \text{for } z \in \mathbb{C}. \hspace{1cm} (4.1)$$

Its gradient is $\nabla g(z) = \Im$. This can be seen by “treating” $\Im$ as a constant and differentiating with respect to $z$.

Any $z \in \mathbb{C}$, can be written as $z = x + iy$ for $x, y \in \mathbb{R}$. So, we have $g(z) = g(x+iy) = x^2 + y^2$ for $x, y \in \mathbb{R}$. This is a function mapping reals to reals. We can equivalently define

$$\tilde{g}(\begin{pmatrix} x \\ y \end{pmatrix}) := x^2 + y^2 = g(x + iy). \hspace{1cm} (4.2)$$

This is a loss function as per Definition 4.1. We have introduced this function before, confer Figure 4.1a and the previous Example 4.2. The gradient of $\tilde{g}$ is

$$\nabla \tilde{g}(\begin{pmatrix} x \\ y \end{pmatrix}) = 2x + 2y = 2\nabla g(x + iy). \hspace{1cm} (4.3)$$

We have pointed out a connection between $g$ and $\tilde{g}$. This result is important, as it will be generalised in the following.

For the general case, it was shown in [10], that we can transform our loss function to real arguments by “splitting” the arguments into the real and imaginary parts. A function $g : \mathbb{C}^n \to \mathbb{R}$ can be transformed to an $\tilde{g} : \mathbb{R}^{2n} \to \mathbb{R}$ as per

$$\tilde{g}(\begin{pmatrix} x \\ y \end{pmatrix}) := g(x + iy), \hspace{1cm} (4.4)$$

for $x, y \in \mathbb{R}^n$. According to [10], the gradient is given by

$$\nabla \tilde{g}(\begin{pmatrix} x \\ y \end{pmatrix}) = 2\nabla g(x + iy), \hspace{1cm} (4.5)$$

for $x, y \in \mathbb{R}^n$. We can now safely call our function $f$ loss function, because it can be transformed to such, as per this procedure. The function values of $f$ will be called residuals as in the case of loss functions. Our loss function can now be minimised using standard minimisation algorithms. In the following, we present an example of a powerful standard minimisation algorithm.
4. Embedding into standard minimisation algorithms

4.3. BFGS minimisation algorithm

As a minimisation algorithm, we propose the Broyden-Fletcher-Goldfarb-Shanno (BFGS) algorithm \[11\]. We discuss the algorithm in the following, while comparing it to other prominent minimisation algorithms.

First of all, BFGS requires a loss function \(g\) as per Definition 4.1, its gradient and a starting point \(x_0\) as inputs. For \(k = 1, 2, \ldots\), the algorithm approximates a minimiser of \(g\) by iterates \(x_k \in \mathbb{R}^n\), such that

\[
g(x_0) > g(x_1) > \cdots > g(x_k) \geq 0.
\] (4.6)

This is supposed to converge to a minimiser of \(g\). Note that \(g(x) \geq 0\) for \(x \in \mathbb{R}\) by the Definition 4.1 of a loss function.

The BFGS algorithm has multiple properties that make it an appropriate choice compared to other minimisation algorithms in our case. These properties are discussed in the following.

- **Efficiency.** The algorithm does not require any linear system solves. This makes it superior amongst other minimisation algorithms, such as Levenberg-Marquardt. Furthermore, the algorithm memorises the history of iterates, in contrast to other methods, such as Gradient descent. Tracking the iterates enables BFGS to converge to a minimiser efficiently.

- **Improvement.** The algorithm requires a starting point as an input. Because we have already gathered prominent examples of RFFs in Chapter 3, we can use those as a starting point. This is supposed to yield an improved RFF compared to the original RFF [5].

- **Extensibility.** By further conditions on the minimisation problem, the possible solutions can be constrained to obtain different RFFs. The BFGS algorithm is a versatile tool for embedding such conditions. In the following chapter, we study such conditions.

**Extensive analysis of BFGS.** We provide an extensive analysis of the BFGS algorithm in Appendix C. BFGS is not a trivial algorithm, as it incorporates a multitude of advances in minimisation research \[11\]–\[16\].
4.4. Performance of BFGS

To demonstrate the performance of our approach, we compare BFGS to the approach in the original publication by Winkelmann and Di Napoli in the case of box-constrained SLiSe [5]. We have not introduced box-constrained SLiSe yet. This is the aim of the following chapter. However, we refer to the same set-up as in the original paper, which justifies discussing the performance of BFGS in this case upfront.

The projected gradient descent algorithm was used by Winkelmann and Di Napoli [5]. We use the L-BFGS-B algorithm, an extension of BFGS [17]. As in the case of BFGS, projected gradient descent does not involve linear system solves. In contrast to BFGS, projected gradient descent does not memorise the history of iterates. This results in worse performance. For a more extensive analysis of projected gradient descent in the context of RFFs, see the original publication [5]. For the L-BFGS-B algorithm, we used the FORTRAN implementation by the authors of the algorithm [17]–[19]. We employed the most recent version 3.0 in our experiments. For projected gradient descent, we used the implementation of Winkelmann and Di Napoli who kindly granted access.

For a comparison, we refer to the same set-up as in the original publication for box-constraints by Winkelmann and Di Napoli first. Especially, this means that we employed the weight function Box-SLiSe (given in Example B.2) and the 16-pole Zolotarev RFF as the starting point of the minimisation algorithm. This number of poles is the standard choice in FEAST.

In the case of projected gradient descent, the resulting residual is $7.57 \cdot 10^{-4}$. In the case of L-BFGS-B, the resulting residual is $4.72 \cdot 10^{-4}$, which is about 38% smaller. Thus, our approach yields a better RFF in terms of weighted, squared distance. Both algorithms require less than 400 function evaluations, which is a good performance for practical use.

This raises the question, why the algorithms converge to different residuals and RFFs. As SLiSe is a non-convex problem, there may exist different minimisers having different residuals [5]. However, this is not the case, as the resulting RFF of projected gradient descent can be further minimised to a residual of $4.72 \cdot 10^{-4}$ by L-BFGS-B. This is the same residual as in the case of L-BFGS-B before. In fact, projected gradient descent does only slightly minimise the starting residual. Whereas the resulting residual of projected

---

3We complied L-BFGS-B using the supplied MAKEFILE that builds upon gcc, used in version 5.4.0. The processor was an Intel Core i5-4200M. In L-BFGS-B, we used standard parameters for maximum accuracy as per the documentation [18], given by factr = 1e1, m = 20.
4. Embedding into standard minimisation algorithms

![Graphs showing comparison of L-BFGS-B and projected gradient descent]

Figure 4.2.: Comparison of L-BFGS-B and projected gradient descent in box-constrained SLiSe.

Gradient descent is $7.57 \cdot 10^{-4}$, the residual of the starting Zolotarev RFF is $8.09 \cdot 10^{-4}$. So, projected gradient descent does not offer the same accuracy as L-BFGS-B.

Also, the case is different, when another starting point is used. For the 16-pole Gauss-Legendre RFF as the starting point, the results are depicted in Figure 4.2. On the $x$-axis, the number of evaluations of the loss function $f$ after each iteration of the minimisation algorithm is denoted. On the $y$-axis, the residual after each iteration of the algorithm is denoted.

We find that the L-BFGS-B algorithm needs about 500 loss function evaluations, compared to about 900,000 in the case of projected gradient descent. Furthermore, despite fewer loss function evaluations, L-BFGS-B yields a smaller residual of $4.72 \cdot 10^{-4}$ opposed to $7.08 \cdot 10^{-4}$ for projected gradient descent. L-BFGS-B results in the same residual and only about 100 function evaluations more as for the Zolotarev RFF as the starting point. In contrast, projected gradient descent results in a better (smaller) residual compared to before, but a much larger number of function evaluations. Nevertheless, the resulting residual of projected gradient descent is not better (smaller) than in the case of L-BFGS-B.

We have also tested different number of poles and different weight functions. However, we found similar results in these cases. We conclude that our approach significantly increases the resilience of minimisation against the choice of parameters in the minimisation process. L-BFGS-B outperforms projected gradient descent in both performance and accuracy.
Constrained rational filter functions

In the preceding chapter, we have derived how to embed SLiSe into standard minimisation algorithms. As a prominent example of such, we studied the BFGS algorithm. This opens the opportunity to make use of further features of such minimisation algorithms: Adding constraints. This means that we are not interested in any RFF in SLiSe minimisation, but rather in one subject to certain constraints to further improve RFFs. In other words, we study modifications to the original SLiSe minimisation problems (3.10). The BFGS algorithm allows to implement constraints relatively easily.

In the following, we introduce three different types of constraints: In Section 5.1, we improve the performance of performing a single FEAST iteration, when SLiSe RFFs are used. In Section 5.2, we present constraints to shape RFFs. In Section 5.3, we constrain RFFs using a given probability distribution to improve the performance of RFF for a particular set of HIEPs.
5. Constrained rational filter functions

5.1. Box-constraints

5.1.1. Problem

Recall that the usage of RFFs in FEAST results in solving linear systems of the form

\[ \alpha (A - zI)^{-1} v, \quad (5.1) \]

for vectors \( v \in \mathbb{C}^n \setminus \{0\} \) and \( \alpha \in \mathbb{C}, \quad z \in \mathbb{C} \setminus \mathbb{R} \), as per (2.5).

This is a problem, if a pole \( z \) of an RFF approaches an eigenvalue of \( A \) in the minimisation process. In this case, the condition number of the matrix \( \alpha (A - zI) \) becomes very large. This yields slow convergence for iterative linear system solvers in FEAST.

In the following, we analyse this condition number further. We neglect the scalar \( \alpha \), as it is a constant factor in this analysis. The condition number of the remainder is given by

\[ \text{cond}(A - zI) = \max_i |\lambda_i - z| \min_j |\lambda_j - z|, \quad (5.2) \]

where \( \lambda_1, \ldots, \lambda_n \) denote the eigenvalues of \( A \).

We rewrite and estimate

\[ \text{cond}(A - zI) = \frac{\max_i |\lambda_i - z|}{\min_j |\lambda_j - \Re(z) - i\Im(z)|} \leq \frac{\max_i |\lambda_i - z|}{|\Im(z)|}, \quad (5.3) \]

as all eigenvalues \( \lambda_j \) of the Hermitian matrix \( A \) are real. Recall that \( \Re \) denotes the real, respectively \( \Im \) the imaginary part.

We assume \(|z| < 1\), as we will only consider RFFs with such poles \( z \). This is related to the search interval being \((-1, 1)\) in a CHIEP. Then, we can further simplify using the triangle inequality

\[ \text{cond}(A - zI) < \frac{\max_i |\lambda_i| + 1}{|\Im(z)|}. \quad (5.4) \]

As \( \max_i |\lambda_i| + 1 \) is a constant factor, we neglect this scalar and define the following quantity.

\[ ^{6}\text{Herein, we analyse the condition number with respect to the 2-norm. This is a natural choice in the context of complex numbers. Moreover, the matrix } A \text{ is assumed to be Hermitian, which implies that } A - zI \text{ is normal. In this case, our claim holds.} \]
5.1. Box-constraints

**Definition 5.1** (Worst-case condition number). Let \( r \) be an RFF. Then, the worst-case condition number in FEAST is (up to a constant factor)

\[
\text{cond}_{\text{worst}}(r) := \max_{z \text{ is pole of } r} \frac{1}{|\Im(z)|}. \tag{5.5}
\]

### 5.1.2. Solution

Fix an RFF \( r^{\beta,w} \) for some \( \beta \in \mathbb{C}^m, w \in (\mathbb{C} \setminus \mathbb{R})^m \) and \( m \in \mathbb{N} \), parametrised as in (2.3). Recall that the values \( w_1, \ldots, w_m \) characterise the poles of the RFF \( r^{\beta,w} \) up to symmetries.

To limit the worst-case condition number, we introduce a *lower bound* \( lb > 0 \) on the absolute imaginary parts of the poles of the RFF \( r^{\beta,w} \) as per

\[
|\Im(w_i)| \geq lb, \quad \text{for } i = 1, \ldots, m. \tag{5.6}
\]

In this case, as of Definition 5.1, we have

\[
\text{cond}_{\text{worst}}(r^{\beta,w}) \leq \frac{1}{lb}. \tag{5.7}
\]

For a given lower bound \( lb > 0 \), the previously studied minimisation problem (3.10) can be reformulated as

\[
\argmin_{\beta \in \mathbb{C}^m, w \in (\mathbb{C} \setminus \mathbb{R})^m} f(\beta, w), \tag{5.8a}
\]

subject to:

\[
|\Im(w_i)| \geq lb, \quad \text{for } i = 1, \ldots, m, \tag{5.8b}
\]

as introduced in [5]. In a general minimisation environment, such bounds are known as *box-constraints*. This is demanding arbitrary lower and upper bounds on the components of the sought solution. For the solution of box-constrained problems, there exists a well-known extension to BFGS, the L-BFGS-B algorithm [17].

For more background on box-constrained minimisation in the case of L-BFGS-B, see Appendix C.
5. Constrained rational filter functions

5.1.3. Performance

We have previously discussed the performance of our implementation of box-constraints in Section 4.4. Compared to the current implementation of box-constraints in SLiSe, our L-BFGS-B approach has significantly improved both performance and accuracy. In this subsection, we discuss the impact of different lower bounds on both the residual and the worst-case condition number in terms of Definition 5.1 of RFFs.

We employ the same set-up as in the original SLiSe publication [5] for box-constrained minimisation: We use the Box-SLiSe weight function in the minimisation problem. This weight function was explicitly designed for box-constrained minimisation. Moreover, we choose the 16-pole Zolotarev RFF as the starting point of the minimisation for two reasons. First, the number of 16 poles results is the default value in FEAST, as it performs well in practice [1]. Second, the minimum absolute imaginary of the poles of this RFF is only about 0.0022, which is low compared to other RFFs. This can be seen as follows: Using the notation as of (2.3), i.e. only employing the poles in the upper-left complex half-plane, we can denote the 16-pole Zolotarev RFF $r^{β,w}$ as

| Poles $w$          | Coefficients $β$                    |
|-------------------|-------------------------------------|
| $-0.999998 + 0.0021993i$ | $0.00089892 - 0.00000198i$         |
| $-0.999851 + 0.0172345i$     | $0.00524579 - 0.0000904i$         |
| $-0.993336 + 0.115256i$       | $0.0346254 - 0.00401754i$        |
| $-0.739835 + 0.672789i$       | $0.150517 - 0.136877i$          |

For a comparison to the other studied RFFs, see Appendix A. There, these RFFs are denoted.

As minimisation algorithm, we use L-BFGS-B in the same set-up as in Section 4.4. We have computed both the worst-case convergence rates, as well as the residuals for 100 equidistant lower bounds in [0, 0.0022]. In the case of the Zolotarev RFF, lower bounds larger than 0.0022 are not feasible, as L-BFGS-B requires that the starting point lies in the bounds.

The results are depicted in Figure 5.1. For $lb = 0.0022$, we obtain a residual of about $4.72 \cdot 10^{-4}$ and a worst-case condition number of about $6.13 \cdot 10^5$. Conversely, for $lb = 0.0011$, we find a residual of about $3.80 \cdot 10^{-4}$ and a worst-case condition number of about $17.8 \cdot 10^5$, which is thrice as much.
5.2. Shape constraints

We have seen examples of RFFs before, i.e. the Gauss-Legendre and the Zolotarev RFF. They share a feature, that is desirable in practice: They have non-increasing extrema outside the search interval \((-1, 1)\). This matches the intuition of an RFF quite well: An RFF delivers fast convergence in FEAST, if the eigenvalues outside the search interval are not close its endpoints. An RFF with a different behaviour may contradict the intuition of the FEAST user.
5. Constrained rational filter functions

There exist SLiSe RFFs having increasing extrema. An example of such is depicted in Figure 5.2. The Gauss-Legendre RFF has non-increasing extrema, whereas the “Increasing RFF” has a local extremum at about 2 with a larger absolute value than the extrema inside [0, 2).

In the following, we present a method to prevent such RFFs in SLiSe minimisation. To achieve this, we introduce a set of constraints to be added to the original minimisation problem (3.10) in the following.

Let $\beta_0 \in \mathbb{C}^m, w_0 \in (\mathbb{C} \setminus \mathbb{R})^m$ characterise the starting RFF $r^{\beta_0,w_0}$ used in the minimisation algorithm, e.g. BFGS as per Section ???. Choose $k \in \mathbb{N}$ evaluation points, $1 < x_1 < \cdots < x_k$. Then for each evaluation point $x_i$, we add a constraint to the minimisation problem as follows

$$|r^{\beta,w}(x_i)| \leq (1 + c) \cdot |r^{\beta_0,w_0}(x_i)|,$$

(5.9)

where $c \in (0, 1)$ controls the percentage of deviation of the resulting RFF from the starting RFF at $x_i$.

Note, that it is sufficient to choose a small number of evaluation points $x_i$ near the endpoints of the search interval: On the one hand, an RFF is a continuous function, which limits the steepness of change in function value. However, the larger the degree of the sought RFF, the more evaluation points and constraints are required, as such RFFs offer more degrees of freedom. On the other hand, an RFF converges to zero for both large positive and negative values as pointed out before.
5.2. Shape constraints

We note that the values on the right hand sides of the in-equations (5.9) are constant. So, we can rewrite

$$|r^{\beta,w}(x_i)| \leq C_i,$$

(5.10)

defining the constants

$$C_i := (1 + c) \cdot |r^{\beta_0,w_0}(x_i)|,$$

(5.11)

for a control parameter $c \in (0, 1)$ and $i = 1, \ldots, k$.

Faster convergence in minimisation algorithms can be achieved, if both the loss function and the constraints are differentiable; RFFs are, but the absolute value is not. Instead of (5.10), we could add the following two constraints to the minimisation problem

$$r^{\beta,w}(x_i) \leq C_i,$$

(5.12a)

$$-r^{\beta,w}(x_i) \leq C_i,$$

(5.12b)

for $i = 1, \ldots, k$.

We will refer to this type of constraints as shape constraints, because they enforce the shape of the sought RFF in the minimisation process.

The resulting minimisation problem can be phrased as

$$\arg\min_{\beta \in \mathbb{C}^m, \omega \in (\mathbb{C} \setminus \mathbb{R})^m} f(\beta, \omega),$$

(5.13a)

subject to: $\pm r^{\beta,w}(x_i) \leq C_i$, for $i = 1, \ldots, k$.

(5.13b)

For instance, this minimisation problem can be solved using the NLOpt minimisation package [20]. This package provides multiple suitable minimisation algorithms, e.g. the BFGS-based SLSQP algorithm [21]. In the following, we will not analyse this type of constraints any further, as they do not improve convergence of FEAST, as per the definition of its convergence rate (2.7). Moreover, these constraints may limit the convergence of the FEAST algorithm, as every added constraint potentially leads to an RFF having a larger residual in SLiSe minimisation. This means that a resulting RFF would be supposed to perform worse in FEAST. However, for gathering RFFs ready for production and the end-user, this technique might be considered.
5. Constrained rational filter functions

![Graphs showing normal and uniform distributions](image)

(a) Normal distribution having variance 1/9.  (b) Uniform distribution on [-5, 5].

Figure 5.3.: Probabilistic RFFs with 16 poles.

5.3. Probabilistic rational filter functions

The convergence rate of FEAST (2.7) determines the performance of FEAST. Previously, we have assumed to have no prior knowledge of the underlying eigenvalue distribution, in the design of RFFs to suit a variety of CHIEPs.

There are cases, where we have prior knowledge of the probability distribution of the eigenvalues, for instance in self-consistent field calculations from material science [1]. In this case, a probability distribution can be employed to obtain Probabilistic RFFs as follows.

Assume a continuous probability distribution $D$ and its corresponding probability density function $h : \mathbb{R} \rightarrow [0, \infty)$ that indicates the eigenvalue distribution of the studied HERMITIAN matrix $A$. As in the case of the ZOLOTAREV RFF in Section 3.2, we assume a gap parameter $G \in (0, 1)$.

For given independent random variables $X, Y$ distributed according to $D$ and an RFF $r^{\beta, \omega}$, we define

$$I := [-G, G].$$

(5.14)

For values inside the search interval, we introduce

$$O := [-\infty, -G^{-1}] \cup [G^{-1}, \infty].$$

(5.15)

For given independent random variables $X, Y$ distributed according to $D$ and an RFF $r^{\beta, \omega}$,
we can determine the expected convergence rate as of

$$E(\beta, w) := \mathbb{E}\left[\frac{r_{\beta,w}(Y)}{r_{\beta,w}(X)} \mid X \in I, Y \in O\right],$$

(5.16)

parametrising an RFF by $\beta \in \mathbb{C}^m, w \in (\mathbb{C} \setminus \mathbb{R})^m$ and $m \in \mathbb{N}$ as per (2.3).

For independent random variables, the conditional expectation (5.16) is defined as

$$E(\beta) = \frac{1}{P[X \in I] \cdot P[Y \in O]} \int_I \int_O \left|\frac{r_{\beta,w}(y)}{r_{\beta,w}(x)}\right| h(y) h(x) \, dy \, dx$$

(5.17a)

$$= \frac{1}{P[X \in I] \cdot P[Y \in O]} \int_I \left|h(x)\right| \frac{1}{\left|r_{\beta,w}(x)\right|} \, dx \cdot \int_O \left|r_{\beta,w}(y)\right| h(y) \, dy.$$  (5.17b)

As $E(\beta, w)$ is non-negative, this directly motivates the minimisation problem

$$\arg\min_{\beta \in \mathbb{C}^m, w \in (\mathbb{C} \setminus \mathbb{R})^m} E(\beta, w).$$

(5.18)

It is possible to compute the value of $E(\beta, w)$ by numerical methods. We have implemented a numerical approach in MATLAB and tested different probability distributions of eigenvalues. Two Probabilistic RFFs are depicted in Figure 5.3, for a gap parameter $G = 0.99$. However, they do not yet perform well in practice and require further research on the right choice of parameters and the computation of the occurring integrals. So, we will not focus on them in the analysis of different RFF in the following chapter.

However, if we had computed a solution to (5.18), this would yield both a well-performing RFF and the expected convergence rate.
“I [...] am rarely happier than when spending an entire day programming my computer to perform automatically a task that would otherwise take me a good ten seconds to do by hand.”

— D. Adams, Last Chance to See

6

Algorithmic design of weight functions

We have previously seen that the Gauss-Legendre RFF aims at providing a good behaviour on average, whereas the Zolotarev RFF is for the worst-case convergence scenario. In this chapter, we improve the Gauss-Legendre RFF to ensure fast convergence of FEAST in practice.

Our improvements yield a new RFF, the Enhanced $\gamma$-SLiSe RFF, which is denoted in Appendix A. This RFF was obtained using the BFGS algorithm, as outlined in Section 6.1. In Section 6.2, we compare the worst-case performance of our new RFF to state-of-art RFFs as introduced in Chapter 3. In Section 6.3, we examine the performance in practice on a large problem set.

6.1. Minimum weight functions

The SLiSe minimisation problems aim at minimising the weighted, squared distance to the indicator function. However, this does not necessarily result in an RFF performing well in FEAST, as this process depends on the chosen weight function. In the following, we introduce a criterion for identifying well-performing weight functions. We call this criterion the worst-case convergence rate of weight functions.
6. Algorithmic design of weight functions

We will use this worst-case convergence rate of a weight function to improve the $\gamma$-SLiSe weight function. This particular weight function was proposed by Winkelmann and Di Napoli to obtain SLiSe RFFs to replace the Gauss-Legendre RFF. For $x \in \mathbb{R}$, this weight function is defined as

$$G_{\gamma\text{-SLiSe}}(x) := \begin{cases} 
1, & \text{if } |x| < 0.95, \\
0.01, & \text{if } 0.95 \leq |x| < 1.05, \\
10, & \text{if } 1.05 \leq |x| < 1.4, \\
20, & \text{if } 1.4 \leq |x| < 5, \\
0, & \text{otherwise.}
\end{cases} \quad (6.1)$$

In particular, we focus on the case of 16 poles, as this is the standard choice in FEAST.

We proceed as follows: First, we introduce the worst-case convergence rate of an RFF. Second, we define the worst-case convergence rate of a weight function. Third, we motivate a minimisation problem of the worst-case convergence rate of weight functions. Fourth, we study how to solve the new minimisation problem numerically.

1. **Worst-case convergence rate of RFFs.** The worst-case convergence rate has previously been studied for RFFs in FEAST. From the convergence rate of FEAST as per (2.7), the worst-case convergence rate was derived in [2] as

$$\text{worstcase}(r, G) = \frac{\max_{x \in [G^{-1}, \infty]} |r(x)|}{\min_{x \in [0, G]} |r(x)|}, \quad (6.2)$$

for an RFF $r$ and a gap parameter $G \in (0, 1)$, assuming there were no eigenvalues in $[-G^{-1}, -G] \cup [G, G^{-1}]$.

As in Definition 3.2 of the Zolotarev RFF, a gap parameter is required for this definition. As before, this is necessary for a meaningful notion of worst-case convergence rate, as RFFs are continuous functions.

2. **Worst-case convergence rate of weight functions.** We now use the worst-case convergence rate of an RFF as per (6.2), to assign a worst-case convergence rate to a weight function.

Let $\mathcal{G}$ be a weight function. Then, we can use $\mathcal{G}$ in a SLiSe minimisation (3.10) with the 16-pole Gauss-Legendre RFF as the starting point. We choose this RFF as a fixed starting point, as we are interested in improving this RFF. The SLiSe
6.1. Minimum weight functions

minimisation using the weight function $\mathcal{G}$ yields a new RFF $r$. For this RFF $r$, we have already derived the worst-case convergence rate as per (6.2), so we can define

$$\text{worstcase}(\mathcal{G}) := \text{worstcase}(r, G), \quad (6.3)$$

where $G \in (0, 1)$ is a fixed gap parameter.

The worst-case convergence rate requires a gap. We suggest a moderate choice of $G = 0.95$, as this yields good results in practice.

3. Weight functions as a minimisation problem. We want to improve the previously introduced $\gamma$-SLiSe weight function in terms of worst-case convergence rate. To achieve this improvement, we generalise the weight function (6.1) to improve to

$$\mathcal{G}^{v, w}(x) := \begin{cases} v_1, & \text{if } |x| < w_1, \\ v_2, & \text{if } w_1 \leq |x| < w_1^{-1}, \\ v_3, & \text{if } w_1^{-1} \leq |x| < w_2, \\ v_4, & \text{if } w_2 \leq |x| < w_3, \\ v_5, & \text{otherwise,} \end{cases} \quad (6.4)$$

for $x \in \mathbb{R}$, where $v \in (0, \infty)^5$, $w_1 \in (0, 1)$, $1 < w_1^{-1} < w_2 < w_3$.

The parameters $v_1, \ldots, v_5$ denote different positive weights. The values $w_1, w_1^{-1}$ indicate gaps around $\pm 1$. The remaining parameters $w_2, w_3$ offer some more degrees of freedom in the choice of steps of the weight function.

An optimal choice of vectors $v, w$ can be defined as the minimum worst-case convergence rate of the induced weight function $\mathcal{G}^{v, w}$. This is supposed to yield a better weight function compared to the original $\gamma$-SLiSe weight function in SLiSe. We define the function

$$h(v, w) := \text{worstcase}(\mathcal{G}^{v, w}), \quad (6.5)$$

where $v \in (0, \infty)^5$, $w_1 \in (0, 1)$, $w_1^{-1} < w_2 < w_3$.

This is a loss function without derivatives as the convergence rate is always non-negative. This motivates the following minimisation problem of 8 variables

$$\arg\min_{v \in (0, \infty)^5, \ w_1 \in (0, 1), \ w_1^{-1} < w_2 < w_3} h(v, w). \quad (6.6)$$
6. Algorithmic design of weight functions

| Gap $G$ | Poles | GAUSS-LEGENDRE  | $\gamma$-SLiSe  | Enhanced $\gamma$-SLiSe |
|--------|-------|-----------------|-----------------|------------------------|
| 0.95   | 16    | $2.42^{-2}$     | $9.44^{-4}$     | $1.64^{-4}$            |
|        | 24    | $1.99^{-2}$     | $2.97^{-4}$     | $2.80^{-5}$            |
|        | 32    | $1.79^{-3}$     | $8.04^{-5}$     | $5.31^{-6}$            |
| 0.98   | 16    | $2.96^{-1}$     | $6.73^{-2}$     | $3.32^{-2}$            |
|        | 24    | $4.83^{-2}$     | $1.32^{-2}$     | $9.21^{-3}$            |
|        | 32    | $2.44^{-2}$     | $6.50^{-3}$     | $5.11^{-3}$            |
| 0.99998| 16    | $9.99^{-1}$     | $9.91^{-1}$     | $9.63^{-1}$            |
|        | 24    | $9.97^{-1}$     | $7.91^{-1}$     | $4.96^{-1}$            |
|        | 32    | $9.96^{-1}$     | $1.75^{-1}$     | $1.04^{-1}$            |

Table 6.1.: Worst-case convergence rates for different RFFs, gaps and numbers of poles. (smaller is better)

4. Solving the minimisation problem. The minimisation problem (6.6) can be solved using standard derivative-free minimisation algorithms. However, the minimisation problem is computationally difficult, because (i) the minimisation problem is non-linear, (ii) the loss function $h$ has no derivatives and (iii) the function evaluations of $h$ are rather expensive. Evaluating $h$ involves a SLiSe minimisation and solving the two minimisation problems in (6.2). The performance can be increased by using the weights and intervals of the $\gamma$-SLiSe weight function as a starting point in the minimisation (6.6). This is a natural choice, as we want to improve the $\gamma$-SLiSe weight function in terms of worst-case convergence rate to obtain a replacement candidate for the GAUSS-LEGENDRE RFF.

In the end, we obtained a weight function, the Enhanced $\gamma$-SLiSe, which can be found in Example B.3. This new weight function yields a new RFFs via SLiSe minimisation. We analyse our new Enhanced $\gamma$-SLiSe RFFs in the following. For the standard choice of 16 poles in FEAST, our new RFF is denoted in Appendix A.

6.2. Worst-case performance

In the previous section, we obtained a new weight function via minimisation of its worst-case convergence rate. In this section, we analyse the worst-case convergence rates as per (6.2) of the resulting Enhanced $\gamma$-SLiSe RFFs. To achieve this, we compare to its competitors, i.e. the GAUSS-LEGENDRE and the $\gamma$-SLiSe RFF. GAUSS-LEGENDRE is the
6.3. Performance in practice

In the following, we analyse the performance of our new Enhanced $\gamma$-SLiSe RFF in practice. As before, we compare to its competitors, i.e. the GAUSS-LEGENDRE RFF and the $\gamma$-SLiSe RFF.

The performance of FEAST in practice has been tested using a set of 2117 different HIEPs. This is the same set as used by WINKELMANN and DI NAPOLI in [5]. This set was obtained from the sparse, HERMITIAN Si2 matrix, part of the matrix collection of the UNIVERSITY OF FLORIDA [22]. From this matrix, there were selected 2117 different search intervals, each containing between 5 and 20 percent of the eigenvalues of the Si2 matrix.
6. Algorithmic design of weight functions

![Figure 6.2: FEAST iterations for eigenvalue count multiplier $C = 1.1$ and 2117 HIEPs.](image)

FEAST was used in the most-recent version 3.0, compiled using the Intel Compiler 17.0.0 and run on an Intel Core i7-6900K. We used the scsrevx method of FEAST for solving HIEPs of sparse matrices and embedding RFFs. Furthermore, the target accuracy of the eigenvalues was adjusted to $10^{-13}$. In the end, we used the same set-up as in [5].

As discussed in Section 2.2, a required argument of FEAST is an upper bound on the number of eigenvalues in the search interval of a given HIEP. Recall that in FEAST, a smaller upper bound yields a better performance in solving the reduced eigenvalue problems, but a worse convergence rate depending on the chosen RFF as per (2.7). So, we have tested different upper bounds. For all the studied HIEPs, we determined the actual eigenvalue count in the search interval and scaled it by a factor $C > 1$. Thus, a smaller $C$ indicates faster FEAST iterations.

The results are depicted in Figure 6.1. For every one of the 2117 problems, all RFFs assured the convergence of FEAST to the sought eigenvalues. We notice that our new Enhanced $\gamma$-SLiSe RFF outperforms the other RFFs, notably for a small $C$. For $C \geq 1.1$, the number of required iterations stays almost constant.

For the case $C = 1.1$, we have also compared the actually required counts of FEAST iterations, see Figure 6.2. We note that the GAUSS-LEGENDRE RFF terminates after a much larger number of iterations than in the case of the RFFs obtained via weighted, squared approximation. The new Enhanced $\gamma$-SLiSe RFF requires only 3 iterations for most of the HIEPs in contrast to the $\gamma$-SLiSe RFF, which needs 4 iterations in most cases.

We conclude that our new RFFs perform well in FEAST in terms of worst-case and practice.

---

7In fact, in [5], the Intel Compiler was used in version 16.0.2. We used the most recent version 17.0.0.
We have discussed SLiSe minimisation for designing RFFs, recently introduced in [5]. In particular, we focussed on current drawbacks of SLiSe, i.e.

1. Incompatibility with standard minimisation algorithms,

2. Impracticable performance of box-constraints,

3. Choice of suitable weight functions,

as mentioned in the introductory Section 1.1.

In this thesis, we have solved these open issues of SLiSe and obtained the following results.

1. **Embedding into standard minimisation algorithms.** The SLiSe minimisation problems have been embedded into standard minimisation algorithms, in particular the BFGS algorithm. This specific algorithm offers the efficiency and extensibility required for SLiSe. For SLiSe minimisation via BFGS, instead of hours, only seconds are needed for obtaining an RFF on an average computer architecture.

2. **Improving the performance of box-constraints.** Box-constraints help reducing the condition numbers in FEAST for SLiSe RFFs. We have improved the original implementation of box-constraints in SLiSe using the L-BFGS-B algorithm. Compared to the original implementation of box-constraints in SLiSe, our approach offers a performance suitable for practice.

We have tested and compared different set-ups of box-constrained SLiSe. In these set-ups, our L-BFGS-B approach requires no more than 500 steps, whereas the original implementation requires up to 900,000 steps. Furthermore, we have shown that our constrained SLiSe RFFs perform significantly better than previous ones, as L-BFGS-B offers a better accuracy compared to the original implementation.
7. Conclusions

3. Algorithmic choice of weight functions. The choice of weight functions as a parameter of SLiSe is crucial for obtaining well-performing RFFs via SLiSe minimisation. We defined the worst-case convergence rate of weight functions as a criterion for indicating well-performing weight functions. We derived new RFFs using a weight function with a minimum worst-case convergence rate in SLiSe.

Our new RFFs offer a better performance in FEAST compared to state-of-art RFFs, such as GAUSS-LEGENDRE and former SLiSe RFFs. Using our new RFFs, the FEAST algorithm requires up to one quarter fewer iterations on average, tested on a large set of benchmark problems.

Further work. For further research, Probabilistic RFFs are certainly of major interest. We have presented applications, a mathematical foundation and first, auspicious results of this approach. The numerical computation of Probabilistic RFFs still requires further examination. In the end, we expect both well-performing RFFs and an estimate of the required iterations of FEAST as a result of this approach.
Appendices
Ready-to-use rational filter functions

In the following, we present the studied RFFs, denoted as in (2.3).

| Poles $w$ | Coefficients $\beta$ |
|-----------|-----------------------|
| $-0.9980552138505067 + 0.062336105956370486i$ | $0.02525791710871586 - 0.001577548191004564i$ |
| $-0.9494253842988177 + 0.3139927382100546i$ | $0.05278354977406013 - 0.017456507483534722i$ |
| $-0.734899387554323 + 0.67818638770961i$ | $0.05763496444397823 - 0.05318789432545047i$ |
| $-0.2841679239019292 + 0.9587745256428074i$ | $0.02576577438829884 - 0.0869329930919054i$ |

Table A.1.: The 16-pole Gauss-Legendre RFF.

| Poles $w$ | Coefficients $\beta$ |
|-----------|-----------------------|
| $-0.999997581539606 + 0.0021993013049440135i$ | $0.0008989201462643977 - 1.977001032029609E-6i$ |
| $-0.9998514744807556 + 0.017234528675274002i$ | $0.005245791227192865 - 9.042216932920706E-5i$ |
| $-0.993358764099828 + 0.11525552757595411i$ | $0.03462538525214074 - 0.004017540430714314i$ |
| $-0.7398348571484926 + 0.6727885136861876i$ | $0.1505137271560608 - 0.13687697801045523i$ |

Table A.2.: The 16-pole Zolotarev RFF.

| Poles $w$ | Coefficients $\beta$ |
|-----------|-----------------------|
| $-0.9999983713139353 + 0.0022i$ | $0.001090570464617412 - 1.4902889756769852E-6i$ |
| $-0.999847656269521 + 0.023174916170735475i$ | $0.007300520076462563 - 0.00010162408356932002i$ |
| $-0.989797942578154 + 0.15300422557734145i$ | $0.0435127109551866 - 0.006058193629191226i$ |
| $-0.6868662884959791 + 0.7440732728350293i$ | $0.1353339692180714 - 0.14590122484259907i$ |

Table A.3.: The 16-pole L-BFGS-B Box-SLiSe RFF, obtained from and to replace the Zolotarev RFF using a lower bound of $lb = 0.0022$. 

### A. Ready-to-use rational filter functions

| Poles $w$                                                                 | Coefficients $\beta$                                      |
|--------------------------------------------------------------------------|-----------------------------------------------------------|
| $-0.9997180876994749 + 0.010064168904151764i$                            | 0.005218903896671892 $- 0.0003275342117714203i$       |
| $-0.985330269864567 + 0.0834401564640276i$                            | 0.019780578125967584 $- 0.005308415315997665i$       |
| $-0.8908400599591626 + 0.30261876848986174i$                            | 0.053241710348050676 $- 0.03215097589453323i$       |
| $-0.4358745582039683 + 0.6982671139969543i$                            | 0.05378661362857605 $- 0.12118676200021669i$       |

Table A.4.: The 16-pole BFGS $\gamma$-SLiSe RFF, obtained from and to replace the GAUSS-LEGENDRE RFF.

| Poles $w$                                                                 | Coefficients $\beta$                                      |
|--------------------------------------------------------------------------|-----------------------------------------------------------|
| $-0.995102777784057 + 0.01971965034279112i$                              | 0.007451889566376135 $- 0.0023538898767857387i$       |
| $-0.9656137585011698 + 0.098224598880633161i$                            | 0.019581536492404246 $- 0.00823771601370859i$       |
| $-0.8531623369434934 + 0.30357032990253513i$                            | 0.04865850681408789 $- 0.033809650419106246i$       |
| $-0.4113331147792164 + 0.6641012378282691i$                            | 0.04909233881671418 $- 0.11480784939181093i$       |

Table A.5.: The 16-pole BFGS Enhanced $\gamma$-SLiSe RFF, obtained from and to replace the GAUSS-LEGENDRE RFF.
Considered weight functions

Example B.1 ($\gamma$-SLiSe). WINKELMANN and DI NAPOLI introduced the $\gamma$-SLiSe function in [5], given by

$$G_{\gamma\text{-SLiSe}}(x) := \begin{cases} 1, & \text{if } |x| < 0.95, \\ 0.01, & \text{if } 0.95 \leq |x| < 1.05, \\ 10, & \text{if } 1.05 \leq |x| < 1.4, \\ 20, & \text{if } 1.4 \leq |x| < 5, \\ 0, & \text{otherwise}, \end{cases} \quad (B.1)$$

for all $x \in \mathbb{R}$. The minimiser of the resulting minimisation problem is to replace the Gauss-Legendre RFF as of Section 3.1.

Example B.2 (Box-SLiSe). WINKELMANN and DI NAPOLI introduced the Box-SLiSe function in [5], given by

$$G_{\text{Box-SLiSe}}(x) := \begin{cases} 1, & \text{if } |x| < 0.95, \\ 4, & \text{if } 0.95 \leq |x| < 0.995, \\ 2, & \text{if } 0.995 \leq |x| < 1.005, \\ 4, & \text{if } 1.005 \leq |x| < 1.05, \\ 0.6, & \text{if } 1.05 \leq |x| < 1.1, \\ 1, & \text{if } 1.1 \leq |x| < 1.3, \\ 0.3, & \text{if } 1.3 \leq |x| < 1.8, \\ 0.1, & \text{if } 1.8 \leq |x| < 3, \\ 0, & \text{otherwise}, \end{cases} \quad (B.2)$$

for all $x \in \mathbb{R}$. The minimiser of the resulting minimisation problem is to replace the
B. Considered weight functions

ZOLOTAREV RFFs as of Section 3.2 when subject to box-constraints.

Example B.3 (Enhanced $\gamma$-SLiSe). For the analysis, we have come up with a new weight function as per

$$
G_{\text{Enhanced } \gamma\text{-SLiSe}}(x) := \begin{cases} 
0.7, & \text{if } |x| < 0.96, \\
0.00092, & \text{if } 0.96 \leq |x| < 1.0417, \\
887, & \text{if } 1.0417 \leq |x| < 1.4, \\
20, & \text{if } 1.4 \leq |x| < 10, \\
0, & \text{otherwise}, 
\end{cases}
$$

(B.3)

for all $x \in \mathbb{R}$. The minimiser of the resulting minimisation problem is to replace the GAUSS-LEGENDRE RFF as of Section 3.1.
Details of BFGS minimisation

In Section 3.3, we have seen how to describe “good” approximations of the indicator function by RFFs as per (2.3) in terms of a loss function as per Definition 4.1. We expect that minimisers of this loss function yield fast convergence in eigenvalue computation. We present how to find minimisers of such functions efficiently, employing the BFGS minimisation algorithm. We first introduce a general minimisation scheme and then present the BFGS algorithm.

To minimise a loss function $f : \mathbb{R}^n \to [0, \infty)$ of $n \in \mathbb{N}$ variables in terms of Definition 4.1, for $k = 0, 1, 2, \ldots$, one approximates a minimiser of $f$ by iterates $x_k \in \mathbb{R}^n$, such that

$$f(x_0) > f(x_1) > \cdots > f(x_k) \geq 0. \quad \text{(C.1)}$$

The only question is how to obtain these iterates. We proceed as shown in Figure C.1. Given a starting iterate $x_k$, we want to find a next iterate $x_{k+1}$ such that $f(x_k) > f(x_{k+1})$. This yields a better approximation to a local minimiser. However, this equivalent to finding a descent direction $p_k \in \mathbb{R}^n$. A descent direction is a vector that “points” from $x_k$ into a direction where $f$ attains a smaller value. It can be shown by fundamental methods

Start: Iterate $x_k$

1. Gather descent direction
2. Line search for new iterate

Descent direction $p_k$

Figure C.1.: General scheme of minimisation
C. Details of BFGS minimisation

Contour plot of $x^2 + y^2$

Figure C.2.: Steps of optimisation in Example C.3.

of calculus, i.e. first-order TAYLOR expansion, that this is equivalent to

$$\nabla f(x_k)^T p_k < 0. \quad (C.2)$$

This vector $p_k$ only shows the direction to a smaller function value of $f$ at $x_k$. In order to gather a smaller function value and thus a next iterate $x_{k+1}$, we have to move along the vector $p_k$. This process is called line search as we search along the line

$$\alpha \mapsto f(x_k + \alpha p_k), \quad \text{for } \alpha \in (0, \infty) \quad (C.3)$$

to gather an $\alpha_k \in (0, \infty)$ such that $f(x_k) > f(x_k + \alpha_k p_k)$. An $\alpha_k$ is called step length. In the end, we set $x_{k+1} := x_k + \alpha_k p_k$ and repeat the process for $x_{k+1}$ instead of $x_k$.

Example C.1. A simple example of a descent direction at $x_k$ is given by the negative gradient $-\nabla f(x_k)$. Obviously, this satisfies (C.2), if and only if $\nabla f(x_k) \neq 0$. However, this constraint is no problem. If we have $\nabla f(x_k) = 0$, we have already found (local) minimiser if it is no saddle points of $f$. In practical implementations, this assured by the right choice of the starting iterate $x_0$.

Example C.2. To illustrate a descent direction, consider the following 2D case: If we want to find the minimiser of a convex function, e.g. $f(x) := x^2$, we can simply “follow” the gradient $-\nabla f(x) = -2x$: For any $x \in \mathbb{R} \setminus \{0\}$, this indicates the direction to the minimiser of $f$. 
Example C.3. As an example for minimisation of a loss function, we study the function $f(x, y) := x^2 + y^2$ for $x, y \in \mathbb{R}$ as in Example 4.2 and Figure 4.1a.

All the following steps are depicted in Figure C.2. The gradient of $f$ is $\nabla f(x, y) = (2x, 2y)$. Suppose, our current iterate was $x_k = (1, 1)$. Then, to gather a next iterate, we will compute a descent direction at $x_k$. For this, we are going to use the negative gradient of $f$ at $x_k$ as in Example C.1. We have for the descent direction $p_k := -\nabla f(x_k) = (-2, -2)$. We cannot just use $x_k + p_k$ as the next iterate as we have $f(x_k + p_k) = f(-1, -1) = f(1, 1)$, but we are searching for a decrease in function value. For instance, we choose $\alpha_k = 0.25$. Then, we set $x_{k+1} := x_k + \alpha_k p_k = (0.5, 0.5)$.

**Line search**

In Example C.1, we have shown how to obtain a descent direction. Following Figure C.1, we have to perform a line search to gather a new iterate. In this section, we study the line search as per (C.3) more deeply. We note that for an arbitrary choice of step lengths $\alpha_k$ in (C.3), this does not necessarily yield a minimiser.

Example C.4. As an example of a non-converging line search, consider the loss function $f(x) := x^2/2$, for $x \in \mathbb{R}$. The gradient of $f$ is given by $\nabla f(x) = x$. To obtain a minimiser, we choose $x_0 := -3$ as the starting point.

If we choose $x_{k+1}$ such that $x_{k+1} - x_k = 2^{-k}$ in every iteration, we have

$$x_{k+1} = x_0 + \sum_{n=0}^{k} 2^{-n} \quad \text{(C.4)}$$

We remember from calculus, that

$$\sum_{k=0}^{\infty} 2^{-k} = 2. \quad \text{(C.5)}$$

In other words,

$$\lim_{k \to \infty} x_k = -1 \neq 0. \quad \text{(C.6)}$$

Hence, we never reach the minimiser of $f$.

If the decrease in $f$ is not sufficiently large, we may never reach a minimiser (nor even get close to it).
To solve this issue, in 1969, Philip Wolfe combined two conditions, that help avoiding no or slow convergence during line search [15], [16]: We have seen in the previous Example C.4 that decrease in function value cannot be arbitrarily. The first Wolfe condition states that there must be so-called sufficient decrease. To phrase this, note that for a descent direction $p_k$ the term $\nabla f(x_k)^T p_k$ indicates the “steepness” of the descent at $x_k$, i.e. the directional derivative. We now want for the function value at the next iterate $x_{k+1}$ to lie below the slope $c_1 \alpha_k \nabla f(x_k)^T$ where $c_1 \in (0, 1)$ is a control parameter. This imposes on the step length $\alpha_k$ and thus the next iterate $x_{k+1} = x_k + \alpha_k p_k$ the condition that

$$f(x_{k+1}) \leq f(x_k) + c_1 \alpha_k \nabla f(x_k)^T p_k.$$  

The condition is also known as the Armijo rule, introduced in 1966 [12]. Per se, this condition is not sufficient as any step length small enough satisfies the condition.

**Example C.5.** An example is depicted in Figure C.3. There, the function and the slope, that shall bound the function, are shown. We find that for $\alpha \in [0, 1] \cup [2, 2.5]$ the first Wolfe condition as per (C.7) is fulfilled.

We know that any minimiser of $f$ satisfies $\nabla f(x) = 0$. Thus, we would like to ensure sufficient decrease in the gradient as well. This second Wolfe condition is known as curvature condition and helps during minimisation to reach a minimiser potentially faster. For instance, we would like for the descent direction $p_k$ at the next iterate $x_{k+1}$, that it is at least $c_2 \in (0, 1)$ percent as steep as at the current iterate $x_k$. This can be phrased as

$$c_2 \nabla f(x_k)^T p_k \leq \nabla f(x_{k+1})^T p_k \leq 0$$  

(C.8)
**Definition C.6** (Wolfe conditions). Let \( n \in \mathbb{N} \) and \( f \) a loss function of \( n \) variables. Furthermore let \( x \in \mathbb{R}^n \) and \( p \) be a descent direction of \( f \) at \( x \), i.e. \( \nabla f(x)^T p < 0 \). Then, a step length \( \alpha \in (0, \infty) \) of a line search as per (C.3) is said to satisfy the Wolfe conditions, if

\[
\begin{align*}
  f(x + \alpha p) &\leq f(x) + c_1 \alpha \nabla f(x)^T p, \\
  c_2 \nabla f(x)^T p &\leq \nabla f(x + \alpha p)^T p,
\end{align*}
\]

(C.9a) (C.9b)

for fixed parameters \( 0 < c_1 < c_2 < 1 \).

According to Nocedal and Wright [11], a good choice for the mentioned parameters is \( c_1 = 10^{-4} \) and \( c_2 = 0.9 \).

Now, the Definition C.6 of the Wolfe condition raises two questions: Does there always exist a step length satisfying the Wolfe conditions and if so, is this step length computable with a finite number of steps? In fact, this is true. For details, see Proposition D.2. Basically, the Proposition states that there always exists an interval \( I \subseteq (0, \infty) \) of step lengths satisfying the Wolfe conditions. Such an interval can be found in finitely many steps.

There exists a variety of algorithms computing such a step size, confer [11, pp. 60–62], [14]. Especially, the latter presents a popular and efficient implementation. There are also other approaches to line search that perform very well. One of such is the method of Hager and Zhang [13] that does not always assure first Wolfe condition (C.9a) and achieves good results in practice.

**BFGS algorithm**

Now that we know how to find “good” step lengths in a line search as in (C.3), we would like to find out how to gather “good” descent directions. Recall, that, given a current iterate \( x_k \), our goal is to find to next iterate \( x_{k+1} \) such that \( f(x_k) > f(x_{k+1}) \).

In minimisation, in each iteration, one usually employs an approximation of \( f \), called model. We do not need a model of the entire \( f \), but only for values “close” to the current iterate \( x_k \). In the end, our hope is that this model will be easier to minimise than \( f \). Even more, we believe that a minimiser of the model will yield the direction to a minimiser of
C. Details of BFGS minimisation

We have seen before that this is called a descent direction. Say, the minimiser of the model was a variable called \( x_{\text{min}} \). Then, the descent direction to analyse is \( p_k := x_{\text{min}} - x_k \). Recall Figure C.1. We can now do a line search for the next iterate along \( p_k \). We have to do that as \( x_{\text{min}} \) does not need to be a minimiser of \( f \). We have to verify that. Even more, we would like to ensure the WOLFE conditions as introduced in the previous section in Definition C.6.

For the model, it is a straightforward idea to use a second-order Taylor approximation of \( f \) at \( x_k \). This is a quadratic approximation of \( f \) in the neighbourhood of \( x_k \) and is given by

\[
f(x) \approx \tilde{f}(x) := f(x_k) + \nabla f(x_k)^T x + \frac{1}{2} x^T \nabla^2 f(x_k) x, \quad x \in \mathbb{R}^n, \tag{C.10a}
\]
at each iteration \( k \).

We assume the Hessian \( \nabla^2 f(x_k) \) to be symmetric positive-definite. We make this assumption as any positive-definite matrix is non-singular. It follows that the unique minimiser of \( \tilde{f} \) is given by

\[
\tilde{p}_k = -\nabla^2 f(x_k)^{-1} \nabla f(x_k). \tag{C.10b}
\]

This approach is called Newton’s method [11] and usually gives a good approximation of \( f \). The computational costs, i.e. solving the linear system (C.10b), are quite high. In the case of our eigenvalue minimisation, the Hessians usually have a large condition number. This means that numerically solving (C.10b) can only be accomplished with little accuracy.

There exist multiple efficient approaches to replacing the Hessians \( \nabla^2(x_k) \) by approximations \( B_k \). This means that we use the model

\[
f(x) \approx m_k(x) := f(x_k) + \nabla f(x_k)^T x + \frac{1}{2} x^T B_k x, \quad x \in \mathbb{R}^n. \tag{C.11a}
\]

This is called a quasi-Newton minimisation. The BFGS algorithm is a powerful example

\[
\begin{align*}
\text{Input: } &B_k, \text{ current iterate } x_k \\
\text{BFGS model} & \downarrow \\
\text{Output: } &\text{Descent direction } p_k
\end{align*}
\]

Figure C.4.: Scheme of the BFGS model.
of such. The key feature of this method is the preservation of the positive-definiteness of a starting Hessian approximation $B_0$. In general, the identity matrix $I_n$ is a sufficiently good $B_0$. In each iteration, we can again find the unique minimiser of (C.11a) as

$$p_k = -B_k^{-1}\nabla f(x_k),$$  \hspace{1cm} (C.11b)

because the positive-definite matrix $B_k$ is non-singular. A scheme of the resulting BFGS algorithm and its required input and produced output is depicted in Figure C.4.

Note that a positive-definite $B_k$ yields

$$\nabla f(x_k)^T p_k = -\nabla f(x_k)^T B_k^{-1}\nabla f(x_k) < 0.$$ \hspace{1cm} (C.11c)

Thus, $p_k$ is a descent direction as per (C.2), which is necessary to be able to obtain a new iterate $x_{k+1}$ via line search.

It seems like solving a linear system was needed to obtain this descent direction $p_k$. In fact, it is possible to compute the inverse of $B_k$ efficiently and analytically. We will denote this inverse as $H_k = B_k^{-1}$. In the end, (C.11b) becomes

$$p_k = -H_k \nabla f(x_k).$$ \hspace{1cm} (C.11d)

We now know how to compute the next descent direction from a given inverse Hessian approximation $H_k = B_k^{-1}$ and the current iterate $x_k$, see also Figure C.4. It remains to show how to obtain the next inverse Hessian approximation.

For the very first iteration of the BFGS algorithm, i.e. $k = 0$, we just assume a symmetric positive-definite $H_0$ as an input, e.g. the identity matrix. From this, we can gather the very first descent direction $p_k$ easily as of the previous equation (C.11d). This then yields

![Figure C.5.: Scheme of BFGS minimisation.](image-url)
the next iterate $x_{k+1}$ via line search.

We now have to acquire a next inverse HESSIAN approximation $H_{k+1}$. For this, we use the previously gathered results to update $H_k$ to a new $H_{k+1}$. This is the BFGS update step and given by

$$H_{k+1} = (I_n - \frac{s_k y_k^T}{y_k^T y_k})H_k(I_n - \frac{y_k s_k^T}{y_k^T y_k}) + \frac{s_k s_k^T}{y_k^T y_k} \tag{C.12}$$

where $s_k := x_{k+1} - x_k$ and $y_k := \nabla f(x_{k+1}) - \nabla f(x_k)$.

It can be shown that the BFGS update maintains the symmetric positive-definiteness of a starting inverse HESSIAN approximation $H_0$, see Theorem D.3.

We can update Figure C.4 to show the entire minimisation procedure for the BFGS algorithm using and producing the previously mentioned inputs and outputs in Figure C.4, see Figure C.5. Eventually, we gather the following algorithm

---

**Algorithm 2 (Unconstrained BFGS Algorithm).**

**Input:** Loss function $f$ of $n \in \mathbb{N}$ variables and its gradient $\nabla f$, $x \in \mathbb{R}^n$, symmetric positive-definite $H \in \mathbb{R}^{n \times n}$, $\varepsilon > 0$.

**Output:** $x \in \mathbb{R}^n$ such that $f(x) \leq \varepsilon$.

1: function BFGS($f, \nabla f, x, H, \varepsilon$)
2: while $f(x) > \varepsilon$ do
3:  $p \leftarrow -H \nabla f(x)$ \Comment{Compute descent direction}
4:  $\alpha \leftarrow$ Step length of a line search (C.3) along $p$ satisfying (C.9)
5:  $x_{\text{pre}} \leftarrow x$
6:  $s \leftarrow \alpha p$
7:  $x \leftarrow x_{\text{pre}} + s$
8:  $y \leftarrow \nabla f(x) - \nabla f(x_{\text{pre}})$
9:  $H \leftarrow$ BFGS update of $H$ according to (C.12)
10: return $x$

---

**Observation C.7.** Let $f$ be a loss function of $n \in \mathbb{N}$ variables and assume that the evaluation of $\nabla f$ and $\nabla^2 f$ can be achieved in constant time and the line search in $\mathcal{O}(g(n))$ for some polynomial $g$. Then, one iteration of the BFGS Algorithm 2 has a time complexity of $\mathcal{O}(n^2 + g(n))$ in contrast to $\mathcal{O}(n^3 + g(n))$ in NEWTON’s method (C.10). However, possibly, NEWTON’s method requires less iterations as no HESSIAN approximation is used.

---

xii
Handling box-constraints

In Section 5.1, we have seen how to improve SLiSe RFFs by box-constraints. In a general real minimisation environment, box-constraints are known as demanding arbitrary upper and lower bounds on the minimiser. For the $i$-th component of an $x \in \mathbb{R}^n$, we would like to have

$$l_i \leq x_i \leq u_i,$$  \hspace{1cm} (C.13)

where $l_i, u_i \in [-\infty, \infty]$. Here, $l_i$ denotes a lower and $u_i$ an upper bound. This means, that for a loss function $f$ of $n \in \mathbb{N}$ variables, we would like to solve the minimisation problem

$$\arg\min_{x \in \mathbb{R}^n} f(x)$$  \hspace{1cm} (C.14a)

subject to: $l_i \leq x_i \leq u_i$, \hspace{1cm} for $i = 1, \ldots, n.$  \hspace{1cm} (C.14b)

The lower and upper bounds are called box-constraints. It is called “box” as indeed the values in the bounds lie in a box of the common sense.

Example C.8. An example of a box is depicted in Figure C.6. Here, the box of values lying in the bounds is denoted as $C$.

Example C.9. Suppose, we want to impose constraints on an minimisation problem in $\mathbb{R}^2$. For instance, we would like to have for the first dimension that $l_1 = 2 \leq x_1 \leq 8 = u_1$ and for the second dimension that $l_2 = -5 \leq x_2 \leq \infty = u_2$. Thus, all these values lie in a
C. Details of BFGS minimisation

set given by

\[ C = [2, 8] \times [-5, \infty). \] \hfill (C.15)

For the solution of box-constrained problems, there is a very well-known algorithm, called L-BFGS-B [17]. In terms of the BFGS scheme in Figure C.5, mainly, the used model is altered to incorporate box-constraints yielding the method shown in Figure C.7. We will shortly describe the main idea behind this algorithm:

At the current iterate \( x_k \), similar to (C.11a), the algorithm forms a quadratic model in the neighbourhood of \( x_k \) using a Hessian approximation \( B_k \) yielding some function

\[ q_k(x), \quad \text{for } x \in \mathbb{R}^n. \] \hfill (C.16)

Consequently, the algorithm identifies the components of \( x_k \) that are going to violate the bounds in the next iterate \( x_{k+1} \) as follows. A projected line search along the gradient \( \nabla f \) at \( x_k \) is used. This can be phrased as

\[ q_k(P(x_k - \alpha \nabla f(x_k))), \quad \text{for } \alpha \in (0, \infty) \] \hfill (C.17)

where

\[ P(x)_i = \begin{cases} l_i, & \text{if } x_i < l_i, \\ x_i, & \text{if } l_i \leq x_i \leq u_i, \\ u_i, & \text{if } u_i < x_i. \end{cases} \] \hfill (C.18)

The latter function is a projector into the box-constraints.

The algorithm just choose the first local minimiser along this line (C.17), called CAUCHY point.

**Definition C.10 (Cauchy point).** Let \( g : [0, \infty) \rightarrow \mathbb{R} \). Then we call a local minimiser

![Figure C.7.: Scheme of constrained BFGS minimisation.](image-url)
$x \in \mathbb{R}$ of $g$ the Cauchy point of $g$, denoted $x_c(g)$, if for every local minimiser $y \in \mathbb{R} \setminus \{x\}$ of $g$ it holds that $x < y$.

It is then possible, to find the Cauchy point $x_c$ of the projected line search (C.17) analytically. Some of the components of $x_c$ might reach their bounds during this process. We keep these components fixed while doing an unconstrained minimisation of the quadratic model $q_k$ starting at $x_c$ using the remaining components. It is not needed to be exact during this minimisation. Projection as per (C.18) is then used to fix violated bounds yielding a value $\tilde{x}_{k+1}$.

Eventually, the new descent direction for a line search is given by $p_k := \tilde{x}_{k+1} - x_k$. For more details see [11, ch. 18.7].
Lemma D.1. Let $\gamma : [0,1] \to \mathbb{C}$ be a closed, positively-oriented, non-self-intersecting path in $\mathbb{C}$ enclosing $(a,b)$. Then, it holds that

$$i_{(a,b)}(x) = \frac{1}{2\pi i} \int_{\gamma} \frac{1}{\zeta - x} \, d\zeta, \quad x \in \mathbb{R} \setminus \text{Ima}(\gamma). \quad (D.1)$$

Proof. Fix $z \in \mathbb{C} \setminus \text{Ima}(\gamma)$. From the Laurent expansion, it follows that $\zeta \mapsto \frac{1}{\zeta - z}, \quad \zeta \in \mathbb{C} \setminus \{z\}$ has one residue of 1 at $z$. Then, the residue theorem implies the result for complex $z$ and thus for real ones as well. \qed

Proposition D.2. Assume the preliminaries of Definition C.6. Then, there always exists a non-empty interval $I \subseteq (0, \infty)$ such that any $\alpha \in I$ satisfies the Wolfe conditions.

Proof. Define $\Phi(\alpha) := f(x - \alpha p) - (f(x) - c_1 \alpha \nabla f^T p)$, for $\alpha \in \mathbb{R}$. Thus, we have that $\Phi'(\alpha) = (\nabla f(x + \alpha p) - c_1 \nabla f(x))^T p$, for $\alpha \in \mathbb{R}$. As $p$ is a descent direction, we have $\Phi'(0) < 0$. Now, there exists an $\alpha_1 > 0$ such that $\Phi'(\alpha) < 0$ for $\alpha \in [0, \alpha_1]$ as $\Phi$ is continuously differentiable. Hence, $\Phi(\alpha_1) < 0$ as well. Then, as $f(x) \geq 0$ for $x \in \mathbb{R}^n$, it is

$$\Phi(\alpha) \geq -(f(x) - c_1 \alpha \nabla f^T p) \geq -f(x). \quad (D.2)$$

For $\alpha \to \infty$, the middle term diverges to $\infty$ and so does $\Phi$. Thus, we can find an $\alpha_2 > \alpha_1$ such that $\Phi(\alpha_2) = 0$ by the intermediate value theorem. Choose the smallest such $\alpha_2$. We have that $\Phi(\alpha) < 0$ and hence $\alpha$ satisfies the first Wolfe condition (C.9a) for $0 < \alpha < \alpha_2$.

Now, by Rolle’s theorem, there exists an $\alpha_3 \in (0, \alpha_2)$ such that $\Phi'(\alpha_3) = 0$, i.e.

$$\nabla f(x + \alpha_3 p)^T p = c_1 \nabla f(x)^T p > c_2 \nabla f(x)^T p, \quad (D.3)$$

in other words, the second Wolfe condition (C.9b), as $c_1 < c_2$. The continuity of both $f$ and $\nabla f$ ensures that there is an entire interval $I \subseteq (a_3, a_2)$, which proves the claim. \qed
D. Further details

**Theorem D.3.** Let \( k \in \mathbb{N}_0 \), \( f \) be a loss function of \( n \in \mathbb{N} \) variables and \( H_k \in \mathbb{R}^{n \times n} \) symmetric positive-definite. Let \( x_k \) be the current iterate, \( p_k := -H_k \nabla f(x_k) \) the descent direction in a line search \( \alpha \mapsto f(x_k + \alpha p_k) \) and \( \alpha_k \in (0, 1) \) chosen to satisfy the Wolfe conditions (C.9) for some parameters \( 0 < c_1 < c_2 < 1 \). Then the next iterate is given by \( x_{k+1} := x_k + \alpha p_k \). Define \( s_k := x_{k+1} - x_k \) and \( y_k := \nabla f(x_{k+1}) - \nabla f(x_k) \), then the BFGS update \( H_{k+1} \) of \( H_k \) as per (C.12) is symmetric positive-definite.

**Proof.** As the symmetric matrices form a group, from (C.12) the symmetry of \( H_{k+1} \) follows immediately. By the second Wolfe condition (C.9b) and as \( p_k \) is a descent direction we find

\[
\nabla f(x_k)^T p_k < c_2 \nabla f(x_k)^T p_k \leq \nabla f(x_{k+1})^T p_k. \tag{D.4}
\]

By the definition of \( s_k \), it follows that

\[
\nabla f(x_k)^T s_k < \nabla f(x_{k+1})^T s_k. \tag{D.5}
\]

Thus, it is

\[
y_k^T s_k > 0. \tag{D.6}
\]

By definition of \( H_{k+1} \), and as \( H_k \) is positive-definite, we have

\[
\frac{v^T H_k v + (s_k^T z)^2 (y_k^T s_k)^{-1}}{>0, \text{ by (D.6)}} \geq 0, \tag{D.7}
\]

where

\[
v := z - s_k^T z. \tag{D.8}
\]

This implies that \( H_{k+1} \) is positive definite and the claim holds. \( \square \)

**Theorem D.4.** Let \( \mathcal{G} \) a piece-wise constant weight function. Furthermore, let \( \beta \in \mathbb{C}^m, w \in (\mathbb{C} \setminus \mathbb{R})^m \). For the function \( f \) in (3.8), it then holds that

\[
f(\beta, w) = 2\Re[\beta^T((X - Z)\beta + (W - Y)\beta - 2\theta)] + \frac{1}{2} \int_{-\infty}^{\infty} \mathcal{G}(x) |h(x)|^2 dx \tag{D.9}
\]

and for the gradient,

\[
\nabla_\beta f(\beta, w) = 4 [\beta^T (\nabla X - \nabla Z) + \beta^T (\nabla W - \nabla Y)] I_\beta, \tag{D.10a}
\]

\[
\nabla_w f(\beta, w) = 4 [\beta^T (X - Z) + \beta^T (W - Y) - \theta]^H, \tag{D.10b}
\]

xviii
where

\[
W_{k,l} := \int_{-\infty}^{\infty} \frac{\mathcal{G}(x)}{(x-w_k)(x-w_l)} \, dx
\]

\[
X_{k,l} := \int_{-\infty}^{\infty} \frac{\mathcal{G}(x)}{(x-w_k)(x-w_l)} \, dx
\]

\[
Y_{k,l} := \int_{-\infty}^{\infty} \frac{\mathcal{G}(x)}{(x-w_k)(x+w_l)} \, dx
\]

\[
Z_{k,l} := \int_{-\infty}^{\infty} \frac{\mathcal{G}(x)}{(x-w_k)(x+w_l)} \, dx
\]

\[
\theta_{k} := \int_{-\infty}^{\infty} \frac{\mathcal{G}(x) i_{\gamma}(x)}{(x-w_k)^2} \, dx
\]

\[
\nabla W_{k,l} := \int_{-\infty}^{\infty} \frac{\mathcal{G}(x)}{(x-w_k)(x-w_l)^2} \, dx
\]

\[
\nabla X_{k,l} := \int_{-\infty}^{\infty} \frac{\mathcal{G}(x)}{(x-w_k)(x-w_l)^2} \, dx
\]

\[
\nabla Y_{k,l} := \int_{-\infty}^{\infty} \frac{\mathcal{G}(x)}{(x-w_k)(x+w_l)^2} \, dx
\]

\[
\nabla Z_{k,l} := \int_{-\infty}^{\infty} \frac{\mathcal{G}(x)}{(x-w_k)(x+w_l)^2} \, dx
\]

\[
\nabla \theta_{k} := \int_{-\infty}^{\infty} \frac{\mathcal{G}(x) i_{\gamma}(x)}{(x-w_k)^2} \, dx
\]

are standard definite integrals, for \( k, l = 1, \ldots, m \).

Proof. Confer [5].
Bibliography

[1] E. Polizzi, “Density-matrix-based algorithm for solving eigenvalue problems”, *Physical Review B*, vol. 79, no. 11, pp. 115112–115117, 2009. DOI: 10.1103/PhysRevB.79.115112.

[2] S. Güttel, E. Polizzi, P. T. P. Tang, and G. Viaud, “Zolotarev quadrature rules and load balancing for the feast eigensolver”, *SIAM Journal on Scientific Computing*, vol. 37, no. 4, A2100–A2122, 2015. DOI: 10.1137/140980090.

[3] E. Di Napoli, E. Polizzi, and Y. Saad, “Efficient estimation of eigenvalue counts in an interval”, *Numerical Linear Algebra with Applications*, vol. 23, no. 4, pp. 674–692, 2016. DOI: 10.1002/nla.2048.

[4] L. Krämer, E. Di Napoli, M. Galgon, B. Lang, and P. Bientinesi, “Dissecting the feast algorithm for generalized eigenproblems”, *Journal of Computational and Applied Mathematics*, vol. 244, pp. 1–9, 2013. DOI: 10.1016/j.cam.2012.11.014.

[5] J. Winkelmann and E. Di Napoli, “Non-Linear Least-Squares Optimization of Rational Filters for the Solution of Interior Eigenvalue Problems”, *ArXiv e-prints*, 2017. arXiv: 1704.03255.

[6] Y. Xi and Y. Saad, “Computing partial spectra with least-squares rational filters”, *SIAM Journal on Scientific Computing*, vol. 38, no. 5, A3020–A3045, 2016. DOI: 10.1137/16M1061965.

[7] Y. Saad, *Numerical methods for large eigenvalue problems*, 2nd ed., ser. Classics in Applied Mathematics. SIAM, 2011, ISBN: 9781611970739.

[8] P. T. P. Tang and E. Polizzi, “Feast as a subspace iteration eigensolver accelerated by approximate spectral projection”, *SIAM Journal on Matrix Analysis and Applications*, vol. 35, no. 2, pp. 354–390, 2014. DOI: 10.1137/13090866X.

[9] W. Dahmen and A. Reusken, *Numerik für ingenieure und naturwissenschaftler*, 2nd ed. Springer, 2008, ISBN: 9783540764939. DOI: 10.1007/978-3-540-76493-9.

[10] L. Sorber, M. V. Barel, and L. D. Lathauwer, “Unconstrained optimization of real functions in complex variables”, *SIAM Journal on Optimization*, vol. 22, no. 3, pp. 879–898, 2012. DOI: 10.1137/110832124.

[11] J. Nocedal and S. Wright, *Numerical optimization*, 2nd ed. Springer, 2006, ISBN: 9780387303031. DOI: 10.1007/978-0-387-40065-5.

[12] L. Armijo, “Minimization of functions having lipschitz continuous first partial derivatives.”, *Pacific Journal of Mathematics*, vol. 16, no. 1, pp. 1–3, 1966. DOI: 10.2140/pjm.1966.16.1.

[13] W. W. Hager and H. Zhang, “A new conjugate gradient method with guaranteed descent and an efficient line search”, *SIAM Journal on Optimization*, vol. 16, no. 1, pp. 170–192, 2005. DOI: 10.1137/030601880.
Bibliography

[14] J. J. Moré and D. J. Thuente, “Line search algorithms with guaranteed sufficient decrease”, ACM Transactions on Mathematical Software, vol. 20, no. 3, pp. 286–307, 1994. DOI: 10.1145/192115.192132.

[15] P. Wolfe, “Convergence conditions for ascent methods”, SIAM Review, vol. 11, no. 2, pp. 226–235, 1969. DOI: 10.1137/1011036.

[16] ——, “Convergence conditions for ascent methods. ii: Some corrections”, SIAM Review, vol. 13, no. 2, pp. 185–188, 1971. DOI: 10.1137/1013035.

[17] R. H. Byrd, P. Lu, J. Nocedal, and C. Zhu, “A limited memory algorithm for bound constrained optimization”, SIAM Journal on Scientific Computing, vol. 16, no. 5, pp. 1190–1208, 1995. DOI: 10.1137/0916069.

[18] C. Zhu, R. H. Byrd, P. Lu, and J. Nocedal, “Algorithm 778: L-bfgs-b: Fortran subroutines for large-scale bound-constrained optimization”, ACM Transactions on Mathematical Software, vol. 23, no. 4, pp. 550–560, 1997. DOI: 10.1145/279232.279236.

[19] J. L. Morales and J. Nocedal, “Remark on algorithm 778: L-bfgs-b: Fortran subroutines for large-scale bound constrained optimization”, ACM Transactions on Mathematical Software, vol. 38, no. 1, 7:1–7:4, 2011. DOI: 10.1145/2049662.2049669.

[20] S. G. Johnson, The nlopt nonlinear-optimization package, Aug. 6, 2017. [Online]. Available: http://ab-initio.mit.edu/wiki/index.php/Main_Page.

[21] D. Kraft, “Algorithm 733: Tomp–fortran modules for optimal control calculations”, ACM Transactions on Mathematical Software, vol. 20, no. 3, pp. 262–281, 1994. DOI: 10.1145/192115.192124.

[22] T. A. Davis and Y. Hu, “The university of florida sparse matrix collection”, ACM Transactions on Mathematical Software, vol. 38, no. 1, 1:1–1:25, 2011. DOI: 10.1145/2049662.2049663.
Approximation, 10
BFGS, 22, 31
  Constrained, 27
  Iterate, 22
  L-BFGS-B, 23, 27, 28
  Starting point, 22
Box-constraint, 2, 23, 27
CHIEP, see HIEP
Complex numbers, 4
Condition number, 26
Conditional Expectation, 33
Conjugate transpose, 4
Constraint, 25
Convergence rate, 9
Eigenpair, 5
Eigentrace, 9
Eigenvalue, 5
Eigenvalue problem, 5
  Hermitian interior, see HIEP
Eigenvector, 5
FEAST, 1, 23, 26, 28, 31, 36, 39, 40
  Convergence rate, 9
  Worst-case condition number, 26
Gap, 13
  Parameter, 13, 32, 36
Gauss-Legendre quadrature, 12
Gauss-Legendre RFF, see RFF
Gradient descent, 22
Hermitian, 15
HIEP, 6
Indicator function, 10
Iterate, 22
L-BFGS-B, see BFGS
Levenberg-Marquardt, 22
Loss function, 15, 20
  Quadratic, 20
Lower bound, see Box-constraint
Minimisation problem, 2, 4, 13, 16, 20,
  22, 27, 31, 33, 36, 37
Numerical integration, 11
Optimisation problem, see Minimisation
  problem
Pole, 7
Projected
  Gradient descent, 22
  Projected gradient descent, 23
QR algorithm, 8
Rational
  Filter function, see RFF
  Subspace Iteration, 8
Residual, 20, 21, 23, 28
RFF, 1, 6
  Gauss-Legendre, 13, 24, 35, 42
  Non-increasing extrema, 29
  Pole, 7
  Probabilistic, 32, 42
  Properties, 7
  Starting, 22
  Symmetry, 7
  Worst-case convergence rate, 36
  Zolotarev, 14, 23, 28
Shape constraint, 31
SLiSe, 14, 23, 36, 41
  Loss function, 21
  Residual, 21
  RFF, see RFF
Starting point, 22
Step function, 16
Subspace iteration, 8
Weight function, 2, 15, 35
Worst-case convergence rate
  RFF, 36
  Weight function, 35
Zolotarev RFF, see RFF