University of Potsdam

Bachelor Thesis

Investigation of Functionals of the Eigenvalues of Unitary Matrices

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Abstract

The eigenvalues of large matrices are of interest for a large variety of use cases. Their calculation however grows increasingly complex with increasing matrix sizes. Therefore, we seek to simplify this process by approximating functionals over the spectrum of a matrix. This thesis is focussed on the spectral density or Denisty of States (DoS) among those. It has already been applied to real symmetric matrices. This work aims to go one step further and apply the findings to unitary matrices with the help of the cayley transform.

Contents

Introduction

To kick off this investigation we first need to look closer at unitary matrices and their properties. Then we will reiterate over the cayley transform to finally close in on the spectral density. Upon this we should have all requirements to start the investigation afterwards.

1.1 Unitary Matrices

Let's begin with a definition that will be relevant in later chapters. The index ^{T} marks the transpose of a matrix. As common in a lot of literature, I_n denotes the identity matrix of size n.

Definition 1 (Orthogonal matrix)**.** Let A be a real, square matrix of size n. Then A is called *orthogonal* if $A^T \cdot A = I_n$.

For the entirety of this thesis, let A always be a complex, square matrix of size n unless stated otherwise. Note that A^* is *conjugate transpose* of the matrix A with all of its entries complex conjugated and transposed.

Definition 2 (Unitary matrix)**.** A matrix A is called *unitary* if $A^* \cdot A = I_n$.

We will oftentimes denote unitary matrices by using U as a reference. It is easy to see that orthogonal matrices are a special case of unitary matrices, since $A^T = A^*$ for all real matrices.
Now, let's assume we have a unitary matrix U and are trying to find its eigenvalues. That means we have to solve the equation

$$U \cdot v = \lambda \cdot v \tag{1.1}$$

for a complex vector $v \neq \mathbf{0}$ of size n and a scalar $\lambda \in \mathbb{C}$. The complex conjugate of this equation is

$$v^* \cdot U^* = v^* \cdot \lambda^* = \lambda^* \cdot v^* \tag{1.2}$$

Put together, we calculate

$$\begin{aligned} v^* \cdot v &= v^* \cdot U^* \cdot U \cdot v \\ &= v^* \cdot \lambda^* \cdot \lambda \cdot v \\ &= \lambda^* \cdot \lambda \cdot v^* \cdot v \\ &= |\lambda|^2 \cdot v^* \cdot v \end{aligned}$$

Since we have that $v \neq \mathbf{0}$ it follows that $v^* \cdot v \neq 0$. Therefore, we can divide by $v^* \cdot v$ to obtain

$$1 = |\lambda|^2 = |\lambda| \tag{1.3}$$

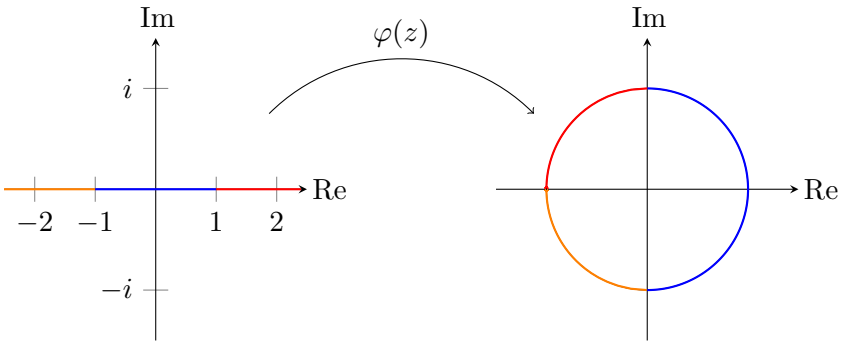
meaning that all eigenvalues of unitary matrices have a length of 1 and are thus situated on the unit circle. For orthogonal matrices, this means their eigenvalues are either 1 or -1. This is an important property, as it justifies that we can make use of the Cayley transfrom introduced in the following section.

1.2 Cayley Transform

The Cayley transform or Cayley transformation is given by the simple function

$$\varphi(z) = (i - z)(i + z)^{-1}$$

This function maps the real line to the unit circle, and more specifically, the interval $[-1, 1]$ to the semi circle $\{z = e^{i\theta} : \theta \in [-\pi/2, \pi/2]\}$ as shown below



This will be relevant later, as we can then use φ to transform unitary matrices into symmetric once and vice versa. Now, let's look how the spectral density is defined in the next section.

1.3 Spectral Density

To get to the notion of the spectral density, we will first need some more basic definitions to build on.

Definition 3 (linear functional)**.** Let V be a vectorspace over a field $\mathbb{K}$. A *linear functional* T is a linear function $T : V \to \mathbb{K}$. The space over all linear functionals $V \mapsto \mathbb{K}$ is called the *dual space* V'.

A simple example for such a functional would be

$$T : \mathcal{C}^\infty(\mathbb{R}) \to \mathbb{R}, \qquad f \mapsto f(0) \tag{1.4}$$

A more special case is the integral.

$$T_g : \mathcal{C}^\infty(\mathbb{C}) \to \mathbb{C}, \qquad f \mapsto \int_{\mathbb{C}} g \cdot f \, \mathrm{d}x \tag{1.5}$$

This definition leads to the concept of a distribution which was introduced to get a method to differentiate where differentiation in the classical sense is not possible.

Definition 4 (distribution)**.** Let $\emptyset \neq \Omega \subset \mathbb{R}^n$ be open. Let $\mathcal{E}$ be the space of *test functions* over Ω. A *distribution* T is a function $T : \mathcal{E} \to \mathbb{C}$ where for all $g, g_1, g_2, \{g_n\}_{n\in\mathbb{N}} \in \mathcal{E}$ with $\lim\limits_{n\to\infty} g_n \to g$ it holds:

$$T(g_1 + \lambda g_2) = T(g_1) + \lambda T(g_2) \quad \text{und} \quad \lim_{n\to\infty} T(g_n) \to T(g)$$

So, put shortly: A distribution T is a continuous and linear functional on $\mathcal{E}$. Now the path is clear to define the so called Dirac delta distribution

Definition 5 (Dirac delta function)**.** Let $\mathcal{E} = \mathcal{C}^\infty(\Omega)$ with $0 \in \Omega \subset \mathbb{R}^n$. Then

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

An important feature of this definition is:

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

This distribution is often misleadingly labled as a function inspite of being decidedly not that.
We can now finally define the spectral density.

Definition 6 (spectral density)**.** Let $A \in \mathbb{R}^{n\times n}$, $A^T = A$ and A sparce. Then, the spectral density is defined as

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

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

The number of eigenvalues in an intervall $[a, b]$ can then be expressed as follows:

$$\nu_{[a,b]} = \int_a^b \sum_j \delta(t - \lambda_j) \, \mathrm{d}t \equiv \int_a^b n\phi(t) \, \mathrm{d}t \tag{1.6}$$

Definition 7 (Schwartz-space over $\mathbb{R}$)**.** The Schwartz-space over $\mathbb{R}$ contains all smooth functions f, which fall fast enough against 0, when $|x|$ gets closer to ∞. [4] In Formeln

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

Im Weiteren werde ich das Symbol $\mathcal{S}$ als Abkürzung für $\mathcal{S}(\mathbb{R})$ benutzen, da sich diese Arbeit allein mit dem reellen Kontext befasst.

Motivation

2.1 Motivation

Calculating the spectral density of a matrix is trivial, when its eigenvalues are already known. However, this is mostly not the case and calculating eigenvalues of very large matrices is time- and energy intensive. At the same time, the DOS as a kind of probability density over the distribution of eigenvalues is of great interest in many fields. Thus, there is a need for methods which approximate the spectral density at low cost. The problem with this is that $\phi(t)$ the Delta distribution is not a *function* as we know it, that can be evaluated at each point.
A more intuitive idea would be to choose an intervall $I \in \mathbb{R}$ such that the spectrum of A, $\sigma(A)$, is a subset of I. Now choose k points t_i in I, such that the intervall is divided in sub intervals:

$$\{t_i\}_{i=1}^{k} \subset I \quad \text{mit} \quad \bigcup_{i=1}^{k-1} [t_i, t_{i+1}] = I$$

Now count the eigenvalues in every sub interval. Then calculate the average value of $\phi(t)$ in every intervall with $\nu_{[a,b]}$ from equation 1.6. The results is histograms, which with increasingly smaller subintervalls, that is to say bigger k and $(t_{i+1} - t_i) \longrightarrow 0$, approach the spectral density.
To count the eigenvalues in the intervals, there is means like for example the Sylvestreschen Trägheitssatz. The details of this method are not part of this work, it would be necessary to calculate a decomposition of $A - t_i I = LDL^T$ for all t_i [3]. We prefer a method in which A is multiplied with vectors, which is in bigger dimensions.
For simplicity we are going to assume, that A is szmmetric and real. The extension to hermetian matrices is simple in comparison.

Bibliography

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