University of Potsdam

Bachelor Thesis

Investigation of Functionals of the Eigenvalues of Unitary Matrices

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July 26, 2025

Abstract

The eigenvalues of large matrices are of interest in a large variety of use cases. However, their computation becomes increasingly challenging as matrix size grows. This thesis focuses on the investigation of functionals over the eigenvalues of unitary matrices, with particular emphasis on the spectral density, or density of states (DoS) among those. While established methods exist for real symmetric matrices, this work extends these approaches to unitary matrices with the help of the Cayley transform. The aim is to develop and analyze efficient techniques for approximating spectral functionals in this broader context.

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Chapter 1

Introduction

The importance of eigenvalues in mathematics and physics is well established. For very large matrices, however, computing all eigenvalues can be prohibitively expensive. In many applications, it suffices to know only a few extremal eigenvalues, certain functionals of the eigenvalues, or the overall distribution of eigenvalues, leading to the concept of the spectral density.

The spectral density, as defined below, provides an exact representation of the eigenvalue distribution. Because it is formulated using the Dirac delta distribution—which is not a conventional function—it must be regularized for practical computations. While efficient techniques exist for real symmetric matrices, our aim is to extend these ideas to the unitary case. To do so, we first revisit Hermitian matrices, introduce the Cayley transform as a link to unitary matrices, and then develop the spectral density framework for unitary matrices. This foundation enables us to address the main algorithm.

1.1 Unitary Matrices

We begin with a basic definition of real symmetric matrices, which we then extend to the complex case. The superscript ^{T} denotes the transpose of a matrix, while * indicates the *conjugate transpose*, also called the *adjoint*, obtained by taking the transpose and then complex conjugating all entries. As is common in the literature, I_n denotes the identity matrix of size n.

Definition 1 (Symmetric matrix)**.** Let $A \in \mathbb{R}^{n\times n}$ be a real, square matrix of size n. Then A is called *symmetric* if $A^T = A$.

This definition naturally leads us to the complex equivalent of a real symmetric matrix.

Definition 2 (Hermitian matrix)**.** Let $A \in \mathbb{C}^{n\times n}$ be a complex square matrix of size n. Then A is called *Hermitian* if $A^* = A$.

Throughout this thesis, A will denote a complex, square matrix of size n, unless stated otherwise. When referring to a Hermitian matrix, we will use the letter H.

We now examine the eigenvalues of Hermitian matrices.

Let $H = H^*$ and $Hv = \lambda v$ for a complex vector $v \in \mathbb{C}^n \setminus \{\mathbf{0}\}$ and a scalar $\lambda \in \mathbb{C}$. Consider now the inner product v^*v. With $(AB)^* = B^*A^*$ and obviously $(A^*)^* = A$

we have that

$$\lambda v^* v = v^* (\lambda v) = v^* (Hv) = (v^* H) v = (H^* v)^* v = (Hv)^* v = (\lambda v)^* v = \overline{\lambda} v^* v.$$

Since we required that $v \neq \mathbf{0}$, it follows that $v^* v \neq \mathbf{0}$ and therefore we can divide the equation by the inner product to obtain $\lambda = \overline{\lambda}$, that is to say λ is real. This means that all eigenvalues of Hermitian matrices are real numbers. It follows that all eigenvalues of symmetric matrices are also real numbers, since they are a special case of Hermitian matrices.

We go on to define the complex matrices central to this thesis:

Definition 3 (Unitary matrix)**.** A matrix A is called *unitary* if $A^* A = A A^* = I_n$. The real equivalent is called an *orthogonal matrix*, where $A^T A = A A^T = I_n$.

We will oftentimes denote unitary matrices by using U as a reference.

Consider a unitary matrix U and an eigenpair (λ, v) of U. The complex conjugate of the eigenvalue equation $Uv = \lambda v$ is

$$v^* U^* = v^* \overline{\lambda} = \overline{\lambda} v^*.$$

We calculate

$$v^* v = v^* I_n v = v^* U^* U v = v^* \overline{\lambda} \lambda v = \overline{\lambda} \lambda v^* v = |\lambda|^2 v^* v$$

With the identical argument as above, we can divide by $v^* v$ to obtain

$$1 = |\lambda|^2 \implies |\lambda| = 1$$

meaning that all eigenvalues of unitary matrices have a length of 1 and are thus situated on the unit circle. As they are a special case of unitary matrices, the same goes for orthogonal matrices. This property is crucial, as it enables the application of the Cayley transform, introduced in the following section.

There is a special group of matrices that all the matrices we have defined so far belong to.

Definition 4 (Normal matrix)**.** A matrix A is called *normal* if it commutes with its conjugate transpose, that is to say $A^* A = A A^*$.

It is straightforward to see that both Hermitian and unitary matrices are normal matrices and that the notion includes real symmetric and orthogonal matrices as special cases. The spectral theorem states that normal matrices can be diagonalized by a unitary matrix [3, Thm. 7.24, p. 218]. That means, for any normal matrix A, there exists a unitary matrix U such that $A = U \Lambda U^*$, where $\Lambda = \operatorname{diag}(\lambda_1, \ldots, \lambda_n)$ with $\lambda_1, \ldots, \lambda_n$ being the eigenvalues of A. This is essential for applying a function to a matrix, which is discussed in the next section.

1.2 Cayley Transform

Before giving the central definition of this section, we first extend the concept of functions to normal matrices, allowing us to map one matrix to another.

Definition 5 (Matrix function of normal matrices)**.** Let A be a normal matrix and let $f : \mathbb{C} \to \mathbb{C}$ be a function that is defined on the spectrum of A, $\sigma(A) = \{\lambda_1, \ldots, \lambda_n\}$. Then the *matrix function* $f(A)$ is defined as

$$f(A) := U f(\Lambda) U^* = U \operatorname{diag}(f(\lambda_1), \ldots, f(\lambda_n)) U^*,$$

where U is the matrix of eigenvectors of A and $\Lambda = \operatorname{diag}(\lambda_1, \ldots, \lambda_n)$ is the diagonal matrix of eigenvalues.

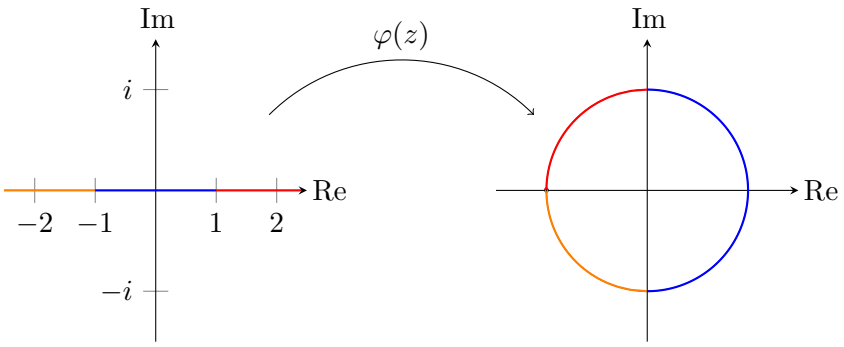
This definition is a special case of the more general definition of matrix functions via Jordan canonical form given by Higham in [4, p. 3]. For normal matrices, the Jordan canonical form is diagonal, so Higham's general definition reduces to the spectral decomposition used here.

Now we can define the *Cayley transform*, which is a specific matrix function, that establishes a correspondence between Hermitian and unitary matrices, allowing spectral properties to be translated between these two important classes.

For a complex number $z \in \mathbb{C}$ with $z \neq -i$, the Cayley transform is defined as

$$\varphi(z) = \frac{i - z}{i + z}.$$

This function maps the real line to the unit circle in the complex plane.



For matrices, the Cayley transform maps a Hermitian matrix H (with $i + H$ invertible) to a unitary matrix U via

$$U = (iI_n - H)(iI_n + H)^{-1}.$$

The condition of $iI_n + H$ being invertible is the same as requiring that H does not have $-i$ as an eigenvalue. If (and only if) that were the case, then we had $Hv = -iv$ for some eigenvector $v \neq \mathbf{0}$, and therefore

$$(iI_n + H)v = iI_n v + Hv = iv + (-iv) = 0.$$

Since Hermitian matrices have only real eigenvalues as discussed above, $-i$ can never be an eigenvalue. Conversely, given a unitary matrix U (with $U \neq -I_n$), the inverse Cayley transform yields a Hermitian matrix:

$$H = i(I_n - U)(I_n + U)^{-1}.$$

This will be relevant later, as we can then use φ to transform unitary matrices into symmetric ones and vice versa.

1.3 Spectral Density

To get to the notion of the spectral density, we will first need some more basic definitions to build on. The reader is assumed to be familiar with the concepts of distributions. Let us also recap that for $\Omega \subset \mathbb{C}^n$ open and non-empty, a *test function* is a smooth function with compact support defined on Ω. The space of all test functions on Ω is usually denoted by $\mathcal{E}$.

We will now look at an important case of a distribution

Definition 6 (Dirac delta distribution)**.** Let $\mathcal{E} = \mathcal{C}^\infty(\Omega)$ with $0 \in \Omega \subset \mathbb{R}^n$. Then

$$\delta : \mathcal{E} \to \mathbb{R}, \quad f \mapsto f(0) \quad \text{with} \quad \delta(f) = \langle \delta, f \rangle = f(0)$$

this distribution is often mistakenly referred to as a function, although it is not a function in the classical sense.

The Dirac delta is characterized by the following property:

$$\int_{-\infty}^{\infty} f(x)\delta(x-a)\,\mathrm{d}x = \int_{-\infty}^{\infty} f(x)\delta(a-x)\,\mathrm{d}x = f(a) \implies \int_{-\infty}^{\infty} \delta(x-a)\,\mathrm{d}x = 1.$$

This means that the Dirac delta distribution is zero everywhere except at the point a, where it is infinitely high, such that the integral over it equals 1. We now have all the tools we need to define the central concept of this thesis:

Definition 7 (Spectral density)**.** Let H be hermitian and sparse. For $x \in \mathbb{R}$, the *spectral density* is then defined as

$$\phi(x) = \frac{1}{n}\sum_{j=1}^{n} \delta(x - \lambda_j)$$

where δ is the Dirac delta distribution and λ_j are the eigenvalues of H in non-descending order.

The summation over the n eigenvalues of H creates a spike at each eigenvalue λ_j, resulting in a distribution that is zero everywhere except at the eigenvalues of H. The division by n ensures that the spectral density is normalized, meaning that the integral over the entire real line equals 1. This is an important property, as it allows us to interpret the spectral density as a probability density function.

The number of eigenvalues ν in an interval $[a, b]$ can then be counted in the following manner:

$$\nu_{[a,b]} = \int_a^b \sum_j \delta(t - \lambda_j)\,\mathrm{d}t \equiv \int_a^b n\phi(t)\,\mathrm{d}t \tag{1.1}$$

Lastly, we will need the notion of the Schwartz space, which we will use as the space of test functions in the following sections.

Definition 8 (Schwartz space over $\mathbb{R}$)**.** The *Schwartz space* over $\mathbb{R}$ consists of all smooth functions f that decay rapidly to zero as $|x|$ approaches infinity [6]. Formally,

$$\mathcal{S}(\mathbb{R}) := \left\{ f \in \mathcal{C}^\infty(\mathbb{R}) \mid \forall p, k \in \mathbb{N}_0 : \sup_{x \in \mathbb{R}} \left| x^p f^{(k)}(x) \right| < \infty \right\}$$

Chapter 2

Motivation

Because of its ability to capture the distribution of eigenvalues, the spectral density of a matrix is a crucial concept in various fields. For example, in quantum mechanics, it describes the density of energy states; in statistics, it is related to the distribution of principal components; and in machine learning, it provides insight into the behavior of large neural networks. However, two main challenges arise when defining and computing the spectral density for a matrix H:

Firstly, the eigenvalues of H are typically not known in advance. If they were, computing the spectral density would be straightforward, but this is rarely the case for large matrices. Secondly, the spectral density is defined using the Dirac delta distribution, which is not a conventional function and cannot be evaluated pointwise. This makes direct computation infeasible, especially for large matrices where eigenvalue decomposition is prohibitively expensive.

To address these challenges, a fundamental idea is to replace the delta distribution by a regular function f with similar properties:

$$\int_{\mathbb{R}} f(x)\,dx = 1, \tag{2.1}$$

where $f(x)$ is very small or zero for most $x \neq 0$, and finite but large near $x = 0$. This regularization enables numerical approximation of the spectral density and is central to many practical algorithms.

For real symmetric matrices, a variety of efficient methods have been developed to approximate the spectral density, often relying on this regularization principle. However, many problems in mathematics and physics naturally lead to complex Hermitian or even unitary matrices, for which the spectral density is less straightforward to compute. In this thesis, we generalize the established approaches from the real symmetric case to the Hermitian case, and further broaden the scope to unitary matrices. This is achieved by first applying the Cayley transform, which provides a bridge between Hermitian and unitary matrices and allows us to transfer techniques and insights between these classes.

One intuitive approach is to select an interval $I \subset \mathbb{R}$ containing the spectrum of H, and divide it into k subintervals using points $\{t_i\}_{i=1}^{k}$. By counting the number of eigenvalues in each subinterval and calculating the average value of $\phi(x)$ using $\nu_{[a,b]}$ from equation 1.1, one obtains a histogram that approximates the true spectral density as the subintervals become smaller.

To count the eigenvalues in the intervals, methods such as Sylvester's law of inertia can be used, which require computing a decomposition of $A - t_i I = LDL^T$ for all t_i [2]. While this is efficient for certain structured matrices, it becomes computationally expensive or impractical for large, unstructured matrices.

This motivates the development of efficient numerical methods that can approximate the spectral density using only matrix-vector multiplications, which scale better with matrix size. In this thesis, we explore such methods, focusing on regularization techniques and polynomial approximations that make the computation of spectral densities feasible for large-scale problems. These advances have the potential to impact a wide range of scientific and engineering disciplines where understanding the spectral properties of large matrices is crucial.

Chapter 3

Kernel Polynomial Method

We consider a class of methods, each with its own variants. All these methods are collectively referred to as the Kernel Polynomial Method (KPM).

As the name suggests, the KPM is a polynomial extension of the spectral density. The coefficients of the polynomials are derived from the method of moments, in order to obtain an estimator function as in statistics.

We previously motivated the replacement of the Dirac delta distribution with a regular function f, and now turn to polynomial approximations for this purpose.

3.1 Basic properties of Chebyshev polynomials

Among the possible choices, Chebyshev polynomials are particularly well-suited due to their favorable mathematical properties, which we will outline below. We note that these properties are not unique, as Legendre polynomials or Hermite polynomials are examples of other good candidates.

First, let's look how Chebyshev polynomials are defined. Using the trigonometric functions, they can be expressed as follows:

$$T_k(x) = \begin{cases} \cos(k \arccos(x)) & \text{for } k \in [-1, 1] \\ \cosh(k \operatorname{arcosh}(x)) & \text{for } k > 1 \\ (-1)^k \cosh(k \operatorname{arcosh}(-x)) & \text{for } k < -1 \end{cases} .$$

For simplicity, we only want to use the formula $T_k(x) = \cos(k \arccos(x))$. This means to only consider matrices which have eigenvalues within the intervall $[-1, 1]$. In the case that this condition should not be fulfilled, the eigenvalues can be transformed accordingly.

For this, let λ_{lb} and λ_{ub} be the lower and upper bound for the eigenvalues of A, respectively. To find these, well-established methods like the Gershgorin circle theorem can be used.

Define

$$c := \frac{\lambda_{lb} + \lambda_{ub}}{2} \quad \text{and} \quad d := \frac{\lambda_{ub} - \lambda_{lb}}{2}$$

Then, the matrix $B = \frac{A - c * I_n}{d}$ has eigenvalues in the interval $[-1, 1]$. A visualization of this is linked in the appendix.

Another way to define Chebyshev polynomials is by calculating them using the recursion formula

$$T_k(x) = 2xT_{k-1}(x) - T_{k-2}(x),$$

where the starting conditions are given by $T_0(x) = 1$ and $T_1(x) = x$.

Now, let

$$h(x) := \frac{1}{\sqrt{1-x^2}} \tag{3.1}$$

be a weight function. Another property of Chebyshev polynomials is that they are *orthogonal* in terms of the scalar product weighted with h:

$$\langle f, g \rangle = \int_{-1}^{1} \frac{1}{\sqrt{1-x^2}} \cdot f(x) \cdot g(x) \, \mathrm{d}x.$$

This means that

$$\int_{-1}^{1} \frac{1}{\sqrt{1-t^2}} \cdot T_k(t) \cdot T_l(t) \, \mathrm{d}t = \begin{cases} 0 & \text{for } k \neq l \\ \pi & \text{for } k = l = 0 \\ \frac{\pi}{2} & \text{for } k = l \neq 0 \end{cases} . \tag{3.2}$$

3.2 Approximating the spectral density

We now define the $\hat{\phi}$ as the product of spectral density with the inverse of the weight function 3.1:

$$\hat{\phi}(x) := \sqrt{1-x^2}\phi(x) = \sqrt{1-x^2} \cdot \frac{1}{n} \sum_{j=1}^{n} \delta(x - \lambda_j)$$

Let $g \in \mathcal{S}(\mathbb{R})$, the Schwartz space defined in definition 8, and let $\mu_k \in \mathbb{R}$ coefficients to be determined such that the following equation holds:

$$\int_{-1}^{1} \hat{\phi}(x) g(x) \, \mathrm{d}x = \int_{-1}^{1} \sum_{k=0}^{\infty} \mu_k T_k(x) g(x) \, \mathrm{d}x \tag{3.3}$$

If this is true for arbitrary $g \in \mathcal{S}(\mathbb{R})$, we can simplify our equation 3.3 to

$$\hat{\phi}(x) = \sum_{k=0}^{\infty} \mu_k T_k(x) \tag{3.4}$$

Now utilize the orthogonality of the Chebyshev polynomials, to calculate a specific coefficient μ_k. Note that δ_{k0} in this context denotes the Kronecker delta, and has nothing to do with the Dirac delta distribution.

$$
\begin{aligned}
&\sum_{l=0}^{\infty} \mu_l T_l(x) = \hat{\phi}(x) \\
\implies &\left(\sum_{l=0}^{\infty} \mu_l T_l(x) \right) \cdot T_k(x) = \hat{\phi}(x) \cdot T_k(x) \\
\implies &\int_{-1}^{1} \frac{1}{\sqrt{1-x^2}} \cdot \left(\sum_{l=0}^{\infty} \mu_l T_l(x) \right) \cdot T_k(x) \, \mathrm{d}x = \int_{-1}^{1} \frac{1}{\sqrt{1-x^2}} \cdot \hat{\phi}(x) \cdot T_k(x) \, \mathrm{d}x \\
\implies &\mu_k \cdot \frac{\pi}{2 - \delta_{k0}} = \int_{-1}^{1} \frac{1}{\sqrt{1-x^2}} \cdot \sqrt{1-x^2} \cdot \phi(x) \cdot T_k(x) \, \mathrm{d}x \\
\implies &\mu_k = \frac{2 - \delta_{k0}}{\pi} \cdot \int_{-1}^{1} \phi(x) \cdot T_k(x) \, \mathrm{d}x
\end{aligned}
$$

By applying the Dirac delta distribution we obtain:

$$
\begin{aligned}
\mu_k = \frac{2 - \delta_{k0}}{\pi} \cdot \int_{-1}^{1} \phi(t) \cdot T_k(t) \, \mathrm{d}t &= \frac{2 - \delta_{k0}}{\pi} \cdot \int_{-1}^{1} \frac{1}{n} \sum_{j=1}^{n} \delta(t - \lambda_j) \cdot T_k(t) \, \mathrm{d}t \\
&= \frac{2 - \delta_{k0}}{n\pi} \sum_{j=1}^{n} T_k(\lambda_j) \\
&= \frac{2 - \delta_{k0}}{n\pi} \operatorname{Tr}(T_k(A))
\end{aligned}
$$

This means we are in need of an estimator for $\operatorname{Tr}(T_k(A))$.

3.3 Estimating the trace of Chebyshev polynomials

We want to obtain the corollary of the following generalized theorem:

Theorem 1. Let $A \in \mathbb{C}^{n \times n}$ be a normal matrix with spectral decomposition

$$
A = U \Lambda U^* \quad \text{where} \quad UU^* = I_n \text{ and } \Lambda = \operatorname{diag}(\lambda_1, ..., \lambda_n)
$$

Let $\beta, v \in \mathbb{C}^n$ with $v = U\beta$. Suppose v is a random vector whose entries v_i are independent and identically distributed standard complex normal variables, i.e., $v_i \sim_{\text{i.i.d.}} \mathcal{N}_{\mathbb{C}}(0, 1)$, meaning $\operatorname{Re}(v_i), \operatorname{Im}(v_i)$ are independent $\mathcal{N}(0, \frac{1}{2})$. Then

$$
\mathbb{E}[v] = 0 \quad \text{and} \quad \mathbb{E}[vv^*] = I_n, \tag{3.5}
$$

and it follows that

$$
\mathbb{E}[\beta] = 0 \quad \text{and} \quad \mathbb{E}[\beta\beta^*] = I_n.
$$

Proof of Theorem 1. Since the expectation operator is linear, it holds that

$$\mathbb{E}[v] = \mathbb{E}[U\beta] = U\mathbb{E}[\beta] = 0 \implies \mathbb{E}[\beta] = 0$$

Furthermore it holds that

$$I_n = \mathbb{E}[vv^*] = \mathbb{E}[(U\beta)(U\beta)^*] = \mathbb{E}[U\beta\beta^*U^*] = U\mathbb{E}[\beta\beta^*]U^*$$

Multiplying both sides with U^* and U yields:

$$U^*I_nU = U^*U\mathbb{E}[\beta\beta^*]U^*U = \mathbb{E}[\beta\beta^*]$$

Since U is unitary, we have shown that $\mathbb{E}[\beta\beta^*] = I_n$. □

This theorem has a nice corollary when investigating a matrix function $f(A)$. In that case,

$$\begin{aligned}
\mathbb{E}\left[v^*f(A)v\right] &= \mathbb{E}\left[(U\beta)^*f(U\Lambda U^*)(U\beta)\right] \\
&= \mathbb{E}\left[\beta^*U^*Uf(\Lambda)U^*U\beta\right] \\
&= \mathbb{E}\left[\beta^*f(\Lambda)\beta\right] \\
&= \mathbb{E}\left[\sum_{j=1}^{n} |\beta_j|^2 f(\lambda_j)\right] \\
&= \sum_{j=1}^{n} f(\lambda_j)\mathbb{E}\left[|\beta_j|^2\right] \\
&= \sum_{j=1}^{n} f(\lambda_j)
\end{aligned}$$

or, more concisely,

$$\mathbb{E}\left[v^*f(A)v\right] = \mathrm{Tr}(f(A)). \tag{3.6}$$

We now have a method to calculate the trace of a matrix function $f(A)$, using only vector multiplications with A.

3.4 The Kernel Polynomial Method algorithm

Now let $n_{\mathrm{vec}} \in \mathbb{N}$ and consider random vectors $v_0^{(1)}, v_0^{(2)}, \ldots, v_0^{(n_{\mathrm{vec}})}$, each drawn independently from the standard normal distribution, that is, $\mathbb{E}[v_0^{(k)}] = 0$ and $\mathbb{E}\left[v_0^{(k)}\left(v_0^{(k)}\right)^T\right] = I_n$. It follows from equation 3.6 that

$$\zeta_k = \frac{1}{n_{\mathrm{vec}}}\sum_{l=1}^{n_{\mathrm{vec}}}\left(v_0^{(l)}\right)^T T_k(A)v_0^{(l)}$$

is a good estimator for $\mathrm{Tr}(T_k(A))$ and therefore

$$\mu_k \approx \frac{2-\delta_{k0}}{n\pi}\zeta_k$$

In order to determine the ζ_k, let $v_0 \equiv v_0^{(l)}$. Using the recursion formula for Chebyschev polynomials, we can calculate

$$T_{k+1}(A)v_0 = 2AT_k(A)v_0 - T_{k-1}(A)v_0$$

For $v_k \equiv T_k(A)v_0$ it also holds that

$$v_{k+1} = 2Av_k - v_{k-1}$$

With this we are fully equipped for the final calculation and the goal of the KPM is reached: Instead of having to multiply matrices with other matrices, it now suffices to multiply matrices with vectors. Now we can approximate $\phi(x)$ as closely as we like. As aforementioned, it is not always desirable to have an infinitely exact approximation. Since it holds that

$$\lim_{k\to\infty} \mu_k \to 0$$

and we are only interested in $T_k(x)$ with $k \leq M$
Therefore we estimate ϕ with

$$\tilde{\phi}_M(x) = \frac{1}{\sqrt{1-x^2}} \sum_{k=0}^{M} \mu_k T_k(x) \tag{3.7}$$

The following pseudo code is based on [5, p. 10] and summarizes the steps described above. The implementation is done in Python, and linked in the appendix.

Applying the Cayley transform to an arbitrary unitary matrix U yields a Hermitian matrix H; and as this is the case, the KPM can be applied to unitary matrices as well.

3.5 The Choice of Random Unitary Matrices

When generating random unitary matrices for numerical experiments, it is important to ensure that their eigenvalues are distributed uniformly on the unit circle, as predicted by random matrix theory. A common approach is to generate a random complex matrix A with independent standard normal entries and then construct a unitary matrix from A using either the QR decomposition or the singular value decomposition (SVD). In the QR approach, A is factored as $A = QR$, where Q is unitary and R is upper triangular. The matrix Q is then used as the random unitary matrix. In the SVD approach, A is factored as $A = U\Sigma V^*$, and either U or V (both unitary) can be used as a random unitary matrix. Although both methods produce unitary matrices, their statistical properties differ. The SVD-based approach yields unitary matrices whose eigenvalues are uniformly distributed on the unit circle, matching the theoretical prediction for random unitary matrices (the so-called Haar measure). In contrast, the QR-based approach does not generally produce a uniform distribution of eigenvalues on the unit circle. This distinction is important for applications where the spectral properties of random unitary matrices play a central role, such as in the study of spectral densities. For such purposes, the SVD-based construction is preferable, as it ensures the correct statistical behavior of the eigenvalues.

Algorithm 1 The Kernel Polynomial Method

Require: $A = A^* \in \mathbb{C}^{n \times n}$ with eigenvalues in the intervall $[-1, 1]$
Ensure: Estimated spectral density $\{\tilde{\phi}_M(t_i)\}$

for $k = 0 : M$ **do**
  $\zeta_k \leftarrow 0$
end for
for $l = 1 : n_{\text{vec}}$ **do**
  Choose a random new vector $v_0^{(l)}$; ▷ $v_{0_i}^{(l)} \sim$ i.i.d. $\mathcal{N}(0, 1)$
  for $k = 0 : M$ **do**
    Calculate $\zeta_k \leftarrow \zeta_k + \left(v_0^{(l)}\right)^T v_k(l)$;
    if $k = 0$ **then**
      $v_1^{(l)} \leftarrow A v_0^{(l)}$
    else
      $v_{k+1}^{(l)} \leftarrow 2A v_k^{(l)} - v_{k-1}^{(l)}$ ▷ Three term recursion
    end if
  end for
end for
for $k = 0 : M$ **do**
  $\zeta_k \leftarrow \frac{\zeta_k}{n_{\text{vec}}}$
  $\mu_k \leftarrow \frac{2 - \delta_{k0}}{n\pi} \zeta_k$
end for
Evaluate $\tilde{\phi}_M(t_i)$ with equation 3.7

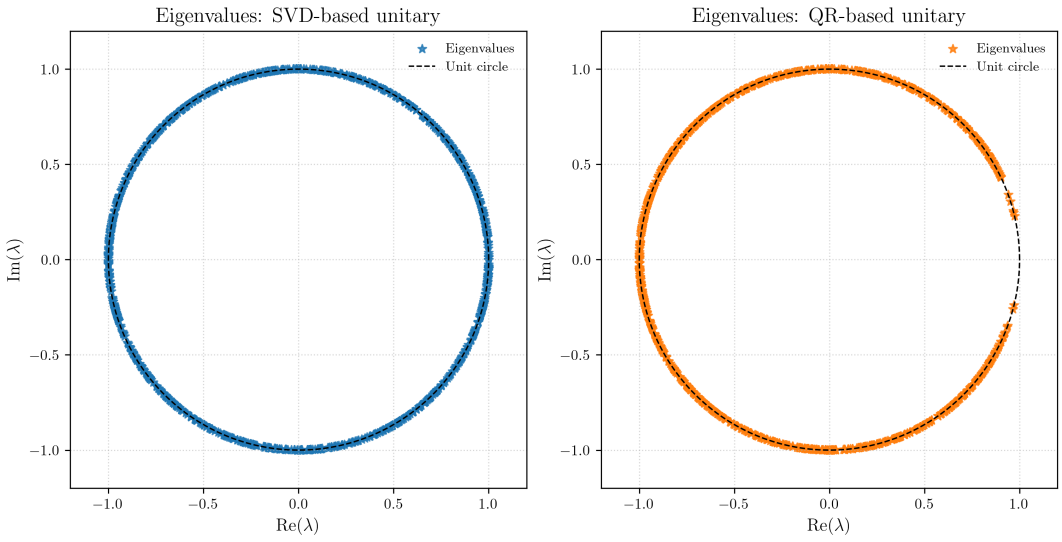


Figure 3.1: Eigenvalue distributions of random unitary matrices generated via SVD and QR.

Chapter 4

Quality Analysis

Let $\tilde{\phi}(t)$ be a regular function, that estimates the spectral density. Since $\phi(t)$ is no function in the classical sense, but all approximations are continuous functions,

$$\left|\left|\phi(t) - \tilde{\phi}(t)\right|\right|_{L^p}$$

is not defined, to estimate the error. In the following, we will introduce two methods to circumvent this problem. The first one uses the fact that $\delta(t)$ is a distribution that can be applied to test functions from the Schwartz space $\mathcal{S}(\mathbb{R})$, while the second one regularizes δ-functions by replacing them with continuous and smooth functions. These two approaches are closely related, as we will see later.

4.1 Resolution

In practice, there is often no need to approximate all eigenvalues of A exactly. This would even be highly discontinuous, as we recall the intuitive approach with histograms. The accuracy of the approximation should be oriented towards the desired *resolution*. This means that often only the eigenvalues in a certain subinterval $[a, b] \subset \sigma(A)$ are of interest in a certain context. The size $b - a$ is then called the resolution of the estimate. This insight should be taken as a parameter in our further considerations.

4.2 Restriction on the Schwartz space

In this first method, we consider $\delta(t)$ as a distribution. Let $g \in \mathcal{C}^\infty(\mathbb{R})$ be a test function from the Schwartz space $\mathcal{S}(\mathbb{R})$ defined in Definition 8. Then we have

$$\langle \delta(\cdot - \lambda), g \rangle = \int_{-\infty}^{\infty} \delta(t - \lambda) g(t) \, \mathrm{d}t = g(\lambda)$$

and for all $p, k \in \mathbb{N}_0$

$$\sup_{t \in \mathbb{R}} |t^p g^{(k)}(t)| < \infty$$

The error can therefore be measured as follows:

$$\epsilon_1 = \sup_{g \in \mathcal{S}(\mathbb{R})} \left| \langle \phi, g \rangle - \langle \tilde{\phi}, g \rangle \right|$$

To transfer the concept of resolution to this error, we first consider $\nu_{[a,b]}$ from equation 1.1 and define accordingly

$$\tilde{\nu}_{[a,b]} = \int_a^b n\tilde{\phi}(t)\ \mathrm{d}t$$

with $\tilde{\phi}(t) \in \mathcal{C}^\infty(\mathbb{R})$. Assuming $n = 1$ and thus $\phi(t) = \delta(t)$, an infinite resolution would mean that for arbitrarily small intervals $[a, b]$ the term $\left|\nu_{[a,b]} - \tilde{\nu}_{[a,b]}\right|$ also becomes arbitrarily small. Let $a = -\varepsilon, b = \varepsilon$. From the definition of the δ-function it follows that

$$\lim_{\varepsilon \to 0+} \nu_{[-\varepsilon,\varepsilon]} = 1$$

while for smooth functions $\tilde{\phi}$ it is clear that

$$\lim_{\varepsilon \to 0+} \tilde{\nu}_{[-\varepsilon,\varepsilon]} = 0$$

This shows that no smooth function converges to the spectral density under continuous increase of the resolution. A carefully balanced approximation would therefore be as precise as a constant one. However, as noted earlier, a finite resolution is often sufficient. We can therefore restrict the Schwartz space $\mathcal{S}(\mathbb{R})$. For example, one could only consider Gaussian distributions of the form

$$g_\sigma(t) = \frac{1}{(2\pi\sigma^2)^{\frac{1}{2}}} e^{-\frac{t^2}{2\sigma^2}}$$

and restrict $\mathcal{S}(\mathbb{R})$ to the subspace

$$\mathcal{S}(\mathbb{R})(\sigma; [\lambda_{us}, \lambda_{os}]) = \{g \mid g(t) \equiv g_\sigma(t - \lambda), \lambda \in [\lambda_{us}, \lambda_{os}]\}$$

Here, λ_{us} and λ_{os} are the upper and lower bounds of the eigenvalues of A as in the previous section, while the parameter σ represents the *target resolution*. We can now use the following metric for quality assessment:

$$E\left[\tilde{\phi}; \mathcal{S}(\mathbb{R})\left(\sigma; [\lambda_{lb}, \lambda_{ub}]\right)\right] = \sup_{g \in \mathcal{S}(\mathbb{R})(\sigma; [\lambda_{lb}, \lambda_{ub}])} \left|\langle \phi, g\rangle - \langle \tilde{\phi}, g\rangle\right| \tag{4.1}$$

4.3 Regularizing the Dirac delta distribution

In the second method, we regularize the δ-function. This means that we replace the δ-function with a smooth function $\phi(t)$ that approximates the spectral density. This is done by smoothing the δ-function. For example, we can use the Gaussian distribution with standard deviation σ:

$$\phi_\sigma(t) = \frac{1}{(2\pi\sigma^2)^{\frac{1}{2}}} e^{-\frac{t^2}{2\sigma^2}}$$

This function is smooth and well-defined for all $t \in \mathbb{R}$. It is also normalized, meaning that

$$\int_{-\infty}^{\infty} \phi_\sigma(t)\ \mathrm{d}t = 1$$

This means that $\phi_\sigma(t)$ can be interpreted as a probability density function. The parameter σ controls the width of the Gaussian distribution and thus the resolution of the approximation. This means that the smaller σ is, the more precise the approximation is, but also the more sensitive it is to noise in the data. This is a common approach in numerical analysis to approximate distributions with smooth functions. The function $\phi_\sigma(t)$ is then well-defined and can be used to calculate the error for $p = 1, 2$ and ∞:

$$\epsilon_2 = \left|\left|\phi_\sigma(t) - \tilde{\phi}(t)\right|\right|_p$$

Let

$$\phi_\sigma(t) = \langle \phi(\cdot), g_\sigma(\cdot - t)\rangle = \sum_{j=1}^{n} g_\sigma(t - \lambda_j)$$

This is the convolution of the spectral density with the Gaussian function g_σ. In similar manner, let

$$\tilde{\phi}_\sigma(t) = \langle \tilde{\phi}(\cdot), g_\sigma(\cdot - t)\rangle$$

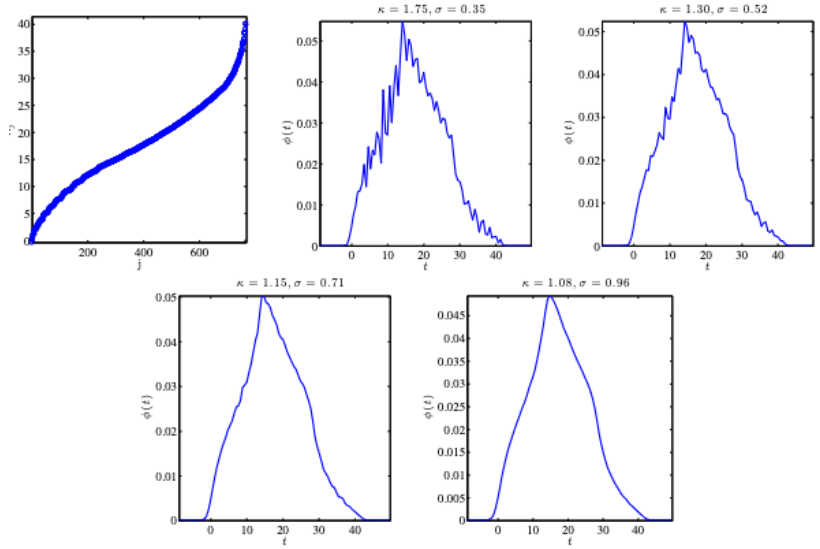
Then

$$E\left[\tilde{\phi}; \mathcal{S}(\mathbb{R})\left(\sigma; [\lambda_{lb}, \lambda_{ub}]\right)\right] = \sup_{g \in \mathcal{S}(\mathbb{R})(\sigma; [\lambda_{lb}, \lambda_{ub}])} \left|\phi_\sigma(t) - \tilde{\phi}_\sigma(t)\right|$$

is the L^∞ error between two well-defined functions. Just like in the other method, σ controls the resolution: the larger the σ, the smoother but also less accurate the approximation. For smaller values, one obtains coarser functions, where small peaks can be detected exactly where the eigenvalues are located. The following graphic is taken from [5, p. 6] and illustrates this effect for four different values of σ: Sei also

$$\phi_\sigma(t) = \langle \phi(\cdot), g_\sigma(\cdot - t)\rangle = \sum_{j=1}^{n} g_\sigma(t - \lambda_j)$$

Dies ist dann nicht anderes als die "Weichzeichnung" der Spektraldichte durch Gauß-Funktionen der Breite σ.



4.4 The condition of non-negativity

As a probability distribution, the spectral density is non-negative, meaning

$$\forall g \in \mathcal{S}(\mathbb{R}), g \geq 0 : \langle \phi, g \rangle \geq 0$$

Some numerical approximations break this property, including the Kernel Polynomial Method. This leads to large errors and must be considered carefully. Methods to mitigate these negative effects would exceed the scope of this work.

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