



DIPLOMARBEIT

Modeling of Signals by using Matrix-valued Optimal Mass Transport

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Kurzfassung

Optimaler Massentransport (OMT) ist eine Methode, um zu beschreiben, wie man die Werte einer ersten gegebene Funktion f verschieben muss, um eine zweite gegebene Funktion g zu erhalten. Wir können ein Ähnlichkeitsmaß zwischen f und g definieren, indem wir messen, wieviel wir von f verschieben müssen, um g zu erhalten. Mithilfe dieses Maßes können wir nun eine weitere Funktion bestimmen, die f und g so ähnlich wie möglich ist und dementsprechend als Mischung der beiden Funktionen gesehen werden kann. Im klassischen Fall ist OMT für nichtnegative, reellwertige Funktionen definiert. In dieser Arbeit erweitern wir OMT auf Funktionen, die in die Menge der hermiteschen, positiv semidefiniten Matrizen abbilden. Diese Funktionen repräsentieren beispielsweise multidimensionale Signale. Wir betrachten Signale als stochastische Prozesse und sind an ihren statistischen Eigenschaften interessiert, insbesondere an der Autokovarianz und Kreuzkovarianz. Der Satz von Herglotz liefert einen Zusammenhang zwischen der Autokovarianz und dem Spektralmaß. erweitern die Aussage auf den multidimensionalen Fall, indem wir auch die Kreuzkovarianzen einbeziehen. Wir zeigen, dass die Matrix der Kreuzspektralmaße positiv semidefinit und daher ein Kandidat für die Methoden des OMT ist. Als Anwendung wollen wir mithilfe von OMT in einem Raum mit einer Signalquelle und zwei Sensoren jenes Signal modellieren, das in der Mitte der beiden Sensoren gemessen werden würde. Für diesen Zweck implementieren wir OMT in MATLAB. In der Formulierung von OMT wird nach einem optimalen Weg gesucht, um q aus f zu erhalten. Dementsprechend müssen wir nun ein konvexes Optimierungsproblem lösen. Die Berechnung benötigt eine kurze Rechenzeit. Wir erhalten Ergebnisse, die den tatsächlichen Messungen an der untersuchten Stelle entsprechen könnten und haben somit eine vielversprechende Methode entwickelt, um Signale zu modellieren.

Abstract

Given two functions f and g, optimal mass transport (OMT) is a method of describing how we can rearrange the values of f in order to obtain g. By considering how much we have to rearrange to obtain g, we define a measure of similarity between f and g. This can be used to determine a function that is as similar as possible to both f and g and hence represents a mixture of the two functions. In the classical setting, OMT is defined for non-negative, real-valued functions. In this thesis, we redefine optimal mass transport for functions that map to the Hermitian, positive semi-definite matrices. These functions can represent, e.g., multidimensional signals. We consider signals as stochastic processes and are interested in their statistical properties, in particular the autocovariance and cross-covariance. Herglotz's theorem provides a connection between autocovariance and spectral measure, however we extend the statement to the multidimensional case by considering cross-covariances. We show that the matrix of the cross-spectral measures is positive semi-definite and thus is a candidate for the methods of optimal mass transport. As an application, a room with a signal source and two sensors is given. We use OMT to model the signal that would be measured in the middle of the two sensors. For this purpose, we implement OMT in MATLAB. In the formulation of OMT, we need to find an optimal way of obtaining g from f. Hence, this requires solving a convex optimization problem. The computation can be done in a short time. We obtain results that could resemble actual measurements at the considered location and hence we have developed a promising method of modeling signals.

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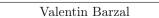
I want to thank my parents for enabling me to change my studies to Technical Mathematics. It was a decision that I have never regretted for a single day.

Last but not least, I want to thank my colleagues that I met during my studies. You were not only a great support in discussing and understanding mathematical problems (special thanks go to Paula Hilbert), but you also became good friends and therefore I always enjoyed spending time at the university.

Eidesstattliche Erklärung

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Wien, am 14. Mai 2025



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Introduction

Optimal mass transport (OMT) provides a way to rearrange the values of a given function fin order to obtain another given function g. More precisely, given two non-negative functions $f,g:[a,b]\to\mathbb{R}_0^+$ that satisfy $\int_a^b f(x)\,dx=\int_a^b g(y)\,dy$, we try to find a transport plan $m:[a,b]\times[a,b]\to\mathbb{R}_0^+$ satisfying

$$\int_{a}^{b} m(x,y) dy = f(x), \qquad \int_{a}^{b} m(x,y) dx = g(y).$$

Loosely speaking, the value m(x,y) tells how much of f(x) we have to take from location x and transport to location y. Based on [NGT14], we describe how we can extend OMT to functions μ that map to the Hermitian, positive semi-definite matrices. In order to ensure the existence of a transport plan, we have to redefine the properties of a transport plan and therefor consider tensor products and corresponding mappings. Our new transport plan will be a function $m:[a,b]\times[a,b]\to\mathbb{C}^{n\times n}\otimes\mathbb{C}^{n\times n}$. Since the transport plan is not unique, we want to find the best one, i.e., the transport plan that moves the least but still satisfies the required constraints. For this purpose, we introduce the cost of each transport plan and select the one with the lowest cost. Finding this optimal transport plan is a convex optimization problem. If our given functions μ_0 and μ_1 are similar, we can find a cheap transport plan, i.e., a transport plan that just moves a little. However, the optimal transport plan of two very different μ_0 and μ_1 will have a high cost. Hence, the optimal cost $\mathcal{T}_{2,\lambda}(\mu_0,\mu_1)$ (i.e., the cost of the optimal transport plan) between μ_0 and μ_1 acts as a measure of similarity between the two functions. Apart from the triangle inequality, $\mathcal{T}_{2,\lambda}$ satisfies all properties of a metric. We can use this measure of similarity to determine a function $\mu_{0.5}$ that minimizes the sum

$$\mathcal{T}_{2,\lambda}(\mu_0,\mu) + \mathcal{T}_{2,\lambda}(\mu,\mu_1)$$

over all μ . This $\mu_{0.5}$ is as similar as possible to our given μ_0 and μ_1 and hence can be seen as a mixture of them. Later, we want to apply these methods to multidimensional signals in order to determine intermediate signals. But first, we need to discuss the theoretical basics about signals.

We consider signals as stochastic processes. In this thesis, we only deal with discrete-time, wide-sense stationary stochastic processes. We are interested in their statistical properties, in particular in the autocovariance and cross-covariance. Herglotz's theorem provides the existence of a spectral measure, i.e., a measure F that satisfies

$$r_{XX}(t) = \int_{-\pi}^{\pi} \exp(i\omega t) dF(\omega)$$



whereat r_{XX} is the autocovariance function of a process X. In this thesis, we prove the existence of a matrix F of complex measures satisfying

$$R(t) = \int_{-\pi}^{\pi} \exp(i\omega t) dF(\omega),$$

whereat R is the covariance matrix. Furthermore, we prove that the matrix $F([\omega_1, \omega_2])$ is positive semi-definite for any $[\omega_1, \omega_2] \subseteq [-\pi, \pi)$.

After showing that cross-spectral density functions of multidimensional signals can be represented as Hermitian, positive semi-definite matrix-valued functions, we apply our OMT methods. As an example, we consider a room with a source and two sensors. Knowing the signals at the two sensors, we try to model the signal that would be measured in between the two sensors. This corresponds to our aforementioned task of finding $\mu_{0.5}$ between given μ_0 and μ_1 . We see that the computation can be done in reasonable time and yields reasonable

A founding father of OMT was the French geometer Gaspard Monge. In the end of the 18th century, he was considering a place where you could dig up soil and a construction where the soil was needed. Since transportation was expensive, he asked for an optimal way to transfer the soil to the construction, i.e., he wanted to know where exactly the soil extracted from a certain location had to be transported to. In 1942, the later Nobel Prize winner Leonid Kantorovich published a general formulation of OMT, without knowing about Monge's work. Some years later, Kantorovich work was connected to Monge's formulation. That gave rise to a new formulation of the OMT problem, namely the Monge-Kantorovich formulation. See [Vil⁺08, Introduction - 3] and [KPT⁺17, p. 44].

Various literature sources were consulted in the preparation of this thesis. In addition to the bibliography, we also want to mention the most frequently used literature here: The description of the concept of OMT, in particular the concepts of matrix-valued OMT, is based on the paper On Matrix-Valued Monge-Kantorovich Optimal Mass Transport by Lipeng Ning, Tryphon T. Georgiou, and Allen Tannenbaum ([NGT14]). Advanced linear and matrix algebra by Nathaniel Johnston ([Joh21]) offers precise but still colorful explanations regarding linear algebra, e.g., tensor products. Stationary Stochastic Processes: Theory and Applications by Georg Lindgren ([Lin12]) provides a good introduction to stochastic processes and their spectral properties, in particular for continuous-time signals/stochastic processes. German-speaking readers will find a detailed introduction to measure theory in $Ma\beta$ - und Integrationstheorie by Jürgen Elstrodt ([Els18]). Real and Complex Analysis by Walter Rudin ([Rud87]) was consulted for theorems and definitions regarding analysis. Probability by Albert N. Shiryaev ([Shi96]) offers precise mathematical formulations regarding stochastic processes and their spectral representation, e.g., Herglotz's theorem.

In Chapter 2, we introduce OMT for non-negative, real-valued functions. In Chapter 3, we redefine OMT for Hermitian, positive semi-definite matrix-valued functions. In Chapter 4, we give an introduction to one-dimensional signals and their statistical properties. In Chapter 5, we consider multidimensional signals. In Chapter 6, we use our methods from Chapter 3 and apply them to multidimensional signals that we have examined in Chapter 5.

Optimal mass transport

In this chapter, we want to introduce the concept of optimal mass transport (OMT), often simply referred to as "optimal transport". Given two functions f and g that satisfy some assumptions, OMT tries to transport the values or "masses" of f in such a way that we receive q. For example, f could indicate at which position how many goods are currently located and q could indicate where the goods should be located after the transport. This transport should be done in an optimal way, i.e., by transporting as little as possible. By considering how "easy" it is to obtain g from f, we can deduce how similar f and g are. This gives rise to even more exciting applications.

Nowadays, OMT plays an important role in signal processing, see e.g., [FSHE25] and [PLE25]. [Vil03] and [Vil+08], authored by Fields medal winner¹ Cédric Villani, offers a very deep and mathematically profound introduction to OMT. Another publication that includes both basic concepts and different applications of OMT in signal processing and machine learning is $[KPT^{+}17]$.

The problem introduced in this thesis corresponds to the Monge-Kantorovich formulation. However, in Section 2.3.2, we give a short introduction to the Monge formulation.

Before diving into definitions and mathematical details of OMT, we want to start with a simple example.

2.1 Motivation

This section does not contain precise mathematical formulations or reasoning. Instead, it is intended to give a first taste of the terms defined in Section 2.2.

Let us consider two discrete functions² $f, g: \{1, 2, 3, 4\} \to \mathbb{R}_0^+$ with the property

$$\sum_{x=1}^{4} f(x) = \sum_{y=1}^{4} g(y),$$

defined by Table 2.1. The symbol \mathbb{R}_0^+ denotes the non-negative real numbers. The bar graph of this discrete function is shown in Figure 2.1.

x, y	1	2	3	4
$\overline{f(x)} \ g(y)$	1 2	$\frac{3}{\frac{3}{2}}$	2	$\frac{1}{2}$

Table 2.1: We define f and g by stating their values for each element in their domain.

¹https://www.mathunion.org/imu-awards/fields-medal

²In order to match with later notation, the argument of f will be denoted as x and the argument of g will be denoted as y.

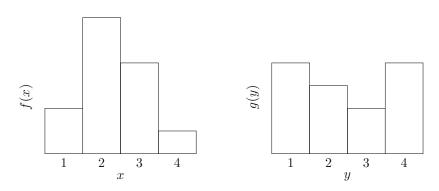


Figure 2.1: Bar graph of f and q

We now want to find out how to deform the first function in order to obtain the second function. Considering the value at each point as mass, we are asking how to move mass of fin order to obtain q. One possible way is shown in Figure 2.2. A suitable way of moving the mass from f so that we obtain g is called transport plan. Such a transport plan can be seen as a function $m:\{1,2,3,4\}\times\{1,2,3,4\}\to\mathbb{R}_0^+$. The mass moved from x to a not necessarily different y is denoted by m(x,y). In Figure 2.2, the values of the transport plan correspond to the height of the moved bars and can be found in Table 2.2. As can be seen in Figure 2.3, a transport plan needs to satisfy

$$\sum_{y=1}^{4} m(x,y) = f(x), \qquad \sum_{x=1}^{4} m(x,y) = g(y)$$
 (2.1)

and an $m:\{1,2,3,4\}\times\{1,2,3,4\}\to\mathbb{R}_0^+$ satisfying these equations is a transport plan.

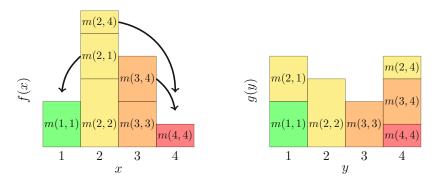


Figure 2.2: Visualization of transport plan m.

Since the "total masses" of the two functions are the same, i.e.,

$$\sum_{x=1}^{4} f(x) = \sum_{y=1}^{4} g(y),$$

it is not surprising that a transport plan exists. However, the transport plan m is not unique,



Transport plan $m(x,y)$								
	y = 1	y = 2	y = 3	y = 4				
x = 1	1	0	0	0				
x = 2	1	$\frac{3}{2}$	0	$\frac{1}{2}$				
x = 3	0	$\bar{0}$	1	$\bar{1}$				
x = 4	0	0	0	$\frac{1}{2}$				

Table 2.2: Values of transport plan m. The mass moved from x to y corresponds to m(x,y).

i.e., there exist other $\widetilde{m} \neq m$ such that

$$\widetilde{m}: \{1, 2, 3, 4\} \times \{1, 2, 3, 4\} \to \mathbb{R}_0^+$$

$$\sum_{y=1}^4 \widetilde{m}(x, y) = f(x), \qquad \sum_{x=1}^4 \widetilde{m}(x, y) = g(y).$$

Since there is more than one transport plan, we want to select the most sensible one. I.e., we seek for a transport plan that moves as little as possible, both in terms of mass and distance. We can implement this by defining costs of transport plans and select the one with the lowest cost. The cost should penalize if we move a lot of mass, i.e., if m(x,y) has a high value, and if we move the mass a long distance, i.e., if |x-y| has a high value. We introduce

$$cost(m) = \sum_{x=1}^{4} \sum_{y=1}^{4} \underbrace{m(x,y)}_{\text{How much}} \cdot \underbrace{|x-y|^2}_{\text{How far do we move?}}.$$

If we do not move anything at all, we have $m \equiv 0$ and hence the cost of m is zero. However, if $f \neq g$, then m will not be a transport plan, i.e., it will not satisfy (2.1).

Optimal mass transport

In this section, we will take our considerations of Section 2.1 and apply it to functions defined on an interval. Hence, we need to consider integrals instead of sums. Our approach is based on the Monge-Kantorovich formulation defined in [NGT14, Section II]. Later, in Section 2.3.1, we will briefly introduce a slightly different version of the Monge-Kantorovich formulation that deals with measures.

Let $f, g : [a, b] \to \mathbb{R}_0^+$ be two functions satisfying

$$\int_{a}^{b} f(x) \, dx = \int_{a}^{b} g(y) \, dy. \tag{2.2}$$

In the spirit of Section 2.1, we want to find a transport plan m, i.e., a function

$$m: [a,b] \times [a,b] \to \mathbb{R}_0^+,$$

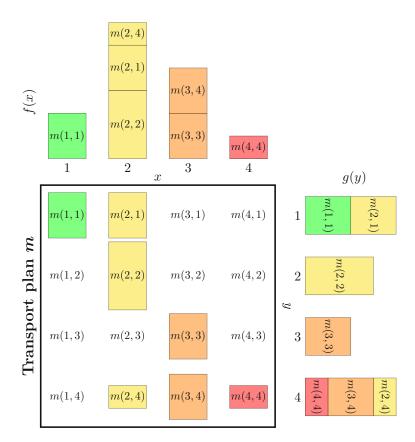


Figure 2.3: The height of each bar represents the value of the transport plan at this position. The functions f and g are the "marginals" of the transport plan m.

satisfying

$$\int_{a}^{b} m(x,y) \, dy = f(x), \qquad \int_{a}^{b} m(x,y) \, dx = g(y). \tag{2.3}$$

Proposition 2.1. Let $f, g : [a, b] \to \mathbb{R}_0^+$ be two functions satisfying (2.2). There exists a transport plan, i.e., there exists a function $m : [a, b] \times [a, b] \to \mathbb{R}_0^+$ satisfying (2.3).

Proof. First, we define $c \in \mathbb{R}_0^+$ as

$$c := \int_{a}^{b} f(x) dx = \int_{a}^{b} g(y) dy.$$

Let us now consider $m:[a,b]\times[a,b]\to\mathbb{R}_0^+$ defined by

$$m(x,y) := \frac{f(x) \cdot g(y)}{c}.$$

We have

$$\int_{a}^{b} \frac{f(x) \cdot g(y)}{c} dy = \frac{f(x)}{c} \cdot \int_{a}^{b} g(y) dy = \frac{f(x)}{c} \cdot c = f(x),$$

$$\int_{a}^{b} \frac{f(x) \cdot g(y)}{c} dx = \frac{g(y)}{c} \cdot \int_{a}^{b} f(x) dx = \frac{g(y)}{c} \cdot c = g(y).$$

Hence, m is a transport plan.

The transport plan defined in the proof of Proposition 2.1 corresponds to distributing the value of each f(x), $x \in [a, b]$ over all $y \in [a, b]$, proportional to the value of g(y), see [Vil03, Introduction - 1].

Since there is at least one transport plan, it makes sense to seek for the "best" of all transport plans, i.e., the one that moves as little as possible in terms of distance and mass. For this purpose, we define the cost of a transport plan as

$$\int_{a}^{b} \int_{a}^{b} d(x, y) m(x, y) dxdy$$

whereat $d:[a,b]\times[a,b]\to\mathbb{R}_0^+$ is a function that gives the cost d(x,y) of moving one unit of mass from the first argument x to the second argument y. It is not required that d is a metric. However, since transport to a close point should be cheaper than transport to a distant point, it makes sense that d behaves similarly to a metric. A common choice of d is $d(x,y) := |x-y|^2$, which we have also chosen in Section 2.1.

For $f, g: [a, b] \to \mathbb{R}_0^+$ satisfying (2.2) and $d: [a, b] \times [a, b] \to \mathbb{R}_0^+$, we define

$$\mathcal{T}_d(f,g) := \inf_{m \in \mathcal{M}(f,g)} \int_a^b \int_a^b d(x,y) m(x,y) \, dx dy \tag{2.4}$$

whereat $\mathcal{M}(f,g)$ denotes the set of all transport plans between f and g. Our function $\mathcal{T}_d(f,g)$ gives the cost of the best transport plan between f and g, i.e., the transport plan with minimal cost. Hence, it acts as a measure of how easily we can transform f in order to obtain g. Thus, it can be seen as a measure of similarity between f and g.

Considering $d(x,y) := |x-y|^2$, we define

$$W_2(f,g) := \left(\inf_{m \in \mathcal{M}(f,g)} \int_a^b \int_a^b |x - y|^2 m(x,y) \, dx dy\right)^{1/2}.$$
 (2.5)

 W_2 is called the 2-Wasserstein metric, see [NGT14, Section II]. The name "Wasserstein metric" might already reveal the statement of the following proposition, see [KPT⁺17, p. $46]^{3}$.

³The notation in [KPT⁺17] is slightly different, see Section 2.3.1. Considering functions whose integrals are the same but not equal to 1, i.e., functions that are not probability densities, do not affect the metric properties, see Remark 2.3.



Proposition 2.2. Let $c \in (0, \infty)$ and let A be defined by

$$\mathcal{A} = \left\{ f : [a, b] \to \mathbb{R}_0^+, \int_a^b f(x) \, \mathrm{d}x = c \right\}.$$

The 2-Wasserstein metric $W_2: \mathcal{A} \times \mathcal{A} \to \mathbb{R}_0^+$ is a metric.

Hence, we have found a metric that allows us to measure the similarity of two functions $f,g\in\mathcal{A}$. We can use this metric to identify functions that are similar to f and g, but we will discuss this idea in detail in Chapter 3.

Remark 2.3. In related literature, e.g., in [NGT14], it is often required that the integrals in (2.2) need to be equal to 1. In that case, our functions are probability densities and many statements become more elegant. For example, in the proof of Proposition 2.1, we could ignore the factor c, since c = 1. However, by simply including such a scaling factor, all formulated statements are true also for our case, i.e., for functions whose integrals are the same but not necessarily equal to 1.

2.3 Other formulations of optimal mass transport

In this section, we want to give another version of the Monge-Kantorovich formulation. Furthermore, we also want to give a very short introduction to the Monge formulation.

2.3.1 Monge-Kantorovich formulation by considering measures

In Section 2.2, we introduced a specific version of the Monge-Kantorovich formulation of OMT, namely by considering $f, g: [a,b] \to \mathbb{R}_0^+$ and $m: [a,b] \times [a,b] \to \mathbb{R}_0^+$. In related literature, e.g., [Vil03], we are not considering such functions on [a, b] but measures on [a, b], i.e., functions on the Borel sets $\mathcal{B}([a,b])$ of [a,b]. Instead of intervals [a,b], we can also choose more general domains. We want to reformulate the Monge-Kantorovich formulation according to [Vil03, Section 1.1.1].

Let $(\Omega_0, \Sigma_0, \mu)$ and $(\Omega_1, \Sigma_1, \nu)$ be two probability spaces and let $d: \Omega_0 \times \Omega_1 \to \mathbb{R}_0^+$ be a measurable function, e.g., a function that penalizes distance. Let $\Pi(\mu, \nu)$ be the set of all probability measures on $\Omega_0 \times \Omega_1$ with marginals μ and ν , i.e.,

$$\Pi(\mu,\nu) := \left\{ \pi : \Sigma_0 \times \Sigma_1 \to \mathbb{R}_0^+, \, \pi(A \times \Omega_1) = \mu(A), \, \pi(\Omega_0 \times B) = \nu(B), \, A \in \Sigma_0, \, B \in \Sigma_1 \right\}.$$

The goal of OMT is finding the infimum

$$\inf_{\pi \in \Pi(\mu,\nu)} \int_{\Omega_0 \times \Omega_1} d(x,y) d\pi(x,y).$$

Using abuse of notation, we can characterize the measures $\pi \in \Pi$ also by the constraint

$$\int_{\Omega_1} 1 d\pi(x, y) = d\mu(x), \qquad \int_{\Omega_0} 1 d\pi(x, y) = d\nu(y),$$

see [Vil03, Introduction - 1]. Considering $\Omega_0 = \Omega_1 = [a, b]$ and f, g, m satisfying (2.2) and (2.3), we have the relation

$$f(x) = d\mu(x), g(y) = d\nu(y) \quad \text{i.e.,} \quad \mu(A) = \int\limits_A f(x) \, dx, \, \nu(B) = \int\limits_B g(y) \, dy,$$

$$m(x,y) = d\pi(x,y) \quad \text{i.e.,} \quad \pi(A \times B) = \int\limits_{A \times B} m(x,y) \, d(x,y),$$

see [KPT⁺17, p. 45]. The advantage of this "measure-version" of Monge-Kantorovich lies in the fact that we can cover more general functions and integration over more general domains, see [KPT $^+$ 17, p. 46]. A "function" f satisfying (2.2) and containing a Dirac delta distribution $\delta(x-s)$ could be realized in the sense of Section 2.3.1 by simply considering a measure μ with $\mu(s) \neq 0$, $s \in [a, b]$.

2.3.2 Monge formulation

Another and even older formulation of OMT is *Monge's* formulation, see [KPT⁺17, p. 45]. Here, two non-negative functions $f:\Omega_0\to\mathbb{R}_0^+,\,g:\Omega_1\to\mathbb{R}_0^+,\,\Omega_0,\Omega_1\subseteq\mathbb{R}^d$ with

$$\int_{\Omega_0} f(x) \, dx = \int_{\Omega_1} g(y) \, dy$$

and a "distance" function $d: \Omega_0 \times \Omega_1 \to \mathbb{R}_0^+$, similar to Section 2.2, are given. Of course, instead of Ω_0, Ω_1 , we can also consider the domain [a, b]. The aim of Monge's formulation is finding the infimum

$$T(f,g) = \inf_{h \in \widetilde{\mathcal{M}}(f,g)} \int_{\Omega_0} d(x,h(x)) f(x) dx$$

where

$$\widetilde{\mathcal{M}}(f,g) := \left\{ h : \int_{x: h(x) \in B} f(x) \, dx = \int_{B} g(y) \, dy \text{ for any } B \subseteq \Omega_{1} \right\}.$$
 (2.6)

This formulation is more restrictive than the Monge-Kantorovich formulation, since for each point x, we transfer the whole mass f(x) only to a single location y, namely to y = h(x), see [KPT⁺17, p. 46]. Hence, it is not surprising that there are cases where there is a transport plan with respect to Proposition 2.1 but no $h \in \mathcal{M}(f,g)$ with respect to (2.6), see [KPT⁺17, p. 45]. Thus, in the following, we are only considering the Monge-Kantorovich formulation.

2.4 Practical considerations regarding transport plans

In this section, the reader should get a first taste of implementation considerations. However, we will not provide any proofs or precise mathematical explanations.

In Section 2.1, we were considering discrete functions and used them as a motivation for Section 2.2, where we were dealing with functions defined on an interval [a,b]. The fact that we are using integrals instead of (weighted) sums has an effect on the structure of the optimal transport plan.

Remark 2.4. Let $f, g: \{x_1, x_2, \dots, x_k\} \to \mathbb{R}_0^+$ be two discrete functions and let the distance between x_{j-1} and x_j be constant for all $j \in \{2, \dots k\}$. If f = g, the optimal transport plan, i.e., the transport plan with the lowest cost, is

$$m(x,y) = \begin{cases} \frac{1}{\Delta} \cdot f(x), & x = y, \\ 0, & x \neq y. \end{cases}$$

In this definition of m, the factor $1/\Delta$ depends on the distance between the elements of the domain. If we consider two functions $f,g:[a,b]\to\mathbb{R}_0^+$ and we have f=g, the optimal "transport plan" would be the "function"

$$m(x,y) = \begin{cases} \delta(0) \cdot f(x), & x = y, \\ 0, & x \neq y. \end{cases}$$

whereat $\delta(.)$ denotes the Dirac delta distribution. Since m is not a function (at least in the classical sense), there is no optimal transport plan m that maps from $[a,b] \times [a,b]$ to the non-negative real numbers \mathbb{R}_0^+ . However, in (2.4), we are seeking for the infimum and not the minimum. Hence, the non-existence of an optimal transport plan $m:[a,b]\times[a,b]\to\mathbb{R}_0^+$ does not necessarily lead to the non-existence of $\mathcal{T}_d(f,g)$. However, considering the formulation and notation in Section 2.3.1, there does exists a suitable π .

When numerically computing the optimal transport cost, we do not have to deal with these considerations, as we will explain soon. But first, we want to define the discretization of a function.

Definition 2.5 (Discretization). Let X be a set, $f:[a,b] \to X$ and $n \in \mathbb{N}$. Consider $x_1 = a, x_n = b$ and $x_j \in [a, b]$ with $x_{j-1} < x_j$ for each $j \in \{2, \ldots, n\}$. The discretization $f_{\mathrm{dis}}: \{x_1, \dots x_n\} \to X$ of f is the function defined by

$$f_{\rm dis}(x_i) = f(x_i)$$

for each $j \in \{1, ..., n\}$. Unless otherwise specified, we will only consider uniformly distributed discretizations, i.e., we furthermore require $x_j - x_{j-1} = \text{const}, j \in \{2, \ldots, n\}$.

If we want to numerically compute the optimal transport plan between two functions $f,g:[a,b]\to\mathbb{R}_0^+$, we always consider discretizations $f_d,g_d:\{x_1,\ldots,x_n\}\to\mathbb{R}_0^+$ instead of our given f and g that are defined on a continuum. Hence, the integrals in (2.3) and (2.4)are weighted sums instead of integrals. We will discuss this in more detail in Section 3.7.2. Thus, our optimal transport plan does not contain any Dirac delta distributions.

In Figure 2.4 and Figure 2.5, we can see two functions f and g and the corresponding optimal transport plan calculated by considering the discretizations of f and g with n = 80. The transport plan is a function $m: \{x_1 = 0, \dots, x_{80} = 1\} \times \{x_1 = 0, \dots, x_{80} = 1\} \to \mathbb{R}_0^+$. We can see that m(x,y)=0 for most pairs $(x,y)\in\{x_1,\ldots,x_{80}\}\times\{x_1,\ldots,x_{80}\}$. This is not surprising, since the optimal transport plan of such a problem has support on a thin set, see [NGT14, Section II, Section IV]. For a detailed and mathematically profound explanation of this phenomenon, see [Vil03, Theorem 2.44] and the required preliminaries in [Vil03].

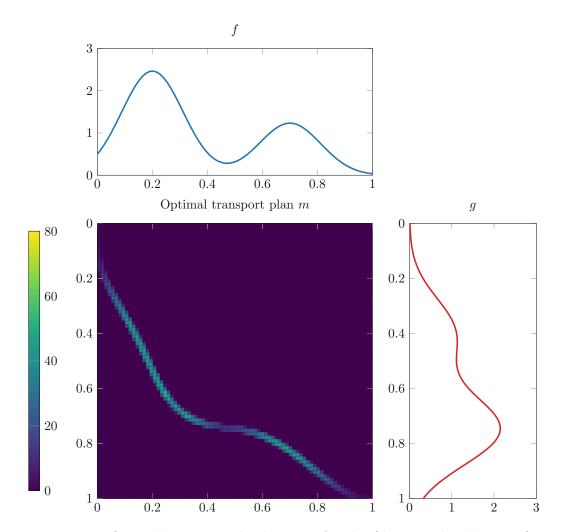


Figure 2.4: Optimal transport plan between f and g (discretized with n = 80).

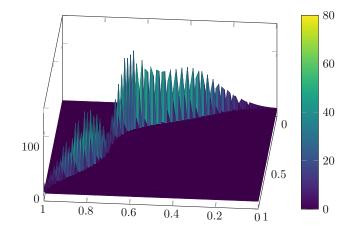


Figure 2.5: 3D view of the transport plan of Figure 2.4.

Optimal mass transport of matrix-valued functions

In Chapter 2, we introduced optimal mass transport between two non-negative, real-valued functions $f,g:[a,b]\to\mathbb{R}_0^+$, $[a,b]\subseteq\mathbb{R}$. In the current chapter, we want to consider a different, even bigger class of functions. The considered functions will map to the Hermitian, positive semi-definite $n \times n$ matrices, $n \in \mathbb{N}$. We will see that the functions of Chapter 2 are a subset of the functions of Chapter 3. However, we need to find a more general definition of transport plan and cost.

The methods in this chapter, in particular in Section 3.1, Section 3.3, Section 3.4, Section 3.5 and Section 3.6, are strongly based on the paper On Matrix-Valued Monge-Kantorovich Optimal Mass Transport by L. Ning, T. Georgiou and A. Tannenbaum, see [NGT14].

3.1 A modified version of optimal mass transport

First, we want to remind the reader of two definitions and two propositions, see [Joh21, Section 1.1, Section 2.1, Section 2.2].

Definition 3.1 (Hermitian matrix). A matrix $A \in \mathbb{C}^{n \times n}$ is called Hermitian matrix or self-adjoint matrix if $A = A^*$, where A^* is the conjugate transpose of A.

Considering Definition 3.1, we see that for each diagonal entry $a_{ii} \in \mathbb{C}$, we have $a_{ii} = \overline{a_{ii}}$. Thus, all diagonal entries a_{ii} , $i \in \{1, ..., n\}$ of an Hermitian matrix are real-valued.

Proposition 3.2 (Eigenvalues of Hermitian matrices). Let $A \in \mathbb{C}^{n \times n}$ be an Hermitian matrix. All eigenvalues of A are real-valued.

If $A \in \mathbb{C}^{n \times n}$ is an Hermitian matrix, then z^*Az is real-valued for any $z \in \mathbb{C}^n$, see [Wer22]. Hence, the following definition is well-defined.

Definition 3.3 (Positive semi-definite matrix). Let $A \in \mathbb{C}^{n \times n}$ be an Hermitian matrix. A is called a positive semi-definite matrix, if we have

$$z^*Az \ge 0 \tag{3.1}$$

for all $z \in \mathbb{C}^n$. If A is positive semi-definite, we denote this by $A \succeq 0$. We denote the set of all $A \succeq 0$ of size $n \times n$ by H_+^n .

Proposition 3.4 (Eigenvalues of positive semi-definite matrices). Let $A \in \mathbb{C}^{n \times n}$ be an Hermitian matrix. $A \succeq 0$ if and only if all eigenvalues of A are non-negative.

We now consider $c \in (0, +\infty)$ and

$$\mathcal{F}_c := \left\{ \mu : [a, b] \to \mathbb{C}^{n \times n} \middle| \mu(x) \in H^n_+, \int_a^b \operatorname{tr}(\mu(x)) \, dx = c \right\}, \tag{3.2}$$

i.e., the set of all functions that map from an interval $[a,b] \subseteq \mathbb{R}$ to the Hermitian, positive semi-definite matrices and have the additional property, that the integral of the trace of the function is equal to c. The trace of an $n \times n$ matrix A is the sum of its n diagonal entries or, equivalently, the sum of its n (not necessarily unique) eigenvalues, see e.g., [Axl24]. We can interpret the trace of a matrix as the "mass" of the matrix, i.e., a scalar value, that indicates how large the eigenvalues are. Hence, all functions in \mathcal{F} have the same "total mass", i.e., the integrals of the sum of the eigenvalues of the matrix-values are the same.

For the case n=1, we have $H_+^1=\mathbb{R}_0^+$ and $\operatorname{tr}(\mu(x))=\mu(x)$. Hence, the functions considered in (2.2) can be seen as a special case of (3.2).

We now want to develop similar methods as in Chapter 2 for elements of \mathcal{F}_c . So let $\mu_0, \mu_1 \in \mathcal{F}_c$. Following the idea of the previous chapter, we would now want to find $m:[a,b]\times[a,b]\to H^n_+$ or at least $m:[a,b]\times[a,b]\to\mathbb{C}^{n\times n}$ with

$$\int_{a}^{b} m(x,y) \, dy = \mu_0(x), \qquad \int_{a}^{b} m(x,y) \, dx = \mu_1(y). \tag{3.3}$$

In contrast to Chapter 2, such an m does not always exist, see [NGT14, Section III-B] or Example 3.5.

Example 3.5. Let $[a,b] \subseteq \mathbb{R}$ be an interval and consider two constant functions $\mu_0, \mu_1, \mu_2, \mu_3, \mu_4, \mu_5$

$$\mu_0(x) = \begin{pmatrix} \frac{1}{b-a} & 0\\ 0 & 0 \end{pmatrix}, \qquad \mu_1(y) = \begin{pmatrix} 0 & 0\\ 0 & \frac{1}{b-a} \end{pmatrix}.$$

It can be readily verified that $\mu_0, \mu_1 \in \mathcal{F}_1$. We want to find $m: [a,b] \times [a,b] \to H^n_+$ such that (3.3) is satisfied. Considering the first entry $m_{11}(x,y)$ of the matrix m(x,y), we want in particular that

$$\int_{a}^{b} m_{11}(x,y) \, dy = \frac{1}{b-a}, \qquad \int_{a}^{b} m_{11}(x,y) \, dx = 0.$$

It follows

$$\int_{a}^{b} \int_{a}^{b} m_{11}(x,y) \, dy dx = \int_{a}^{b} \frac{1}{b-a} \, dx = 1 \neq 0 = \int_{a}^{b} 0 \, dy = \int_{a}^{b} \int_{a}^{b} m_{11}(x,y) \, dx dy$$

which contradicts Theorem of Fubini¹, see e.g., [Els18, Chapter V, Theorem 2.1]. Thus, there is no $m:[a,b]\times[a,b]\to H^n_+$ or $m:[a,b]\times[a,b]\to\mathbb{C}^{n\times n}$ that satisfies (3.3).



¹In order to be very stringent, we have to consider the Riemann integral as a Lebesgue integral.

This example illustrates that it is not enough to just move the values (i.e. the matrices) from x to y. However, it also shows that it might be useful to include the possibility of rotating the matrix-values, so that we can obtain

$$\begin{pmatrix} 0 & 0 \\ 0 & \frac{1}{b-a} \end{pmatrix} \text{ from rotating } \begin{pmatrix} \frac{1}{b-a} & 0 \\ 0 & 0 \end{pmatrix}.$$

Hence, we will try to find transport plans in a "bigger space". For this purpose, we need to examine tensor products.

Tensor products, Kronecker products, partial trace

In this section, we want to provide the required knowledge about tensor products and related mathematical concepts. Tensor products are a very abstract concept and it is not easy to depict them in a descriptive way. However, [Joh21] and [RAG05] offer introductions to this topic worth reading. First, we want to give a general definition of tensor products, see [Izm23, Definition 5.38].

Definition 3.6 (Tensor product). Let V, W, Z be vector spaces. The tensor product of Vand W is a vector space $V \otimes W$ together with a map $\varphi: V \times W \to V \otimes W$ such that for any bilinear map $h: V \times W \to Z$ there is a unique linear map $h: V \otimes W \to Z$ such that $h = h \circ \varphi$, see Figure 3.1.

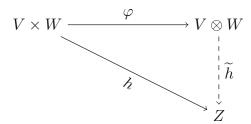


Figure 3.1: For each bilinear map $h: V \times W \rightarrow Z$ there exists a unique linear map $\widetilde{h}: V \otimes W \to Z$ such that $h = \widetilde{h} \circ \varphi$

In the following, we will denote the vector space $V \otimes W$ as a tensor product without mentioning the map φ . It can be shown that for any vector spaces V, W, there exists a tensor product $V \otimes W$ and it is unique up to isomorphism, see [Joh21, Section 3.3.2]. Hence, it makes sense to consider "the" tensor product of two vector spaces.

The elements of the tensor product are called tensors. For each $v \in V, w \in W$, the element $v \otimes w := \varphi(v \times w)$ is a tensor. Tensors of the form $v \otimes w$ are called decomposable tensors or elementary tensors, see [RAG05, Chapter 14, p. 345] and [Joh21, Definition 3.3.1]. However, not every tensor is an elementary tensor, but every tensor can be written as a linear combination of elementary tensors, see [Joh21, Theorem 3.3.1] and [RAG05, Chapter 14, p. 345].

Definition 3.6 might seem very abstract. However, if our considered vector spaces are of the form \mathbb{C}^n or $\mathbb{C}^{n\times m}$, the introduced objects are becoming more concrete. But first, we need to introduce the Kronecker product $A \otimes B$ of two matrices $A \in \mathbb{C}^{m \times n}$ and $B \in \mathbb{C}^{p \times q}$. see [Joh21, Definition 3.1.1].

Definition 3.7 (Kronecker product). Let $A \in \mathbb{C}^{m \times n}$ and $B \in \mathbb{C}^{p \times q}$ be two matrices. The Kronecker product $A \otimes B$ of A and B is the block matrix

$$A \otimes B := \begin{pmatrix} a_{11}B & \dots & a_{1n}B \\ \vdots & \ddots & \vdots \\ a_{n1}B & \dots & a_{nn}B \end{pmatrix} \in \mathbb{C}^{(m \cdot p) \times (n \cdot q)}$$

whereat a_{jk} denotes the (j,k)-entry of A.

The symbol "\oting" in Definition 3.7 denotes something different than before, i.e., the Kronecker product and not the tensor product. However, it is no coincidence that the symbols coincide. Since we can interpret vectors in \mathbb{C}^n as matrices with dimension (n,1) or (1,n), Definition 3.7 can be also used for two vectors $v \in \mathbb{C}^n$, $w \in \mathbb{C}^m$.

Let us consider vector spaces of the form $V = \mathbb{C}^n$, $W = \mathbb{C}^m$. The elementary tensors of the tensor product $\mathbb{C}^n \otimes \mathbb{C}^m$ are up to isomorphism exactly the Kronecker products $v \otimes w$ of $v \in \mathbb{C}^n$, $w \in \mathbb{C}^m$ and the tensor product $\mathbb{C}^n \otimes \mathbb{C}^m$ is the vector space $\mathbb{C}^{n \cdot m}$, see [Joh21, Section 3.3.2]. Since $\mathbb{C}^{k \times \ell} \cong \mathbb{C}^{k\ell}$, analogous properties hold for vector spaces of the form $V = \mathbb{C}^{n \times m}, W = \mathbb{C}^{p \times q}.$

We now want to define the partial trace, see [Joh21, Section 3.A.2]. In order to match with our future notation, we only define it for tensors in $\mathbb{C}^{n\times n}\otimes\mathbb{C}^{n\times n}$. We want to note that $\mathbb{C}^{n\times n}\otimes\mathbb{C}^{n\times n}\cong\mathbb{C}^{n^2}\otimes\mathbb{C}^{n^2}\cong\mathbb{C}^{n^2n^2}\cong\mathbb{C}^{n^2\times n^2}$.

Definition 3.8 (Partial trace). We define the partial traces $\operatorname{tr}_0: \mathbb{C}^{n \times n} \otimes \mathbb{C}^{n \times n} \to \mathbb{C}^{n \times n}$ and $\operatorname{tr}_1: \mathbb{C}^{n\times n} \otimes \mathbb{C}^{n\times n} \to \mathbb{C}^{n\times n} \ by$

$$\operatorname{tr}_0(A \otimes B) := (\operatorname{tr} \otimes I_n)(A \otimes B) := \operatorname{tr}(A) \otimes I_n(B) = \operatorname{tr}(A) \cdot B$$

$$\operatorname{tr}_1(A \otimes B) := (I_n \otimes \operatorname{tr})(A \otimes B) := I_n(A) \otimes \operatorname{tr}(B) = \operatorname{tr}(B) \cdot A$$

for all $A, B \in \mathbb{C}^{n \times n}$. Here, tr(M) denotes the well-known trace of a square matrix M and $I_n(M)$ denotes the identity of an $n \times n$ matrix M.

Although we have only defined the partial traces in an explicit way for elementary tensors, i.e., tensors of the form $A \otimes B \in \mathbb{C}^{n \times n} \otimes \mathbb{C}^{n \times n}$ with $A, B \in \mathbb{C}^{n \times n}$, the partial traces are still well-defined for each tensor in $\mathbb{C}^{n\times n}\otimes\mathbb{C}^{n\times n}$, see [Joh21, Section 3.A.2].

Example 3.9. Let us consider the block matrix

$$A = \begin{pmatrix} A_{11} & \dots & A_{1n} \\ \vdots & \ddots & \vdots \\ A_{n1} & \dots & A_{nn} \end{pmatrix} \in \mathbb{C}^{n^2 \times n^2}$$

whereat each block A_{jk} , $j,k \in \{1,\ldots n\}$, is an $n \times n$ matrix. The partial traces tr_0 and tr_1 of A are

$$\operatorname{tr}_{0}\begin{pmatrix} A_{11} & \dots & A_{1n} \\ \vdots & \ddots & \vdots \\ A_{n1} & \dots & A_{nn} \end{pmatrix} = A_{11} + A_{22} + A_{33} + \dots + A_{nn} \quad \in \mathbb{C}^{n \times n}$$

$$\operatorname{tr}_{1}\begin{pmatrix} A_{11} & \dots & A_{1n} \\ \vdots & \ddots & \vdots \\ A_{n1} & \dots & A_{nn} \end{pmatrix} = \begin{pmatrix} \operatorname{tr}(A_{11}) & \dots & \operatorname{tr}(A_{1n}) \\ \vdots & \ddots & \vdots \\ \operatorname{tr}(A_{n1}) & \dots & \operatorname{tr}(A_{nn}) \end{pmatrix} \quad \in \mathbb{C}^{n \times n},$$

see [Joh21, Section 3.A.2].

We want to state a proposition, see [Joh21, Theorem 3.1.3].

Proposition 3.10. Let $A, B \in \mathbb{C}^{n \times n}$. If $A, B \succeq 0$, then $A \otimes B \succeq 0$.

Proposition 3.11. Let $A \in \mathbb{C}^{n^2 \times n^2}$ be a block matrix,

$$A = \begin{pmatrix} A_{11} & \dots & A_{1n} \\ \vdots & \ddots & \vdots \\ A_{n1} & \dots & A_{nn} \end{pmatrix} \in \mathbb{C}^{n^2 \times n^2}$$

whereat each block A_{jk} , $j, k \in \{1, ... n\}$, is an $n \times n$ matrix.

- (a) We have $\operatorname{tr}(\operatorname{tr}_0(A)) = \operatorname{tr}(\operatorname{tr}_1(A)) = \operatorname{tr}(A)$.
- (b) If $A \succeq 0$, then $\operatorname{tr}_0(A) \succeq 0$.
- (c) If $A \succeq 0$, then $\operatorname{tr}_1(A) \succeq 0$.

(a) This follows immediately from Example 3.9.

(b) For each $z = (z_1^T, \dots, z_n^T)^T \in \mathbb{C}^{n^2}$ with $z_j \in \mathbb{C}^n$, $j \in \{1, \dots, n\}$, we have $z^*Az \geq 0$. Let $j \in \{1, \dots n\}$. For each $w \in \mathbb{C}^n$, we have

$$w^* A_{ij} w = z^* A z \ge 0, \tag{3.4}$$

whereat $z = (z_1^T, \dots, z_n^T)^T$ with $z_j = w$ and $z_k = 0 \in \mathbb{C}^n$, $k \neq j$. Hence, A_{jj} is positive semi-definite and thus $\sum_{j=1}^n A_{jj}$ is positive semi-definite as well.

(c) See [Zha12, Theorem 2.1] in combination with Example 3.9.



3.3 A transport plan

After our interlude in the world of tensors, we now want to come back to our quest for a transport plan. So let us reconsider $\mu_0, \mu_1 \in \mathcal{F}_c$. As already seen in Example 3.5, there is not always an $m:[a,b]\times[a,b]\to H^n_+$ satisfying

$$\int_{a}^{b} m(x, y) \, dy = \mu_0(x), \qquad \int_{a}^{b} m(x, y) \, dx = \mu_1(y).$$

Thus, we are now trying to find a function m that maps to a "bigger" space and has similar properties as the transport plans in Chapter 2.

We attempt to find an m that maps to the tensor product space $\mathbb{C}^{n\times n}\otimes\mathbb{C}^{n\times n}\cong\mathbb{C}^{n^2\times n^2}$. In detail, we define a transport plan between $\mu_0 \in \mathcal{F}_c$ and $\mu_1 \in \mathcal{F}_c$ as a function m satisfying

- 1. $m: [a,b] \times [a,b] \to \mathbb{C}^{n^2 \times n^2}$
- 2. $m(x,y) \succeq 0$ for each $x,y \in [a,b]$.
- 3. The integrals of the partial traces are μ_0 and μ_1 , i.e.,

$$\int_{a}^{b} \operatorname{tr}_{1}(m(x,y)) \, dy = \mu_{0}(x), \qquad \int_{a}^{b} \operatorname{tr}_{0}(m(x,y)) \, dx = \mu_{1}(y). \tag{3.5}$$

Example 3.12. Let $\mu_0, \mu_1 \in \mathcal{F}_c$ and consider $m : [a, b] \times [a, b] \to \mathbb{C}^{n^2 \times n^2}$ defined by

$$m(x,y) := \frac{1}{c} (\mu_0(x) \otimes \mu_1(y)).$$

Since $\mu_0(x)$ and $\mu_1(y)$ are positive semi-definite, $\frac{1}{c}(\mu_0(x)\otimes\mu_1(y))$ is also positive semi-definite, see Proposition 3.10. Furthermore, we have

$$\int_{a}^{b} \operatorname{tr}_{1}\left(\frac{\mu_{0}(x) \otimes \mu_{1}(y)}{c}\right) dy = \frac{1}{c} \int_{a}^{b} \mu_{0}(x) \operatorname{tr}(\mu_{1}(y)) dy = \frac{\mu_{0}(x)}{c} \int_{a}^{b} \operatorname{tr}(\mu_{1}(y)) dy = \mu_{0}(x),$$

$$\int_{a}^{b} \operatorname{tr}_{0}\left(\frac{\mu_{0}(x) \otimes \mu_{1}(y)}{c}\right) dx = \frac{1}{c} \int_{a}^{b} \operatorname{tr}(\mu_{0}(x)) \mu_{1}(y) dx = \frac{\mu_{1}(y)}{c} \int_{a}^{b} \operatorname{tr}(\mu_{0}(x)) dx = \mu_{1}(y).$$

Hence, $m:(x,y)\mapsto \frac{1}{c}(\mu_0(x)\otimes\mu_1(y))$ is a transport plan.

Since tensor products and partial traces are not very descriptive, the transport plan for matrix-valued functions is not as intuitive as for real-valued functions. However, our new definition of transport plans provides for any arbitrary functions $\mu_0, \mu_1 \in \mathcal{F}_c$ at least one transport plan, see Example 3.12. Furthermore, equation (3.5) is strongly reminiscent to (2.3) in Chapter 2.

3.4 Transport cost

Since we just have shown that there always exists a transport plan (with respect to its definition in the previous section), we are now interested in finding an optimal transport plan. Similar to Section 2.2, we first introduce a cost that penalizes moving.

1. We want to consider how much we are moving from $x \in [a, b]$ to $y \in [a, b]$. In Section 2.2, m(x,y) indicated the amount of mass that we are moving from x to y. Now, we consider

as the mass that is moved from x to y.

For example, if $m(x,y) = \frac{1}{c}(\mu_0(x) \otimes \mu_1(y))$, then $\operatorname{tr}(m(x,y)) = \frac{1}{c}(\operatorname{tr}(\mu_0(x)) \cdot \operatorname{tr}(\mu_1(y)))$, see [Joh21, Theorem 3.1.3].

2. We want to consider how far we are moving from $x \in [a, b]$ to $y \in [a, b]$, so how far x and y are apart. For this purpose, we consider the square of the euclidean distance,

$$|x-y|^2$$
.

3. We want to consider the directionality mismatch between $\operatorname{tr}_1(m(x,y))$ and $\operatorname{tr}_0(m(x,y))$. Hence, we are asking if the values of the entries of the matrices $tr_1(m(x,y))$ and $\operatorname{tr}_0(m(x,y))$ are differently distributed with respect to the different entries.

For example, the matrices

$$A = \begin{pmatrix} 1 & 0 \\ 0 & 0 \end{pmatrix} \qquad \text{and} \qquad B = \begin{pmatrix} \frac{8}{10} & 0 \\ 0 & \frac{2}{10} \end{pmatrix}$$

are both positive semi-definite and their highest values are at their top left entries A_{11} and B_{11} , respectively. Hence, their directional mismatch is low. However, the highest values of the two positive semi-definite matrices

$$A = \begin{pmatrix} 1 & 0 \\ 0 & 0 \end{pmatrix} \qquad \text{and} \qquad B = \begin{pmatrix} \frac{1}{10} & \frac{2}{10} \\ \frac{2}{10} & \frac{9}{10} \end{pmatrix}$$

are clearly at different entries (i.e., at A_{11} and B_{22}), hence their directional mismatch is high.

This approach is also connected to the directional mismatch of the eigenvectors of the matrices A and B.

We can quantify the mismatch by considering the squared Frobenius norm² of the difference of the two matrices $\operatorname{tr}_1(m(x,y))$ and $\operatorname{tr}_0(m(x,y))$. In order to not be affected

The Frobenius norm $||A||_F$ of a matrix $A = (a_{jk})_{j \in \{1,...,n\}, k \in \{1,...,m\}} \in \mathbb{C}^{n \times m}$ is defined as the square root of the sum of the squared absolute values of all entries, i.e., $||A||_F = (\sum_{j=1}^n \sum_{k=1}^m |a_{jk}|^2)^{1/2}$, see [Joh21].

by the mass of the matrix (or the length of the eigenvectors), we normalize $\operatorname{tr}_1(m(x,y))$ and $\operatorname{tr}_0(m(x,y))$ by $\operatorname{tr}(m(x,y))$.

For example, for $m(x,y) = \frac{1}{c}(\mu_0(x) \otimes \mu_1(y))$, we have

$$\frac{\operatorname{tr}_{0}(m(x,y))}{\operatorname{tr}(m(x,y))} = \frac{1}{c} \cdot \frac{\operatorname{tr}(\mu_{0}(x)) \cdot \mu_{1}(y)}{\operatorname{tr}(\mu_{0}(x)) \cdot \operatorname{tr}(\mu_{1}(y))} = \frac{1}{c} \cdot \frac{\mu_{1}(y)}{\operatorname{tr}(\mu_{1}(y))}$$
$$\frac{\operatorname{tr}_{1}(m(x,y))}{\operatorname{tr}(m(x,y))} = \frac{1}{c} \cdot \frac{\mu_{0}(x) \cdot \operatorname{tr}(\mu_{1}(y))}{\operatorname{tr}(\mu_{0}(x)) \cdot \operatorname{tr}(\mu_{1}(y))} = \frac{1}{c} \cdot \frac{\mu_{0}(x)}{\operatorname{tr}(\mu_{0}(x))}$$

Considering both the squared Frobenius norm and the normalization, we get

$$\left\| \frac{\operatorname{tr}_0(m(x,y))}{\operatorname{tr}(m(x,y))} - \frac{\operatorname{tr}_1(m(x,y))}{\operatorname{tr}(m(x,y))} \right\|_F^2$$

We now want to combine these three different factors of moving cost and evaluate it for all pairs (x,y) in $[a,b] \times [a,b]$. This gives rise to our definition of the cost of a transport plan m:

$$cost(m) = \int_{a}^{b} \int_{a}^{b} \left(\underbrace{|x-y|^{2}}_{\text{distance}} + \lambda \cdot \underbrace{\left\| \frac{\operatorname{tr}_{0}(m(x,y))}{\operatorname{tr}(m(x,y))} - \frac{\operatorname{tr}_{1}(m(x,y))}{\operatorname{tr}(m(x,y))} \right\|_{F}^{2}}_{\text{direction}} \right) \cdot \underbrace{\operatorname{tr}(m(x,y))}_{\text{mass}} dxdy \quad (3.6)$$

The scalar $\lambda \in (0, +\infty)$ acts as a weighting factor between the impact of the distance cost and the directional cost. Similar to the examples in [NGT14, Section V], we will choose $\lambda = 1/10$ when implementing the method in Chapter 6.

3.5 A distance between μ_0 and μ_1

Let $c \in (0, +\infty)$ and let $\mu_0, \mu_1 \in \mathcal{F}_c$. Considering the cost of a transport plan m, see (3.6), we now define

$$\mathcal{T}_{2,\lambda}(\mu_0, \mu_1) := \inf_{m \in \mathcal{M}(\mu_0, \mu_1)} \operatorname{cost}(m)$$
(3.7)

whereat $\mathcal{M}(\mu_0, \mu_1)$ denotes the set of all transport plans between μ_0 and μ_1 . In Example 3.12, we have already shown that $\mathcal{M}(\mu_0, \mu_1) \neq \emptyset$. As in Chapter 2, we can interpret the cost of the optimal transport plan between μ_0 and μ_1 as a measure of similarity or distance between μ_0 and μ_1 . For $\mu_0, \mu_1 \in \mathcal{F}_c$, we have

- 1. $\mathcal{T}_{\lambda,2}(\mu_0,\mu_1) = \mathcal{T}_{\lambda,2}(\mu_1,\mu_0)$
- 2. $\mathcal{T}_{\lambda,2}(\mu_0,\mu_1) \geq 0$
- 3. $\mathcal{T}_{\lambda,2}(\mu_0,\mu_1) = 0$ if and only if $\mu_0 = \mu_1$,



see [NGT14, Section IV]³. However, the triangle inequality does not hold in general. Thus, $\mathcal{T}_{\lambda,2}$ is not a metric. We want to recall that the 2-Wasserstein metric in Section 2.2 was indeed a metric.

To determine $\mathcal{T}_{\lambda,2}(\mu_0,\mu_1)$, we have to find an infimum of the costs of all transport plans. Hence, finding $\mathcal{T}_{\lambda,2}(\mu_0,\mu_1)$ is an optimization problem. Next, we want to introduce a specific class of optimization problems, see [BV09, Section 4.2.1].

Definition 3.13. An optimization problem is called convex if it is of the form

minimize
$$f_0(x)$$

subject to $f_i(x) \le 0$, $i \in \{1, ..., m\}$
 $h_i(x) = 0$, $i \in \{1, ..., p\}$

where f_0, \ldots, f_m are convex functions and h_1, \ldots, h_p are affine functions.

Convex optimization problems behave nicely: There are fast algorithms for solving convex optimization problems and every local minimizer is also a global minimizer, see [BV09, Section 1.2.1, Section 4.2.2].

The cost in (3.6) can be rewritten as

$$cost(m) = \int_{a}^{b} \int_{a}^{b} |x - y|^{2} \cdot tr(m(x, y)) + \lambda \cdot \frac{\|tr_{0}(m(x, y)) - tr_{1}(m(x, y))\|_{F}^{2}}{tr(m(x, y))} dxdy.$$

Since for each transport plan m, the partial traces $\operatorname{tr}_0(m(x,y))$ and $\operatorname{tr}_1(m(x,y))$ are positive semi-definite and $\operatorname{tr}(\operatorname{tr}_0(m(x,y))) = \operatorname{tr}(\operatorname{tr}_1(m(x,y))) = \operatorname{tr}(m(x,y))$ for each $x,y \in [a,b]$, see Proposition 3.11 (b),(c) and Proposition 3.11 (a), $\mathcal{T}_{\lambda,2}(\mu_0,\mu_1)$ is lower bounded by the minimal value of the optimization problem

minimize
$$\int_{a}^{b} \int_{a}^{b} |x-y|^{2} \cdot m_{tr}(x,y) + \lambda \cdot \frac{\|m_{0}(x,y) - m_{1}(x,y)\|_{F}^{2}}{m_{tr}(x,y)} dxdy$$

subject to $m_{0}, m_{1} : [a,b] \times [a,b] \to \mathbb{C}^{n \times n}, \ m_{tr} : [a,b] \to \mathbb{R}_{0}^{+},$
 $m_{0}(x,y), m_{1}(x,y) \succeq 0 \text{ for each } x,y \in [a,b],$
 $\operatorname{tr}(m_{0}(x,y)) = \operatorname{tr}(m_{1}(x,y)) = m_{tr}(x,y) \text{ for each } x,y \in [a,b],$
 $\int_{a}^{b} m_{0}(.,y) dy = \mu_{0}, \quad \int_{a}^{b} m_{1}(x,.) dx = \mu_{1}.$ (3.8)

However, for an optimal solution $\widehat{m}_0, \widehat{m}_1, \widehat{m}_{tr}$ of (3.8), the tensor $\widehat{m} := \widehat{m}_0 \otimes \widehat{m}_1$ is a valid transport plan, i.e., $\widehat{m} \in \mathcal{M}(\mu_0, \mu_1)$, and $\operatorname{tr}(\widehat{m}(x, y)) = \widehat{m}_{\operatorname{tr}}(x, y)$. Thus, the optimal cost of our original problem (3.7) is the same as the optimal cost of our new optimization problem (3.8).

³In [NGT14], we are only dealing with elements of \mathcal{F}_1 . However, we can scale elements of \mathcal{F}_c by 1/c, so that they are elements of \mathcal{F}_1 . This clearly has no effects on the three statements. Hence, the statements are also valid for elements of \mathcal{F}_c , $c \in (0, +\infty)$.

The optimization problem (3.8) is convex, see [NGT14, Section III-D]. Hence, we can efficiently find the optimal value of (3.8) and therefore also $\mathcal{T}_{\lambda,2}(\mu_0,\mu_1)$. In (3.7), we had to optimize over positive semi-definite $n^2 \times n^2$ matrices. In (3.8), we are optimizing over positive semi-definite $n \times n$ matrices. Thus, because of the lower dimensionality, the computational effort is further reduced.

When implementing $\mathcal{T}_{\lambda,2}$ in Chapter 6, we will therefore solve (3.8) instead of (3.7).

3.6 An intermediate function $\mu_{0.5}$

Given two functions $\mu_0, \mu_1 \in \mathcal{F}_c$, we can determine a distance between f and g that measures the degree of similarity, namely by computing $\mathcal{T}_{\lambda,2}(\mu_0,\mu_1)$. Next, we want to find a function that is as similar as possible to both μ_0 and μ_1 . Since we expect that this function is a mixture between μ_0 and μ_1 , we denote this function as $\mu_{0.5}$. In terms of formulas, we want to determine $\mu_{0.5} \in \mathcal{F}_c$ with

$$\mu_{0.5} = \underset{\mu \in \mathcal{F}_c}{\operatorname{arg\,min}} \left(\mathcal{T}_{\lambda,2}(\mu_0, \mu) + \mathcal{T}_{\lambda,2}(\mu, \mu_1) \right).$$

Finding $\mu_{0.5}$ is a convex optimization problem, see [NGT14, Section V-A]. Before discussing if $\mu_{0.5}$ lies in the middle of μ_0 and μ_1 with respect to $\mathcal{T}_{\lambda,2}$, we want to consider two examples:

Example 3.14. Let (X,d) be a metric space and $x,y \in X$. In particular, d satisfies the triangle inequality. We have

$$d(x,x) + d(x,y) = d(x,y) + d(y,y) = d(x,y) \stackrel{\triangle}{\leq} d(x,z) + d(z,y)$$

for each $z \in X$. Thus, both z = x and z = y minimize the sum

$$d(x,z) + d(z,y)$$
.

Example 3.15. Let $d_2: \mathbb{C} \times \mathbb{C} \to \mathbb{R}_0^+$ be the euclidean metric and let $d_2^2: \mathbb{C} \times \mathbb{C} \to \mathbb{R}_0^+$ be its square. We will not prove the following statement, but one can verify that d_2^2 does not satisfy the triangle inequality anymore and that the sum

$$d_2^2(x,z) + d_2^2(z,y)$$

gets minimized by z = (x + y)/2, but not by z = x or z = y, assuming that $x \neq y$. In fact, z = (x + y)/2 is the only minimizer.

In contrast to Example 3.14, $\mathcal{T}_{\lambda,2}$ does not satisfy the triangle inequality. It also cannot be written as the square of some metric, see [NGT14, Section IV], but we still hope that it behaves similar as d_2^2 in Example 3.15, i.e., that our minimizer $\mu_{0.5}$ lies in the middle of μ_0 and μ_1 (in terms of $\mathcal{T}_{\lambda,2}$). When computing $\mu_{0.5}$ in Section 6.2, we have

$$\frac{\mathcal{T}_{\lambda,2}(\mu_0,\mu_{0.5})}{\mathcal{T}_{\lambda,2}(\mu_0,\mu_{0.5}) + \mathcal{T}_{\lambda,2}(\mu_{0.5},\mu_1)} = 0.500968, \quad \frac{\mathcal{T}_{\lambda,2}(\mu_{0.5},\mu_1)}{\mathcal{T}_{\lambda,2}(\mu_0,\mu_{0.5}) + \mathcal{T}_{\lambda,2}(\mu_{0.5},\mu_1)} = 0.499032.$$

Hence, at least in our example, we have $\mathcal{T}_{\lambda,2}(\mu_0,\mu_{0.5}) \approx \mathcal{T}_{\lambda,2}(\mu_{0.5},\mu_1)$ and thus $\mu_{0.5}$ is indeed in the middle of μ_0 and μ_1 .



3.7 Implementation and Coding

In this section, we discuss theoretical considerations on the numerical implementation of the previous methods. Later, in Chapter 6, we will use MATLAB to compute solutions of given problems and present them in plots.

3.7.1 Functions and dimensions

When implementing a function over an interval [a, b], we will not consider the function as a "function", i.e., a mapping of arbitrary points $x \in [a, b]$ to its range, but as the collection of the evaluation of its discretization, see Definition 2.5. Hence, a function $f:[a,b]\to\mathbb{R}$ is represented by an *n*-dimensional vector $[f(x_1), \ldots, f(x_n)]$. As already mentioned before, we select uniformly distributed points $x_j, j \in \{1, ... n\}$.

We are dealing with matrix-valued functions, where each matrix has size 2×2 . Thus, these functions will be represented by $2 \times 2 \times n$ arrays. A function $m:[a,b] \times [a,b] \to \mathbb{C}^{2\times 2}$ will be represented by a $2 \times 2 \times n \times n$ array, whereat each entry is a complex number.

3.7.2 Numerical integration

Let us consider $f:[a,b]\to\mathbb{C}$ and a discretization $f_{dis}:\{x_1,\ldots x_n\}\to\mathbb{C}$ of f. We want to emphasize that $\{x_1, \ldots x_n\} \in [a, b]$ are uniformly distributed. When computing an integral, we will use the following approximation

$$\int_{a}^{b} f(x)dx \approx \sum_{k=1}^{n} f(x_k)\Delta x,$$

whereat

$$\Delta x \coloneqq \frac{b-a}{n},$$

which is almost⁴ the (left) Riemann rule, see e.g., [Ger11, Section 2.1]. Finding m_1 with

$$\int_{a}^{b} m_1(x, y) dx = \mu_1(y)$$

corresponds to finding m_1 with

$$\Delta x \cdot \sum_{k=1}^{n} m_1(x_k, y) = \mu_1(y).$$

However, in practice we simply try to find an $\widetilde{m_1}$ with

$$\sum_{k=1}^{n} \widetilde{m_1}(x_k, y) = \mu_1(y).$$

⁴The actual Riemann sum consists of n-1 many summands with weight $\frac{b-a}{n-1}$, but here we have n many summands with weight $\frac{b-a}{n}$. In practice, this difference can be neglected.

Here, m_1 and $\widetilde{m_1}$ are related via

$$\widetilde{m_1} = \frac{m_1}{\Delta x}.$$

For most of the calculation, it doesn't matter if we consider m_1 or $\widetilde{m_1}$, as long as we use it consistently. Only when interpreting the cost $\mathcal{T}_{2,\lambda}$, we need to reconsider if we are using m_1 or $\widetilde{m_1}$.

3.7.3 Optimization process

Computing $\mathcal{T}_{2,\lambda}(\mu_0,\mu_1)$ and $\mu_{0.5}$ requires solving a convex optimization problem. There are (at least) two methods to solve such a problem with MATLAB, namely the Optimization Toolbox and the CVX framework. In this thesis, the author used MATLAB versions R2024a and R2024b, CVX version 2.2 and MOSEK version 10.2.8. Hence, all following statements were only tested with those versions. When using other versions, the following statements might not be correct anymore.

Optimization Toolbox

The Optimization Toolbox⁵ of MATLAB allows solving convex optimization problems as well as non-convex problems. However, there are some constraints that need to be considered:

- Clearly, the objective function and all inequality constraints have to be real-valued, otherwise "minimizing" would not make sense. However, the optimization problem must not contain any complex-valued variables at all, even if the objective function and all inequality constraints are real-valued. E.g., the problem $\min \operatorname{Re}(z)^2 + 2 \cdot \operatorname{Im}(z), z \in \mathbb{C}$, is not supported.
 - Instead, complex variables must be split into real and imaginary parts, and both parts need to be considered as independent, real-valued variables. Addition and subtraction of two complex variables can be easily calculated by considering real part and imaginary part separately. However, multiplication of two complex variables in terms of real and imaginary part is more challenging.
- There is no command that explicitly ensures that a matrix-valued optimization variable is positive semi-definite. Instead, this property must be required implicitly. One method is to not search for the positive semi-definite optimization variable A itself, but to find a lower-triangular matrix L (whose diagonal entries are not necessarily non-zero) with the property $A = LL^*$, see [HJ13, Corollary 7.2.9 (Cholesky factorization)]. Hereby, L^* denotes the conjugate transpose of L.
- Some useful MATLAB commands are not supported when using optimization variables, for example permute. However, reshape is supported and can be used to achieve similar results as permute.



⁵Download and documentation: https://se.mathworks.com/products/optimization.html

CVX package

CVX⁶ is a MATLAB-based package for convex optimization. The basic version (which includes two solvers, namely SDPT3 and SeDuMi) can be downloaded for free. In addition to a simple syntax, the package also has other interesting properties:

- Optimization variables can be complex-valued.
- Optimization variables can have the (explicit) constraint to be positive semi-definite.
- Many mathematical expressions need to be stated in terms of CVX-internal functions. E.g., the command x^2 is not allowed but must be replaced with square(x).
- CVX can only deal with problems where every part is convex. E.g., the function $f(x) = 3x^2 - x^2$ is clearly convex, but since $-x^2$ is concave, CVX will not support this function, i.e., it will not support 3*square(x)-square(x). Of course, in this case the function can be easily reformulated as the "fully convex" function $2x^2$, i.e., 2*square(x). However, such a reformulation is not always possible.

As already mentioned, CVX includes two free solvers. However, it also supports some commercial solvers. The MOSEK⁷ solver is a commercial solver, but there are free academic licenses. During the work on this thesis, a specific problem was calculated with both the SDPT3 and the MOSEK solver. Solving the problem with SDPT3 took around half an hour, however, the MOSEK-based solving could be done in less than 10 seconds. Thus, all CVX-based codes in this thesis are using the MOSEK solver.

⁶Download and documentation: https://cvxr.com/cvx/

⁷Download and documentation: https://www.mosek.com/

One-dimensional signals and their statistical properties

In this chapter, we give an introduction to signals in terms of statistical signal processing. For this purpose, we examine their statistical properties and observe an exciting representation of the autocovariance.

In Chapter 3, we were dealing with OMT for matrix-valued functions. We established $\mathcal{T}_{2,\lambda}$ that helps us defining distances between two functions and finding intermediate functions. In Chapter 6 we will use these methods as a tool for our problems. However, we have not yet talked about the actual problems that we will deal with later. In Chapter 4 and Chapter 5, we want to provide the mathematical foundation for the applications in Chapter 6. Thus, those two chapters contain many definitions and theorems and are of theoretical nature.

4.1 Stochastic processes

When thinking about the word "signal", many different meanings could come to your mind. Some might think of audio signals. An audio signal can be seen as a function $f:[t_0,t_1]\to\mathbb{R}$ that gives the current deviation in air pressure at time point $t \in [t_0, t_1]$, see [Kre23]. An illustration can be found in Figure 4.1.

In statistical signal processing, we have a different approach. But first, we want to give two definitions, see [Flo15].

Definition 4.1 (Stochastic process). Given a probability space $(\Omega, \mathcal{F}, \mathbb{P})$, a stochastic process is any collection $\{X(t)\}_{t\in T}$ of random variables $X(t), t\in T$ defined on this probability space. If $T = \mathbb{Z}$, we call $\{X(t)\}_{t \in T}$ a discrete-time stochastic process, if $T = [0, +\infty)$, we call it a continuous-time stochastic process. We refer to the stochastic process $\{X(t)\}_{t\in T}$ as X.

Definition 4.2 (Realization of a stochastic process). Let $\{X(t)\}_{t\in T}$ be a stochastic process on the probability space $(\Omega, \mathcal{F}, \mathbb{P})$ and let $\omega \in \Omega$. Let $X(t)(\omega)$ denote the realization of the random variable X(t) with respect to ω . For $\omega \in \Omega$, the realization of the stochastic process is the function

$$t \mapsto X(t)(\omega)$$

In statistical signal processing, a signal is seen as a stochastic process, see [Sch91, Section 1.6]. A certain measurement of a signal, e.g., the function in Figure 4.1, corresponds to a certain realization of that signal. However, statistical signal processing is not interested in concrete realizations of a signal but in the statistical properties of the signal, see [Sch91].



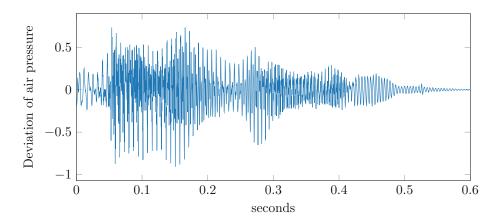


Figure 4.1: The graph shows the deviation in air pressure, while a colleague of the author says the word "Leiwand", which means "nice" in Viennese slang. This function can be seen as a realization of a stochastic process.

4.2 Statistical terms and definitions

In the following, we will assume that all stochastic processes are discrete-time stochastic processes. Unless otherwise stated, all stochastic processes will be complex-valued, i.e., $X(t)(\omega) \in \mathbb{C}$. Furthermore, all stochastic processes in Section 4.2 are sufficiently nice, i.e., all expected values used in the following definitions exist. After recapitulating the definition of covariance, we want to give another definition, see [Shi96].

Definition 4.3. Let X_1 and X_2 be two random variables. Its covariance $Cov(X_1, X_2)$ is defined by

$$Cov(X_1, X_2) = \mathbb{E}((X_1 - \mathbb{E}(X_1))\overline{(X_2 - \mathbb{E}(X_2))})$$

Definition 4.4 (Wide-sense stationary). Let $\{X(t)\}_{t\in T}$ be a discrete-time stochastic process. We call X wide-sense stationary if, for all $t_1, t_2, s \in \mathbb{Z}$,

$$\mathbb{E}(X(t_1)) = \mathbb{E}(X(t_2))$$
$$\operatorname{Cov}(X(t_1+s), X(t_1)) = \operatorname{Cov}(X(t_2+s), X(t_2))$$

Hence, a wide-sense stationary process has a constant expected value, and the covariance of $X(t_1)$ and $X(t_2)$ only depends on the lag between t_1 and t_2 . In addition to our previous assumptions, we will often assume that our considered stochastic processes are wide-sense stationary and the expected value is 0, i.e., $\mathbb{E}(X(t)) = 0$, $t \in T$. Under this assumption, we want to provide more definitions, see [Par18].

Definition 4.5 (Autocovariance). Let $\{X(t)\}_{t\in T}$ be a discrete-time wide-sense stationary stochastic process and let its expected value be 0. For $t, s \in \mathbb{Z}$, the autocovariance r_{XX} of X is defined by

$$r_{XX}(t) := \mathbb{E}\left(X(s+t)\overline{X(s)}\right).$$
 (4.1)

Since X is wide-sense stationary, the expression in (4.1) is well-defined, i.e., it is independent of $s \in \mathbb{Z}$. Definition 4.5 might remind the knowledgeable reader of the autocorrelation of a wide-sense stationary stochastic process. As the expected value of X is 0, the autocorrelation and the autocovariance coincide.

4.3 Spectral representation

In the last section, we have defined the autocovariance r_{XX} of a wide-sense stationary stochastic process X with expected value of 0. The autocovariance can give important information about the process X. In this section, we want to introduce a representation of the autocovariance. We start with an important result, see [Shi96, Section VI-§1, 3. Theorem].

Theorem 4.6 (Herglotz). Let $\{X(t)\}_{t\in T}$ be a discrete-time, wide-sense stationary stochastic process with expected value of 0. Let r_{XX} be its autocovariance. There exists a finite measure F on $([-\pi, \pi), \mathcal{B}([-\pi, \pi))^1$ such that for every $t \in \mathbb{Z}$, we have²

$$r_{XX}(t) = \int_{-\pi}^{\pi} \exp(i\omega t) dF(\omega). \tag{4.2}$$

Definition 4.7 (Spectral measure). Let $\{X(t)\}_{t\in T}$ be a discrete-time, wide-sense stationary stochastic process with expected value of 0. The measure F involved in (4.2) is called the spectral measure.

Although they share the same name, the spectral measure defined in Definition 4.7 is not the same as the spectral measure defined in functional analysis, e.g., in [WKB23, Definition 7.1.1].

The spectral measure F is uniquely defined by the autocovariance function r_{XX} , see [Shi96, Section VI-§1, Remark 1].

In fact, there are many different formulations of Theorem 4.6. Depending on its specific formulation, the Wiener-Khinchin theorem provides a very similar statement to Theorem 4.6, see e.g. [Gub06].

4.3.1 Lebesgue-Stieltjes integral

The integral in (4.2) is a Lebesgue integral with respect to the measure F. In many textbooks, the authors are using integrals with respect to a nondecreasing, right-continuous function. However, the exact meaning of this notation is often omitted. Because of that, proofs of connected theorems (e.g. Theorem 5.8) might become "hand-wavy" and not rigorous. In this subsection, we want to explain this frequently used notation.

The next two definitions and the next proposition are taken from [Shi96, Section II-§3] and [Kus14, Section 6.2].

 $^{{}^{1}\}mathcal{B}([-\pi,\pi))$ denotes the Borel sets of the interval $[-\pi,\pi)$. The Borel sets are a σ -algebra.

²In contrast to Definition 4.2, ω now denotes a frequency, i.e., a value in $[-\pi,\pi)$, and not an element of the probability space Ω .

Definition 4.8 (Lebesgue-Stieltjes measure). A Lebesgue-Stieltjes measure on $(\mathbb{R}, \mathcal{B}(\mathbb{R}))$ is a measure μ such that for every bounded interval $A \subseteq \mathbb{R}$, the measure $\mu(A)$ is finite.

If μ is a finite measure, we have $\mu(A) < \infty$ for every not necessarily bounded $A \in \mathcal{B}(\mathbb{R})$. Hence, every finite measure on $(\mathbb{R}, \mathcal{B}(\mathbb{R}))$ is a Lebesgue-Stieltjes measure.

Definition 4.9 (Generalized distribution function). A generalized distribution function is a function $G: \mathbb{R} \to \mathbb{R}$ that is nondecreasing and right-continuous.

Proposition 4.10. There is a correspondence between Lebesgue-Stieltjes measures μ and generalized distribution functions G by dint of

$$\mu((a,b]) = G(b) - G(a). \tag{4.3}$$

Given a generalized distribution function G, one can define μ by the right-hand side of (4.3). Conversely, if a Lebesgue-Stieltjes measure μ is given, there exists a generalized distribution function G such that (4.3) is satisfied. This G is unique up to an additive constant c.

Next, we want to define what integration with respect to a function G means, see [Shi96, Section II-§6].

Definition 4.11 (Lebesgue-Stieltjes integral). Let $G: \mathbb{R} \to \mathbb{R}$ be a generalized distribution function and let f be an integrable function. Let μ be the corresponding Lebesgue-Stieltjes measure on $(\mathbb{R}, \mathcal{B}(\mathbb{R}))$, as in Proposition 4.10. We define the Lebesgue-Stieltjes integral $\int_{-\infty}^{\infty} f(x) dG(x)$ as the Lebesgue integral with respect to μ , i.e.,

$$\int_{-\infty}^{\infty} f(x) dG(x) := \int_{-\infty}^{\infty} f(x) d\mu(x).$$

So far, all definitions and propositions in this subsection deal with measures μ on $(\mathbb{R}, \mathcal{B}(\mathbb{R}))$ and functions $G: \mathbb{R} \to \mathbb{R}$. However, Remark 4.12 allows us to consider μ on $([a,b), \mathcal{B}([a,b)))$ and $G:[a,b)\to\mathbb{R}$, see [Shi96, Section VI-§1].

Remark 4.12. Let $G:[a,b)\to\mathbb{R}$ be a nondecreasing, right-continuous function and let $G(b) := \lim_{x \to b} G(x)$. We can extend G by

$$\widetilde{G}(x) := \begin{cases} G(x), & x \in [a, b), \\ G(a), & x < a, \\ G(b), & x \ge b, \end{cases}$$

$$(4.4)$$

so we have $\widetilde{G}|_{[a,b)} = G$. Let $\widetilde{\mu}$ be the measure on $(\mathbb{R}, \mathcal{B}(\mathbb{R}))$ that corresponds to \widetilde{G} , see Proposition 4.10. We have

$$\widetilde{\mu}(A) = 0$$
 for every $A \in \mathcal{B}(\mathbb{R} \setminus [a, b))$.

We now define the measure μ on $([a,b),\mathcal{B}([a,b]))$ by

$$\mu(A) := \widetilde{\mu}(A), \quad A \in \mathcal{B}([a,b)) \subseteq \mathcal{B}(\mathbb{R}).$$

Analogously, we can start with a measure μ on $([a,b),\mathcal{B}([a,b)]))$ and extend it to a measure $\widetilde{\mu}$ on $(\mathbb{R}, \mathcal{B}(\mathbb{R}))$ by

$$\widetilde{\mu}(A) = \begin{cases} \mu(A), & A \in \mathcal{B}([a,b)), \\ 0, & A \in \mathcal{B}(\mathbb{R} \setminus [a,b)). \end{cases}$$

The corresponding generalized distribution function \widetilde{G} satisfies (4.4). We define $G:[a,b)\to$ \mathbb{R} as the restriction of G to [a,b), i.e. $G := G|_{[a,b)}$.

Hence, there is a correspondence between nondecreasing, right-continuous functions $G:[a,b)\to\mathbb{R}$ and measures μ on $([a,b),\mathcal{B}([a,b)])$.

Thus, it make sense to consider Lebesgue-Stieltjes integrals with respect to $G:[a,b)\to\mathbb{R}$. In the spirit of Definition 4.11 and Remark 4.12, we can reformulate Theorem 4.6 as

Theorem 4.13. Let $\{X(t)\}_{t\in T}$ be a discrete-time, wide-sense stationary stochastic process with expected value of 0. Let r_{XX} be its autocovariance. There exists a nondecreasing, right-continuous function $F: [-\pi, \pi) \to \mathbb{R}$ such that for every $t \in \mathbb{Z}$, we have

$$r_{XX}(t) = \int_{-\pi}^{\pi} \exp(i\omega t) dF(\omega).$$

In order to not overload the variable name F, let us for now denote the spectral measure, see Definition 4.7, as F_m . As already mentioned, the corresponding nondecreasing, rightcontinuous function is unique up to a constant. $F: [-\pi, \pi) \to \mathbb{R}$, uniquely defined by $F(\omega) := F_m([-\pi, \omega))$, is a nondecreasing, right-continuous function that satisfies (4.3). This gives rise to the next definition, see [Shi96, Section VI-§1].

Definition 4.14 (Spectral function). Let $\{X(t)\}_{t\in T}$ be a discrete-time, wide-sense stationary stochastic process with expected value of 0. Let F_m be its spectral measure. The function $F: [-\pi, \pi) \to \mathbb{R}_0^+$ defined by

$$F(\omega) := F_m([-\pi, \omega])$$

is called the spectral function of X.

For the spectral function F, it immediately follows that $F(-\pi) = 0$.

4.3.2 Spectral density

If the spectral function F is differentiable, we can state another representation of the covariance function. In this subsection, we present this representation without further reasoning. However, in Section 5.3, we will give a more rigorous explanation for a more general situation. For this purpose, we need the concept of complex measure, thus we are not proving it already now. The following result will immediately follow from Corollary 5.20. **Proposition 4.15.** Let $\{X(t)\}_{t\in T}$ be a discrete-time, wide-sense stationary stochastic process with expected value of 0. Let r_{XX} be its autocovariance, F the corresponding spectral function and let λ be the Lebesgue measure. If F is differentiable with F' = f, we have

$$r_{XX}(t) = \int_{-\pi}^{\pi} f(\omega) \exp(i\omega t) d\lambda(\omega).$$

for each $t \in \mathbb{Z}$.

Definition 4.16 (Spectral density). With the notation of Proposition 4.15, we call f = F'the spectral density of the stochastic process X.

Multidimensional signals

In Chapter 4, we have considered single stochastic processes $\{X(t)\}_{t\in T}$, with $X(t)(\omega)\in\mathbb{C}$, whereat $\omega \in \Omega$ denotes an element of the probability space. Now, we want to consider multiple stochastic processes $\{X_1(t)\}_{t\in T},\ldots,\{X_n(t)\}_{t\in T}$. Since we can describe those processes as a single vector-valued process

$$\{X(t)\}_{t \in T} \coloneqq \left\{ \begin{pmatrix} X_1(t) \\ X_2(t) \\ \vdots \\ X_n(t) \end{pmatrix} \right\}_{t \in T}, \tag{5.1}$$

these processes are often described as "multidimensional stochastic processes", "vector-valued stochastic processes", or simply as "vector process", see e.g., [Lin12]. Hence, we call this chapter "Multidimensional signals". Another common name for these signals is vector-valued signals. However, for the sake of clearer notation, we will consider multiple stochastic processes $\{X_j(t)\}_{t\in T}$ with $X_j(t)(\omega)\in\mathbb{C}, j\in\{1,\ldots,n\}, \omega\in\Omega$ instead of a single stochastic process $\{X(t)\}_{t\in T}$ with $X(\omega)\in\mathbb{C}^n$, as in (5.1).

5.1 Statistical terms and definitions

First, we want to extend the definitions of Section 4.2 to multiple stochastic processes, see [Par18].

Definition 5.1 (Jointly wide-sense stationary). Let $\{X(t)\}_{t\in T}$ and $\{Y(t)\}_{t\in T}$ be two discretetime stochastic processes. We call X and Y jointly wide-sense stationary if they are individually wide-sense stationary and if, for all $t_1, t_2, s \in \mathbb{Z}$,

$$\operatorname{Cov}(X(t_1+s),Y(t_1)) = \operatorname{Cov}(X(t_2+s),Y(t_2)).$$

Definition 5.2 (Cross-covariance). Let $\{X(t)\}_{t\in T}$ and $\{Y(t)\}_{t\in T}$ be two discrete-time jointly wide-sense stationary stochastic processes, both with expected value of 0. The cross-covariance $r_{XY}(t)$ of X and Y is defined as

$$r_{XY}(t) := \mathbb{E}(X(s+t)\overline{Y(s)}).$$
 (5.2)

We define $r_{YX}(t)$ in an analogous way.

If two wide-sense stationary processes X and Y are jointly wide-sense stationary, their cross-covariance $Cov(X(t_1), Y(t_2))$ only depends on the lag between t_1 and t_2 . As X and Y are jointly wide-sense stationary, equation (5.2) is well-defined, i.e., independent of the choice of $s \in \mathbb{Z}$.



Proposition 5.3. Let $\{X(t)\}_{t\in T}$ and $\{Y(t)\}_{t\in T}$ be two discrete-time jointly wide-sense stationary stochastic processes, both with expected value of 0. The autocovariance and the cross-covariance satisfy

$$r_{XY}(-t) = \overline{r_{YX}(t)}, \quad r_{XX}(-t) = \overline{r_{XX}(t)}, \quad r_{YY}(-t) = \overline{r_{YY}(t)}$$

Proof. We will only prove the first identity. The other two identities then follow by considering X = Y.

$$r_{XY}(-t) = \mathbb{E}\left(X(s-t)\overline{Y(s)}\right) = \overline{\mathbb{E}\left(Y(s)\overline{X(s-t)}\right)} = \overline{\mathbb{E}\left(Y(s+t)\overline{X(s)}\right)} = \overline{r_{YX}(t)}$$

Definition 5.4 (Covariance matrix). Let $\{X_1(t)\}_{t\in T}, \{X_2(t)\}_{t\in T}, \dots, \{X_n(t)\}_{t\in T}$ be discrete-time, jointly wide-sense stationary stochastic processes with expected value of 0. The covariance matrix is defined as

$$R(t) = \begin{pmatrix} r_{X_1X_1}(t) & r_{X_1X_2}(t) & \dots & r_{X_1X_n}(t) \\ r_{X_2X_1}(t) & r_{X_2X_2}(t) & \dots & r_{X_2X_n}(t) \\ \vdots & \vdots & \ddots & \vdots \\ r_{X_nX_1}(t) & r_{X_nX_2}(t) & \dots & r_{X_nX_n}(t) \end{pmatrix}$$
(5.3)

The diagonal of the covariance matrix consists of the autocovariances of each process X_i , whereat all other entries are the cross-covariances.

5.2 Herglotz theorem for multiple stochastic processes

The goal of this section is obtaining a "multiple process"-version of Herglotz theorem, Theorem 4.6. First, we need to introduce complex measures, total variation and integration with respect to a complex measure, see [Wer11, Section A.4] and [Rud87, Chapter 6].

Definition 5.5 (Complex measure). Let Σ be a σ -algebra. A function $\mu: \Sigma \to \mathbb{C}$ is called a complex measure if μ is σ -additive.

Definition 5.6 (Total variation). Let μ be a complex measure on (X, Σ) . The total variation $|\mu|$ of μ is a finite measure on (X,Σ) defined by the supremum

$$|\mu|(E) = \sup \sum_{i=1}^{\infty} |\mu(E_i)|, \qquad E \in \Sigma$$

taken over all partitions $(E_i)_{i\in\mathbb{N}}$ of E. A partition $(E_i)_{i\in\mathbb{N}}$ of E is a countable collection of elements of Σ such that $\bigcup_{i \in \mathbb{N}} E_i = E$ and $E_i \cap E_j = \emptyset$, $i \neq j$.

We want to emphasize that complex measures are mapping to the complex numbers but not to $+\infty$. In contrast, measures are mapping to $[0,+\infty] \nsubseteq \mathbb{C}$. Hence, not every measure is also a complex measure. However, every finite measure is indeed a complex measure, since the codomain of a finite measure is $[0,+\infty)\subseteq\mathbb{C}$. Next, we want to define integration with respect to a complex measure, see [Wer11, Definition A.4.5].

Definition 5.7 (Integral with respect to a complex measure). Let μ be a complex measure on (X,Σ) and let f be an integrable function with respect to $|\mu|$. Let μ_{Re} and μ_{Im} be the decomposition of μ in real part and imaginary part, i.e., $\mu = \mu_{Re} + i \cdot \mu_{Im}$. Let μ_{Re}^+, μ_{Re}^- and $\mu_{\rm Im}^+, \mu_{\rm Im}^-$ be the corresponding Jordan decomposition of $\mu_{\rm Re}$ and $\mu_{\rm Im}$, respectively. We define the integral by

$$\int f \, d\mu = \int f \, d\mu_{\rm Re}^+ - \int f \, d\mu_{\rm Re}^- + i \cdot \left(\int f \, d\mu_{\rm Im}^+ - \int f \, d\mu_{\rm Im}^- \right).$$

Let μ_1, \ldots, μ_n be complex measures and $z_1, \ldots, z_n \in \mathbb{C}$. Considering the definition of a complex measure,

$$\sum_{j=1}^{n} z_j \mu_j$$

is also a complex measure. If f is integrable with respect to μ_1, \ldots, μ_n , we furthermore have

$$\sum_{j=1}^{n} z_j \int f \, d\mu_j(\omega) = \int f \, d\left(\sum_{j=1}^{n} z_j \mu_j\right)(\omega),\tag{5.4}$$

see [Kal21, Fakta 18.3.16 - 5].

The next theorem and its proof is inspired by the first part of [Lin12, Theorem 7.1 (a)]. However, we are dealing with discrete-time processes instead of continuous-time processes. Furthermore, the proof in [Lin12] does not elaborate what it means to consider a linear combination of integrals with respect to different nondecreasing, right-continuous functions. In this thesis, we try to provide a rigorous argumentation by considering complex measures.

Theorem 5.8. Let $X_1, X_2, ... X_n$ be n-many discrete-time, jointly wide-sense stationary stochastic processes with expected value of 0 and let $R: \mathbb{Z} \to \mathbb{C}^{n \times n}$ be their covariance matrix. There exists a matrix F of complex measures F_{jk} , $j,k \in \{1,\ldots n\}$, on $([-\pi,\pi),\mathcal{B}([-\pi,\pi))$ such that

$$R(t) = \int_{-\pi}^{\pi} \exp(i\omega t) dF(\omega)$$
 (5.5)

for each $t \in \mathbb{Z}$. Furthermore we have $F_{kj}(A) = \overline{F_{jk}(A)}$ for every $j,k \in \{1,\ldots,n\}$, $A \in \mathcal{B}([-\pi,\pi)).$

The notation in (5.5) means that for each R_{jk} with $j, k \in \{1, ..., n\}$, there exists a complex measure F_{jk} such that

$$R_{jk}(t) = \int_{-\pi}^{\pi} \exp(i\omega t) dF_{jk}(\omega).$$
 (5.6)

Proof. Since $R_{jj} = r_{X_j X_j}$ is an autocorrelation function, we can apply Herglotz's Theorem 4.6 and obtain a finite measure F_{jj} , so in particular a complex measure, such that (5.6) is satisfied. The main task of this proof is finding such a complex measure for R_{jk} , $j \neq k$.

Consider the complex vector $z = \{z_1, \dots z_m\} \in \mathbb{C}^n$ and

$$Y(t) = \sum_{j=1}^{n} z_j X_j(t).$$

Y is a discrete-time, wide-sense stationary stochastic process with expected value of 0. Let r_z be its autocovariance function. Theorem 4.6 provides a finite measure G_z such that

$$r_z(t) = \int_{-\pi}^{\pi} \exp(i\omega t) dG_z(\omega).$$

Furthermore, we have

$$\begin{split} r_z(t) &= \mathbb{E}\left(Y(s+t)\overline{Y(s)}\right) = \mathbb{E}\left(\sum_{j=1}^n z_j X_j(s+t) \sum_{k=1}^n \overline{z_k} \overline{X_k(s)}\right) \\ &= \mathbb{E}\left(\sum_{j=1}^n \sum_{k=1}^n z_j X_j(s+t) \overline{z_k} \overline{X_k(s)}\right) = \mathbb{E}\left(\sum_{j,k \in \{1,\dots,n\}} z_j \overline{z_k} X_j(s+t) \overline{X_k(s)}\right) \\ &= \sum_{j,k \in \{1,\dots,n\}} z_j \overline{z_k} \cdot \mathbb{E}\left(X_j(s+t) \overline{X_k(s)}\right) = \sum_{j,k \in \{1,\dots,n\}} z_j \overline{z_k} R_{jk}(t) \end{split}$$

Altogether, we have

$$r_z(t) = \sum_{j,k \in \{1,\dots,n\}} z_j \overline{z_k} R_{jk}(t) = \int_{-\pi}^{\pi} \exp(i\omega t) dG_z(\omega)$$
 (5.7)

for any $z = \{z_1, \dots z_n\} \in \mathbb{C}^n$.

Next, let $j, k \in \{1, ..., n\}$ and consider $v = \{v_1, ..., v_n\}, w = \{w_1, ..., w_n\} \in \mathbb{C}^n$ defined by

$$v_{\ell} = \begin{cases} 1 & \text{if } \ell = j \\ 1 & \text{if } \ell = k \\ 0 & \text{else} \end{cases} \text{ and } w_{\ell} = \begin{cases} i & \text{if } \ell = j \\ 1 & \text{if } \ell = k \\ 0 & \text{else} \end{cases}$$

We have

$$r_{v}(t) = R_{jj}(t) + R_{jk}(t) + R_{kj}(t) + R_{kk}(t) = \int_{-\pi}^{\pi} \exp(i\omega t) dG_{v}(\omega)$$
$$r_{w}(t) = R_{jj}(t) + i \cdot R_{jk}(t) - i \cdot R_{kj}(t) + R_{kk}(t) = \int_{-\pi}^{\pi} \exp(i\omega t) dG_{w}(\omega).$$



Subtraction of $R_{jj}(t)$ and $R_{kk}(t)$ yields

$$R_{jk}(t) + R_{kj}(t) = \int_{-\pi}^{\pi} \exp(i\omega t) dG_v(\omega) - R_{jj}(t) - R_{kk}(t)$$
 (5.8)

$$i \cdot R_{jk}(t) - i \cdot R_{kj}(t) = \int_{-\pi}^{\pi} \exp(i\omega t) dG_w(\omega) - R_{jj}(t) - R_{kk}(t).$$
 (5.9)

Considering (5.4), we can write the right-hand side of (5.8) as

$$\int_{-\pi}^{\pi} \exp(i\omega t) dG_v(\omega) - \int_{-\pi}^{\pi} \exp(i\omega t) dF_{jj}(\omega) - \int_{-\pi}^{\pi} \exp(i\omega t) dF_{kk}(\omega)$$
$$= \int_{-\pi}^{\pi} \exp(i\omega t) d(G_v - F_{jj} - F_{kk})(\omega)$$

and the right-hand side of (5.9) as

$$\int_{-\pi}^{\pi} \exp(i\omega t) dG_w(\omega) - \int_{-\pi}^{\pi} \exp(i\omega t) dF_{jj}(\omega) - \int_{-\pi}^{\pi} \exp(i\omega t) dF_{kk}(\omega)$$
$$= \int_{-\pi}^{\pi} \exp(i\omega t) d(G_w - F_{jj} - F_{kk})(\omega).$$

Adding line (5.8) and (5.9) with factor -i and i, respectively, gives

$$(5.8) - i \cdot (5.9) = 2 \cdot R_{jk}(t)$$

$$= \int_{-\pi}^{\pi} \exp(i\omega t) d(G_v - F_{jj} - F_{kk})(\omega) - i \cdot \left(\int_{\pi}^{\pi} \exp(i\omega t) d(G_w - F_{jj} - F_{kk})(\omega) \right)$$

$$= \int_{-\pi}^{\pi} \exp(i\omega t) d(G_v - F_{jj} - F_{kk})(\omega) + \left(\int_{-\pi}^{\pi} \exp(i\omega t) d(-i \cdot (G_w - F_{jj} - F_{kk}))(\omega) \right)$$

$$= \int_{-\pi}^{\pi} \exp(i\omega t) d(G_v - F_{jj} - F_{kk} - i \cdot (G_w - F_{jj} - F_{kk}))(\omega)$$

and

$$(5.8) + i \cdot (5.9) = 2 \cdot R_{kj}(t)$$

$$= \int_{-\pi}^{\pi} \exp(i\omega t) d(G_v - F_{jj} - F_{kk} + i \cdot (G_w - F_{jj} - F_{kk}))(\omega).$$



Hence, there exist two complex measures

$$F_{jk} := \frac{1}{2} (G_v - F_{jj} - F_{kk} - i \cdot (G_w - F_{jj} - F_{kk})), \tag{5.10}$$

$$F_{kj} := \frac{1}{2} (G_v - F_{jj} - F_{kk} + i \cdot (G_w - F_{jj} - F_{kk})), \tag{5.11}$$

with

$$R_{jk}(t) = \int_{-\pi}^{\pi} \exp(i\omega t) dF_{jk}(\omega), \qquad (5.12)$$

$$R_{kj}(t) = \int_{-\pi}^{\pi} \exp(i\omega t) dF_{kj}(\omega).$$

Equation (5.10) and (5.11) show that $F_{kj} = \overline{F_{jk}}$.

Similar to Definition 4.7 (spectral measure) and Definition 4.14 (spectral function), we want to define the cross-spectral measure and cross-spectral function.

Definition 5.9 (Cross-spectral measure). Let X_i, X_k be discrete-time, jointly wide-sense stationary stochastic processes with expected value of 0. The complex measure F_{jk} involved in (5.12) is called the cross-spectral measure of X_i and X_k .

Definition 5.10 (Cross-spectral function). Let X_i, X_k be discrete-time, jointly wide-sense stationary stochastic processes with expected value of 0 and let $F_{m,jk}$ be the cross-spectral measure of X_j and X_k . The function $F_{jk}: [-\pi, \pi) \to \mathbb{C}$ defined by

$$F_{jk}(\omega) = F_{m,jk}([-\pi,\omega])$$

is called the cross-spectral function of X_j and X_k .

Since the cross-spectral measure is a complex measure, it is clear that the cross-spectral function is in general a complex-valued function. In particular, the cross-spectral function is not nondecreasing. The term "nondecreasing complex-valued function" does not even make sense, because the complex numbers \mathbb{C} are not an ordered field.

Next, we want to investigate whether matrix F has properties related to positive semidefiniteness. But first, we need to state an important theorem, see [Els18, Section VIII-§2, Theorem 2.26. $M_{\text{reg}}(X,\mathcal{B}(X))$ is the space of regular complex measures on $(X,\mathcal{B}(X))$ and $C_0(X)$ is the space of continuous functions in X that vanish at infinity. $C'_0(X)$ denotes its dual space.

¹For the following theorems it is in fact not required to know the exact definition of "regularity", since all complex measures we are dealing with are already regular complex measures. However, the interested reader finds a definition in [Els18] or any other book about measure theory.

Theorem 5.11 (Representation theorem of Riesz for $C'_0(X)$). Let X be a locally compact Hausdorff space. Then

$$\Phi: M_{\text{reg}}(X, \mathcal{B}(X)) \to C'_0(X),$$

$$\Phi(\mu)(f) := \int_X f \, d\mu \qquad f \in C_0(X), \mu \in M_{reg}(X, \mathcal{B}(X))$$

is an isomorphism with

$$\|\Phi(\mu)\| = \|\mu\|,$$

whereat $\|\mu\| := |\mu|(X)$.

Theorem 5.11 is also known as *Riesz-Markov* theorem, see e.g., [WKB23, Theorem 2.3.9]. If X is a compact space, we have $C_0(X) = C(X)$. Furthermore, we want to remind the reader of Stone-Weierstraß's theorem (complex version), see [Rud⁺64, Theorem 7.33] and the required assumptions [Rud⁺64, Definition 7.28, Definition 7.30, Chapter 7].

Definition 5.12 (Algebra, Self-adjoint, Separating points, Vanishing at no point). A family A of complex functions defined on a set E is said to be an algebra if f + g, fg, $cf \in A$ for all $f,g\in\mathcal{A},c\in\mathbb{C}$. It is self-adjoint, if $\overline{f}\in\mathcal{A}$ for all $f\in\mathcal{A}$. It separates points, if for each pair of distinct points $x_1, x_2 \in E$, $x_1 \neq x_2$, there exists a function $f \in A$ such that $f(x_1) \neq f(x_2)$. It vanishes at no point, if for each $x \in E$, there exists a function $f \in A$ such that $f(x) \neq 0$.

Theorem 5.13 (Stone-Weierstraß (complex version)). Let \mathcal{A} be an algebra of complex continuous functions on a compact set K. If A is self-adjoint, separates points and vanishes at no point of K, then A is dense in C(K) with respect to $\|.\|_{\infty}$.

In the proof of Theorem 5.15 we will need the following lemma.

Lemma 5.14. Let μ be a complex measure on $([-\pi,\pi),\mathcal{B}([-\pi,\pi))$. We have $\mu=0$ if and only if

$$\int_{-\pi}^{\pi} \exp(i\omega t) \, d\mu(\omega) = 0$$

for all $t \in \mathbb{Z}$.

Proof. If $\mu = 0$, we clearly have

$$\int_{-\pi}^{\pi} \exp(i\omega t) d\mu(\omega) = 0.$$

To show the other direction, we assume that $\mu \neq 0$ and show that there needs to be a $t \in \mathbb{Z}$, such that $\int_{\pi}^{\pi} \exp(i\omega t) d\omega \neq 0$. Considering the bijection $\varphi: [-\pi, \pi) \to \mathbb{T}, \omega \mapsto \exp(i\omega)$ with $\mathbb{T} := \{z \in \mathbb{C} : |z| = 1\}, \text{ we can identify } [-\pi, \pi) \text{ with } \mathbb{T}, \text{ see e.g., } [Axl20, Section 11A]. Hence,$



we can identify μ with a measure $\widetilde{\mu}$ on $(\mathbb{T}, \mathcal{B}(\mathbb{T}))$ by setting $\mu(A) = \widetilde{\mu}(\exp(iA))$. Since $\mu \neq 0$, we also have $\widetilde{\mu} \neq 0$.

As a compact subset of \mathbb{C} , \mathbb{T} is a compact space, see [KH15, Proposition 12.11.2]. Now $\widetilde{\mu}$ is regular, see [Els18, Chapter VIII, Corollary 1.12] and [Els18, Chapter VIII, Implications 2.22]. According to Theorem 5.11, there exists a function $f \in C_0(\mathbb{T}) = C(\mathbb{T})$ such that

$$\int_{\mathbb{T}} f(\omega) \, d\widetilde{\mu}(\omega) \neq 0.$$

We define

$$\delta := \left| \int_{\mathbb{T}} f(\omega) \, d\widetilde{\mu}(\omega) \right| > 0.$$

As $\widetilde{\mu} \neq 0$ is a complex measure, we have $|\widetilde{\mu}|(\mathbb{T}) \in (0, +\infty)$. The span² of the continuous functions $\{h: \mathbb{T} \to \mathbb{C}, z \mapsto z^t, t \in \mathbb{Z}\}$ is a self-adjoint, point separating, at no point vanishing algebra in $C(\mathbb{T})$. Hence, according to Theorem 5.13, there exists a

$$g(\omega) = \sum_{t=-m}^{m} z_t \cdot \omega^t, \quad z_{-m}, \dots, z_m \in \mathbb{C}$$

such that $||f - g||_{\infty} < \delta/(2 \cdot |\widetilde{\mu}|(\mathbb{T}))$. Furthermore, we have

$$\left| \int\limits_{\mathbb{T}} f(\omega) \, d\widetilde{\mu}(\omega) - \int\limits_{\mathbb{T}} g(\omega) \, d\widetilde{\mu}(\omega) \right| = \left| \int\limits_{\mathbb{T}} f(\omega) - g(\omega) \, d\widetilde{\mu}(\omega) \right| \stackrel{(1)}{<} |\widetilde{\mu}|(\mathbb{T}) \cdot \frac{\delta}{2 \, |\widetilde{\mu}|(\mathbb{T})} = \frac{\delta}{2}$$

whereat inequality (1) holds because of Theorem 5.11 and its implication

$$|\Phi(\widetilde{\mu})(f-g)| \le \|\Phi(\widetilde{\mu})\| \cdot \|f-g\|_{\infty} = \|\widetilde{\mu}\| \cdot \|f-g\|_{\infty} = |\widetilde{\mu}|(\mathbb{T}) \cdot \|f-g\|_{\infty}.$$

The inequality

$$\underbrace{\left| \int_{\mathbb{T}} f(\omega) \, d\widetilde{\mu}(\omega) \right|}_{=\delta} = \left| \int_{\mathbb{T}} f(\omega) \, d\widetilde{\mu}(\omega) - \int_{\mathbb{T}} g(\omega) \, d\widetilde{\mu}(\omega) + \int_{\mathbb{T}} g(\omega) \, d\widetilde{\mu}(\omega) \right| \\
\leq \underbrace{\left| \int_{\mathbb{T}} f(\omega) \, d\widetilde{\mu}(\omega) - \int_{\mathbb{T}} g(\omega) \, d\widetilde{\mu}(\omega) \right|}_{<\frac{\delta}{2}} + \left| \int_{\mathbb{T}} g(\omega) \, d\widetilde{\mu}(\omega) \right|$$

shows that

$$\left| \int_{\mathbb{T}} g(\omega) \, d\widetilde{\mu}(\omega) \right| > \frac{\delta}{2}$$

²The elements of this space are often called "trigonometric polynomials", see e.g. [Rud87].

which leads to

$$0 \neq \int_{\mathbb{T}} g(\omega) \, d\widetilde{\mu}(\omega) = \int_{\mathbb{T}} \sum_{t=-m}^{m} z_t \cdot \omega^t \, d\widetilde{\mu}(\omega) = \sum_{t=-m}^{m} z_t \cdot \int_{\mathbb{T}} \omega^t \, d\widetilde{\mu}(\omega).$$

Thus, there exists a $t \in \mathbb{Z}$ such that

$$\int_{\mathbb{T}} \omega^t \, d\widetilde{\mu}(\omega) \neq 0.$$

As $\{h: \mathbb{T} \to \mathbb{C}, \, \omega \mapsto \omega^t, \, t \in \mathbb{Z}\}$ correspond to $\{h: [-\pi, \pi) \to \mathbb{C}, \, \omega \mapsto \exp(i\omega t), \, t \in \mathbb{Z}\}$, we found a $t \in \mathbb{Z}$ such that

$$\int_{-\pi}^{\pi} \exp(i\omega t) d\mu(\omega) = \int_{\mathbb{T}} \omega^t d\widetilde{\mu}(\omega) \neq 0.$$

The next theorem and its corollary are based on the second part of [Lin12, Theorem 7.1 (a)], which states a similar result for continuous-time stochastic processes. However, we elaborate³ the proof.

Theorem 5.15. Let X_1, X_2, \ldots, X_n be discrete-time, jointly wide-sense stationary stochastic processes with expected value of 0 and let F be the matrix involved in (5.5), i.e.,

$$F(A) = \begin{pmatrix} F_{11}(A) & \cdots & F_{1n}(A) \\ \vdots & \ddots & \vdots \\ F_{n1}(A) & \cdots & F_{nn}(A) \end{pmatrix}, \qquad A \in \mathcal{B}([-\pi, \pi)).$$

Let $[\omega_1, \omega_2] \subseteq [-\pi, \pi)$ be an interval. The matrix $F([\omega_1, \omega_2]) \in \mathbb{C}^{n \times n}$ is positive semi-definite.

Proof. Since $F_{kj}(A) = \overline{F_{jk}(A)}$ (see Theorem 5.8), $F([\omega_1, \omega_2])$ is an Hermitian matrix. Let $z = \{z_1, \dots, z_2\} \in \mathbb{C}^n$. We want to show that

$$z^* F([\omega_1, \omega_2]) z \ge 0. \tag{5.13}$$

Similar to the proof of Theorem 5.84, we consider the stochastic process

$$Y(t) = \sum_{j=1}^{n} \overline{z_j} X_j(t).$$



³In [Lin12] the proof is concentrated to "It is easy to see that $\Delta F(\omega)$ has the stated properties. [...]", without stating any preliminaries as Lemma 5.14. In this thesis, we try to prepare the proof even for people without the required sight.

⁴Due to technical reasons, we consider the process $\sum \overline{z_j} X_j$ instead of $\sum z_j X_j$ as in Theorem 5.8.

and its autocovariance r_z and spectral measure G_z . Hence, we have

$$r_z(t) = \int_{-\pi}^{\pi} \exp(i\omega t) dG_z(\omega).$$

Furthermore, we have

$$\int_{-\pi}^{\pi} \exp(i\omega t) dG_{z}(\omega) = r_{z}(t) \stackrel{(1)}{=} \sum_{j,k \in \{1,\dots,n\}} \overline{z_{j}} z_{k} R_{jk}(t)$$

$$= \overline{(z_{1},\dots z_{n})} \begin{pmatrix} R_{11}(t) & \cdots & R_{1n}(t) \\ \vdots & \ddots & \vdots \\ R_{n1}(t) & \cdots & R_{nn}(t) \end{pmatrix} \begin{pmatrix} z_{1} \\ \vdots \\ z_{n} \end{pmatrix}$$

$$= \overline{(z_{1},\dots z_{n})} \begin{pmatrix} \int \exp(i\omega t) dF_{11}(\omega) & \cdots & \int \exp(i\omega t) dF_{1n}(\omega) \\ \vdots & \ddots & \vdots \\ \int \exp(i\omega t) dF_{n1}(\omega) & \cdots & \int \exp(i\omega t) dF_{nn}(\omega) \end{pmatrix} \begin{pmatrix} z_{1} \\ \vdots \\ z_{n} \end{pmatrix}$$

$$\stackrel{(5.4)}{=} \int_{-\pi}^{\pi} \exp(i\omega t) dF_{n1}(\omega) \begin{pmatrix} \overline{(z_{1},\dots z_{n})} \begin{pmatrix} F_{11} & \cdots & F_{1n} \\ \vdots & \ddots & \vdots \\ F_{n1} & \cdots & F_{nn} \end{pmatrix} \begin{pmatrix} z_{1} \\ \vdots \\ z_{n} \end{pmatrix} \end{pmatrix} (\omega)$$

$$F_{z} :=$$

$$= \int_{-\pi}^{\pi} \exp(i\omega t) dF_{z}(\omega).$$

Equation (1) holds because of (5.7) and the fact that we considered $Y = \sum \overline{z_j} X_j$ instead of $Y = \sum z_j X_j$. As a linear combination of complex measures, F_z is a complex measure. Since

$$\int_{-\pi}^{\pi} \exp(i\omega t) d(G_z - F_z)(\omega) = 0$$

for all $t \in \mathbb{Z}$, Lemma 5.14 provides that $G_z - F_z = 0$, i.e., $G_z = F_z$. Hence, F_z is a measure and

$$\frac{\overline{(z_1, \dots z_n)}}{\overline{(z_1, \dots z_n)}} \begin{pmatrix} F_{11}([\omega_1, \omega_2]) & \dots & F_{1n}([\omega_1, \omega_2]) \\ \vdots & & \ddots & \vdots \\ F_{n1}([\omega_1, \omega_2]) & \dots & F_{nn}([\omega_1, \omega_2]) \end{pmatrix} \begin{pmatrix} z_1 \\ \vdots \\ z_n \end{pmatrix} \\
= \begin{pmatrix} \overline{(z_1, \dots z_n)} \begin{pmatrix} F_{11} & \dots & F_{1n} \\ \vdots & \ddots & \vdots \\ F_{n1} & \dots & F_{nn} \end{pmatrix} \begin{pmatrix} z_1 \\ \vdots \\ z_n \end{pmatrix} ([\omega_1, \omega_2]) = F_z([\omega_1, \omega_2]) \ge 0$$

which shows that the matrix $F([\omega_1, \omega_2])$ is positive semi-definite.



Corollary 5.16. Let $X_1, X_2, \ldots X_n$ be discrete-time, jointly wide-sense stationary stochastic processes with expected value of 0 and let F be the matrix of cross-spectral functions F_{ik} , i.e., $F: [-\pi, \pi) \to \mathbb{C}^{n \times n}$ with

$$F(\omega) = \begin{pmatrix} F_{11}(\omega) & \cdots & F_{1n}(\omega) \\ \vdots & \ddots & \vdots \\ F_{n1}(\omega) & \cdots & F_{nn}(\omega) \end{pmatrix}, \qquad \omega \in [-\pi, \pi).$$

Let $\omega_1 < \omega_2$. The matrix $\Delta F(\omega_1, \omega_2) := F(\omega_2) - F(\omega_1)$ is positive semi-definite.

Proof. Let F_m be the matrix of the spectral measures and cross-spectral measures involved in (5.5). Considering the definition of the spectral function and cross-spectral function, we have $\Delta F(\omega_1, \omega_2) = F(\omega_2) - F(\omega_1) = F_m([\omega_1, \omega_2])$. Theorem 5.15 yields that $F_m([\omega_1, \omega_2])$ is positive semi-definite. Hence, $\Delta F(\omega_1, \omega_2)$ is positive semi-definite.

5.3 Spectral density

In this section, we want to consider a special case, namely that the spectral function Fis differentiable. We will see that this gives very useful properties. But first, we want to discuss some theoretical background, see [Kal21, Definition 18.3.10].

Definition 5.17. Let ν be a measure on (X, Σ) and let μ be a measure or a complex measure on (X,Σ) . We call μ absolutely continuous with respect to ν if $\nu(A)=0$ implies $\mu(A)=0$ whereat $A \in \Sigma$. If μ is absolutely continuous with respect to ν , we will denote this by $\mu \ll \nu$.

We will now formulate the Theorem of Radon-Nikodym, see [Kal21, Theorem 18.3.12]. However, we only consider the case that μ is absolutely continuous with respect to the Lebesgue measure λ .

Theorem 5.18 (Radon-Nikodym). Let μ be a complex measure on $(X, \mathcal{B}(X))$ and let λ be the Lebesgue measure on $(X,\mathcal{B}(X))$. We have $\mu \ll \lambda$ if and only if there exists an integrable function f such that $\mu = f \cdot \lambda$, i.e.

$$\mu(A) = \int_{A} f \, d\lambda, \quad \text{for all } A \in \Sigma.$$
 (5.14)

In this case, f is unique almost everywhere (with respect to λ) and is called density of μ with respect to λ .

If $\mu \ll \lambda$, we can describe integrals with respect to μ as integrals with respect to λ , see [Kal21, Fakta 18.3.16 - 3].

Proposition 5.19. Let λ be the Lebesque measure on $(X, \mathcal{B}(X))$, let μ be a complex measure on $(X,\mathcal{B}(X))$ with $\mu \ll \lambda$ and let f be the density of μ with respect to λ as in 5.14. A function g is integrable with respect to μ if and only if $g \cdot f$ is integrable with respect to λ and we have

$$\int\limits_X g \, d\mu = \int\limits_X g \cdot f \, d\lambda.$$

Let $F: [-\pi, \pi) \to \mathbb{C}$ be the cross-spectral function of two processes X and Y, let F be differentiable with F' = f and let F_m be the corresponding cross-spectral measure. Since F is differentiable, it is also continuous. Hence, F_m is absolute continuous with respect to λ. According to the Fundamental Theorem of Calculus for Lebesgue measures, see [Els18, Theorem VII - 4.14, f is the density of F_m . Together with Proposition 5.19, we have

$$\int_{a}^{b} g(\omega) dF_{m}(\omega) = \int_{a}^{b} f(\omega) \cdot g(\omega) d\lambda(\omega).$$

for any integrable function g. Considering $g(\omega) = \exp(i\omega t)$ gives rise to the following corollary.

Corollary 5.20. Let X, Y be discrete-time, jointly wide-sense stationary stochastic processes with expected value of 0 and let F be the cross-spectral function of X and Y. Let F be differentiable with F' = f. We have

$$\int_{-\pi}^{\pi} \exp(i\omega t) dF(\omega) = \int_{-\pi}^{\pi} f(\omega) \exp(i\omega t) d\lambda(\omega)$$
 (5.15)

whereat the left-hand side is a Lebesque-Stieltjes integral.

If we choose X = Y, Corollary 5.20 gives exactly the same result for the spectral function instead of the cross-spectral function. The function f in (5.15) has a special name, see, e.g., [Lin12].

Definition 5.21 ((Cross-) spectral density). With the notation of Corollary 5.20, we call f the cross-spectral density of X and Y. If X = Y, we call f the spectral density of X.

Corollary 5.20 reveals a very important result, namely that the autocovariance (crosscovariance) is the Fourier transform of the (cross-) spectral density, if the (cross-) spectral density exists. However, the (cross-) spectral density does not always exists. Hence, we included this section only as a special case at the end of this chapter.

Finally, we want to adapt the results of the previous section to the special situation of the current section.

Corollary 5.22. Let $X_1, X_2, \ldots X_n$ be discrete-time, jointly wide-sense stationary stochastic processes with expected value of 0 and let $F_{jk}: [-\pi, \pi) \to \mathbb{R}(\mathbb{C}), j,k \in \{1, \dots n\}$, be their (cross-) spectral functions. For each $j, k \in \{1, \ldots, n\}$, let F_{jk} be differentiable with $f_{jk} := F'_{jk}$ The matrix

$$f(\omega) = \begin{pmatrix} f_{11}(\omega) & \cdots & f_{1n}(\omega) \\ \vdots & \ddots & \vdots \\ f_{n1}(\omega) & \cdots & f_{nn}(\omega) \end{pmatrix}, \qquad \omega \in [-\pi, \pi).$$
 (5.16)

is positive semi-definite for each $\omega \in [\pi, \pi)$.

Proof. Considering the matrix F of the (cross-) spectral functions and $\Delta F(\omega_1, \omega_2) =$ $F(\omega_2) - F(\omega_1)$ (see Corollary 5.16), we have

$$f(\omega) = \lim_{\delta \to 0} \frac{\Delta F(\omega, \omega + \delta)}{\delta}.$$

Corollary 5.16 yields $F(\omega, \omega + \delta)/\delta \succeq 0$ for any $\delta > 0$. Thus, the limit and therefore $f(\omega)$ is positive semi-definite as well.

Definition 5.23 (Spectral density matrix). We call the matrix-valued function f involved in (5.16) spectral density matrix.

In this chapter, we have extended Herglotz's theorem to the multidimensional case by proving the existence of a matrix F of complex measures that satisfies (5.5), see Theorem 5.8. Using Lemma 5.14, we examined the structure of matrix F and proved its positive semi-definiteness, see Theorem 5.15. If the corresponding (cross-) spectral functions are differentiable, the matrix of the densities is also positive semi-definite, see Corollary 5.22.



Modeling intermediate signals

In the previous chapters, we have gained basic knowledge about signals and their spectral representation. Now, we want to apply OMT to solve problems regarding signals and their spectral densities. We provide two examples that were solved numerically with MATLAB and the CVX toolbox, see Section 3.7. Both codes were executed on a standard laptop without GPU with a runtime of less than 15 seconds each. The number of sampling points in the corresponding discretizations was n = 80.

6.1 Scaling

Before introducing concrete applications, we want to discuss how we can manipulate Hermitian, positive semi-definite 2×2 matrix-valued functions $\mu: [a,b] \to H^2_+$ in order to receive functions $\widetilde{\mu} \in \mathcal{F}_c$ for some given $c \in (0, +\infty)$. Of course, the answer is scaling, however there are at least two sensible scaling methods that preserve the positive semi-definiteness.

The most obvious method is defining

$$c_{\mathrm{tr}} \coloneqq \int_{a}^{b} \operatorname{tr}(\mu(x)) dx$$

and

$$\widetilde{\mu} \coloneqq \frac{c}{c_{\mathrm{tr}}} \mu.$$

It can be readily verified that $\widetilde{\mu} \in \mathcal{F}_c$, if $\mu(x) \succeq 0$ for each x.

Another method is defining two constants $c_0, c_1 \in (0, +\infty)$ such that

$$\int_{a}^{b} \frac{\mu_{11}(x)}{c_0^2} + \frac{\mu_{22}(x)}{c_1^2} dx = c,$$

whereat

$$\mu(x) = \begin{pmatrix} \mu_{11}(x) & \mu_{12}(x) \\ \mu_{21}(x) & \mu_{22}(x) \end{pmatrix}.$$

We now define

$$\widetilde{\mu}(x) \coloneqq \begin{pmatrix} \mu_{11}(x)/c_0^2 & \mu_{12}(x)/(c_0c_1) \\ \mu_{21}(x)/(c_0c_1) & \mu_{22}(x)/c_1^2 \end{pmatrix}.$$

Since $\mu(x)$ is positive semi-definite, μ_{11} and μ_{22} are non-negative, see Definition 3.3. The determinant $\mu_{11}\mu_{22} - \mu_{12}\mu_{21}$, which is the product of the eigenvalues, is non-negative. Thus, one can show that both the trace and the determinant of $\widetilde{\mu}$ are non-negative and therefore $\widetilde{\mu}$ is positive semi-definite. Because of our choice of c_0 and c_1 , $\widetilde{\mu}$ is an element of \mathcal{F}_c .



6.2 N-dimensional signals

In Chapter 5, we considered multidimensional signals. In Corollary 5.22, we have seen that for each $\omega \in [-\pi, \pi)$, the value $f(\omega)$ of the spectral density matrix of a multidimensional signal is positive semi-definite. Given some $c \in (0, +\infty)$, we can scale f in order to receive an element of \mathcal{F}_c .

Given two n-dimensional signals X_0 and X_1 and their already scaled spectral density matrices $f_0 \in \mathcal{F}_c$ and $f_1 \in \mathcal{F}_c$, defined by (5.16), we now want to use the method of Section 3.6 to obtain the spectral density matrix $f_{0.5}$ of an "intermediate" signal $X_{0.5}$. A more concrete, special case of this situation will be discussed in Section 6.3.

To give an example, we now assume that two spectral density matrices $f_0, f_1 \in \mathcal{F}_1$ are given. For this purpose, we are using μ_0 and μ_1 from the example in [NGT14, Section V-A].

$$f_0(\omega) := \begin{pmatrix} 1 & 0 \\ \frac{1}{5} \exp(-i\omega) & 1 \end{pmatrix} \cdot \begin{pmatrix} \frac{1}{|a_0(\omega)|^2} & 0 \\ 0 & \frac{1}{100} \end{pmatrix} \cdot \begin{pmatrix} 1 & \frac{1}{5} \exp(i\omega) \\ 0 & 1 \end{pmatrix},$$
$$f_1(\omega) := \begin{pmatrix} 1 & \frac{1}{5} \\ 0 & 1 \end{pmatrix} \cdot \begin{pmatrix} \frac{1}{100} & 0 \\ 0 & \frac{1}{|a_1(\omega)|^2} \end{pmatrix} \cdot \begin{pmatrix} 1 & 0 \\ \frac{1}{5} & 1 \end{pmatrix},$$

with

$$a_0(\omega) = \left(\exp(2i\omega) - \frac{9}{5}\cos\left(\frac{\pi}{4}\right)\exp(i\omega) + \frac{81}{100}\right) \cdot \left(\exp(2i\omega) - \frac{7}{5}\cos\left(\frac{\pi}{3}\right)\exp(i\omega) + \frac{49}{100}\right),$$

$$a_1(\omega) = \left(\exp(2i\omega) - \frac{9}{5}\cos\left(\frac{\pi}{6}\right)\exp(i\omega) + \frac{81}{100}\right) \cdot \left(\exp(2i\omega) - \frac{3}{2}\cos\left(\frac{2\pi}{15}\right)\exp(i\omega) + \frac{9}{16}\right).$$

Figure 6.1 shows f_0 and f_1 together with $f_{0.5}$, computed as in Section 3.6.

Since $f_0, f_1, f_{0.5}$ are matrix-valued functions with complex entries, we cannot display them in a single graph. However, our functions are mapping to the Hermitian matrices. Hence, the diagonal entries $f_{k,11}, f_{k,22}, k \in \{0,1,0.5\}$ are real-valued. Furthermore, the off diagonal entries $f_{k,12}$, $k \in \{0,1,0.5\}$ are the complex conjugates of $f_{k,21}$, $k \in \{0,1,0.5\}$, respectively. Thus, it is sufficient to only display the absolute value $|f_{k,21}|$ (= $|f_{k,12}|$) and the argument $\angle f_{k,21}$ (= $-\angle f_{k,12}$). Therefore, Figure 6.1 displays $f_{k,11}$, $|f_{k,21}|$, $\angle f_{k,21}$ and $f_{k,22}$ for $k \in \{0, 1, 0.5\}$.

 f_0 and f_1 are conjugate symmetric functions, i.e., $f(-t) = \overline{f(t)}$. Hence it is not surprising that $f_{0.5}$ is also a conjugate symmetric function. For this reason, we are computing and plotting $f_{0.5}$ only in the interval $[0, \pi]$.

We can see that $f_{0.5}$ is indeed a mixture of f_0 and f_1 . The peak of $f_{0.5}$ is located in the middle of the peaks of f_0 and f_1 and the height of the peak is approximately the average of the heights of the peaks of f_0 and f_1 . In comparison, the most straightforward way of computing a mixture of f_0 and f_1 would be taking the arithmetic average of each value, i.e., defining $f_{0.5} := (f_0 + f_1)/2$. However, this $f_{0.5}$ would have two peaks that are located above/below the peaks of f_0 and f_1 . Hence, our more complicated computation yields results that better resemble an intermediate function between f_0 and f_1 .

In the plot of $\angle f_{0.5,21}$, we have an almost linear behavior in the interval $[0,\pi/2]$. However, there are high oscillations in the interval $[\pi/2,\pi]$. We should not overrate this strange

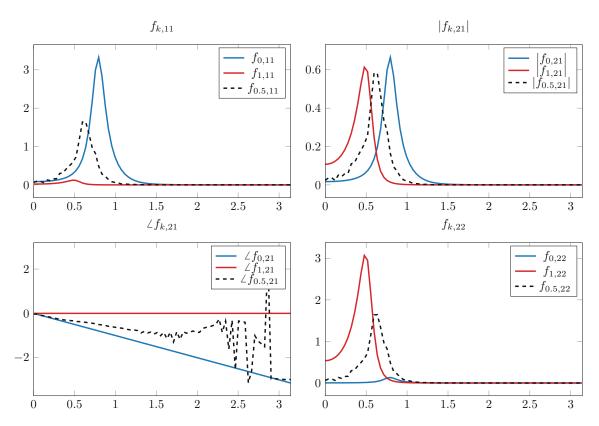


Figure 6.1: The plot on the top left shows the top left entries $f_{k,11}$ of f_k , the plot on the bottom right shows the bottom right entries $f_{k,22}$ of f_k with $k \in \{0,1,0.5\}$. These entries are real-valued. The bottom left entries $f_{k,21}$ are the conjugate transposed of the top right entries $f_{k,12}$, $k \in \{0,1,0.5\}$. In the top right plot we show their absolute values, in the bottom left plot we show their arguments. We can see that $f_{0.5}$ is indeed a mixture between f_0 and f_1 in all four entries.

behavior, since the absolute value $|f_{0.5,21}|$ in this interval is almost zero and the argument of complex numbers that are almost zero is not very relevant.

6.3 Filtered signals

6.3.1 Theoretical setup

In this section, we consider a room with a source and two sensors, see Figure 6.2. The source emits a signal X. The sensors receive signals Y_0 and Y_1 , respectively. Since there is some space between the source and the sensors and there might be, e.g., reflections from the surrounding walls, signal Y_0 and Y_1 are different from signal X. However, there is still some kind of correlation between the emitted signal and the received signals.

The aim of this section is finding an intermediate signal $Y_{0.5}$ that would correspond to a sensor that is located between sensor A and sensor B (gray dot in Figure 6.2).

A very common way of describing such a situation is modeling the interaction by considering

Sensor B

Sensor A

Source

Figure 6.2: A source is emitting a signal X, Sensor A and Sensor B are receiving (presumably) slightly different signals Y_0 and Y_1 . In the middle of the two sensors (gray dot), we assume signal $Y_{0.5}$.

room impulse functions. A detailed motivation can be found in [Smi08]. For this purpose, we assume that there are two room impulse functions $h_0, h_1 : \mathbb{Z} \to \mathbb{C}$ satisfying

$$y_0(t) = h_0(t) * x(t)$$
 and $y_1(t) = h_1(t) * x(t)$, (6.1)

for each outcome ω of the sample space Ω . The functions $x:t\to X(t)(\omega), y_0:t\to \infty$ $Y_0(t)(\omega), y_1: t \to Y_1(t)(\omega)$ are the realizations of X, Y_1, Y_2 with respect to ω . The symbol * denotes the discrete convolution, i.e.,

$$h(t) * x(t) \coloneqq (h * x)(t) \coloneqq \sum_{k=-\infty}^{\infty} h(k)x(t-k),$$

see [PM96, Section 2.3.4]. Since we have (6.1) for each outcome $\omega \in \Omega$, we can write

$$Y_0(t) = h_0(t) * X(t)$$
 and $Y_1(t) = h_1(t) * X(t)$.

Let us assume that the (cross-) spectral densities $f_{XX}, f_{X_kY}, f_{YX_k}, f_{Y_kY_k}, k \in \{0,1\}$ of X, Y_0, Y_1 exist. Furthermore, we denote the Fourier transforms of h_0 and h_1 as H_0 and H_1 , respectively. H_0 and H_1 are often called frequency responses, see e.g., [PM96, Section 4.4]. We have

$$f_{XY_k}(\omega) = \overline{H_k(\omega)} f_{XX}(\omega), \quad f_{Y_kX}(\omega) = H_k(\omega) f_{XX}(\omega), \quad f_{Y_kY_k}(\omega) = |H_k(\omega)|^2 f_{XX}(\omega)$$

for $k \in \{0, 1\}$, see [Pap91, Section 10.3]. For proving these statements, it might be helpful to recall that the autocovariance and cross-covariance are the Fourier transforms of the spectral density and cross-spectral density, respectively, see Section 5.3. We can now reformulate the matrix of the (cross-) spectral densities as

$$\begin{pmatrix} f_{XX}(\omega) & f_{XY_k}(\omega) \\ f_{Y_kX}(\omega) & f_{Y_kY_k}(\omega) \end{pmatrix} = f_{XX}(\omega) \cdot \underbrace{\begin{pmatrix} 1 & \overline{H_k(\omega)} \\ H_k(\omega) & |H_k(\omega)|^2 \end{pmatrix}}_{\mu_k(\omega) :=}, \quad k \in \{0, 1\}.$$



We have already discussed that the left-hand side of this equation is positive semi-definite. If $f_{XX}(\omega) \neq 0$ for all ω , we could deduce that $\mu_k(\omega)$ is also positive semi-definite. However, we can prove the positive semi-definiteness of $\mu_k(\omega)$ without this constraint: We are assuming $Y_0, Y_1 \not\equiv 0$, hence we have $h \not\equiv 0$ and $H \not\equiv 0$. Since the right columns of $\mu_0(\omega)$ and $\mu_1(\omega)$ are multiples of the left columns with factor $\overline{H_0(\omega)}$ and $\overline{H_1(\omega)}$, respectively, $\mu_0(\omega)$ and $\mu_1(\omega)$ are both of rank 1 and therefore have one eigenvalue of 0. As the traces, which are the sums of the eigenvalues, of $\mu_0(\omega)$ and $\mu_1(\omega)$ are positive, the other eigenvalues must be greater than zero. Thus, $\mu_0(\omega), \mu_1(\omega) \succeq 0$ for each $\omega \in [-\pi, \pi]$.

In the spirit of Section 6.1, we can scale $\mu_0(\omega)$ and $\mu_1(\omega)$ such that

$$\int_{-\infty}^{\infty} \operatorname{tr}(\mu_0(\omega)) d\omega = \int_{-\infty}^{\infty} \operatorname{tr}(\mu_1(\omega)) d\omega.$$

Now everything has been arranged for matrix-valued OMT.

6.3.2 Computation of the signal

We assume that two transfer functions \widetilde{H}_0 and \widetilde{H}_1 are already given. Let \widetilde{H}_0 , $\widetilde{H}_1: [-\pi, \pi] \to \mathbb{C}$ be defined as

$$\widetilde{H}_k(\omega) = \frac{\exp(2i\omega)}{(\exp(i\omega) - p_k)(\exp(i\omega) - \overline{p_k})}, \quad k \in \{0, 1\},$$

with

$$p_0 = \frac{9}{10} \cdot \exp\left(\frac{\pi}{6}i\right), \qquad p_1 = \frac{9}{10} \cdot \exp\left(\frac{2\pi}{3}i\right).$$

We do not want to give a detailed interpretation of our choice of $\widetilde{H_0}$ and $\widetilde{H_1}$. However, the knowledgeable reader will recognize that H_0 and H_1 correspond to filters with poles $p_0, \overline{p_0}$ and $p_1, \overline{p_1}$, respectively. A profound interpretation and explanation can be found in [PM96].

We define H_0 and H_1 by scaling H_0 and H_1 ,

$$H_0(\omega) := 2\pi \cdot \frac{\widetilde{H_0}(\omega)}{\int\limits_{-\pi}^{\pi} \widetilde{H_0}(\nu) d\nu}, \qquad H_1(\omega) := 2\pi \cdot \frac{\widetilde{H_1}(\omega)}{\int\limits_{-\pi}^{\pi} \widetilde{H_1}(\nu) d\nu}.$$

The matrix-valued functions $\mu_0, \mu_1 : [-\pi, \pi] \to H^2_+$

$$\mu_0(\omega) = \begin{pmatrix} 1 & \overline{H_0(\omega)} \\ H_0(\omega) & |H_0(\omega)|^2 \end{pmatrix}, \qquad \mu_1(\omega) = \begin{pmatrix} 1 & \overline{H_1(\omega)} \\ H_1(\omega) & |H_1(\omega)|^2 \end{pmatrix}, \tag{6.2}$$

are positive semi-definite for each $\omega \in [-\pi, \pi]$ and satisfy

$$\int_{-\pi}^{\pi} \operatorname{tr}(\mu_0(\omega)) d\omega = \int_{-\pi}^{\pi} \operatorname{tr}(\mu_1(\omega)) d\omega = 4\pi.$$

Hence, $\mu_0, \mu_1 \in \mathcal{F}_{4\pi}$, whereat

$$\mathcal{F}_{4\pi} := \left\{ \mu : [-\pi, \pi] \to \mathbb{C}^{2 \times 2} \mid \mu(\omega) \in H_+^2, \int_{-\pi}^{\pi} \operatorname{tr}(\mu(\omega)) d\omega = 4\pi \right\}.$$

We can now use our methods from Chapter 3 to find an intermediate $\mu_{0.5} \in \mathcal{F}_{4\pi}$,

$$\mu_{0.5}(\omega) = \begin{pmatrix} \mu_{0.5,11} & \mu_{0.5,12} \\ \mu_{0.5,21} & \mu_{0.5,22} \end{pmatrix}.$$

However, it would be favorable if there is an $H_{0.5}$ such that $\mu_{0.5}$ is of the form

$$\mu_{0.5}(\omega) = \begin{pmatrix} 1 & \overline{H_{0.5}(\omega)} \\ H_{0.5}(\omega) & |H_{0.5}(\omega)|^2 \end{pmatrix}. \tag{6.3}$$

In general, $\mu_{0.5}$ will not be of this form. Within the optimization problem of finding an intermediate $\mu_{0.5}$, we can set the constraint that μ is of form (6.3). However, adding this constraint will cause the optimization problem to be no longer convex. Instead, we try a different approach.

1. First, we define

$$\mathcal{F}_{4\pi,1} := \left\{ \mu : [-\pi, \pi] \to \mathbb{C}^{2 \times 2} \, \middle| \, \mu(\omega) \in H^2_+, \, \int_{-\pi}^{\pi} \operatorname{tr}(\mu(\omega)) \, d\omega = 4\pi, \, \, \mu_{11}(\omega) = 1 \right\},$$

so we add the affine constraint that the first entry $\mu_{11}(\omega)$ of $\mu(\omega)$ is equal to 1 for all $\omega \in [-\pi, \pi]$. It can be readily verified that $\mathcal{F}_{4\pi,1} \subseteq \mathcal{F}_{4\pi}$.

- 2. Using the method of Section 3.6, we determine $\widetilde{\mu}_{0.5} \in \mathcal{F}_{4\pi,1}$ that minimizes the sum $\mathcal{T}_{2,\lambda}(\mu_0,\mu) + \mathcal{T}_{2,\lambda}(\mu,\mu_1)$ over all $\mu \in \mathcal{F}_{4\pi,1}$. The function $\widetilde{\mu}_{0.5}$ is still the solution of a convex optimization problem, since the additional constraint is an affine constraint. see [BV09, Section 4.2.1].
- 3. Finally, we want to find $H_{0.5}: [-\pi, \pi] \to \mathbb{C}$ such that

$$\begin{pmatrix} 1 & \overline{H_{0.5}} \\ H_{0.5} & |H_{0.5}|^2 \end{pmatrix} \quad \text{and} \quad \begin{pmatrix} \widetilde{\mu}_{0.5,11} & \widetilde{\mu}_{0.5,12} \\ \widetilde{\mu}_{0.5,21} & \widetilde{\mu}_{0.5,22} \end{pmatrix}$$

are "close" to each other. Hence, we define $H_{0.5}$ by

$$H_{0.5} = \underset{H:[-\pi,\pi]\to\mathbb{C}}{\arg\min} \int_{-\pi}^{\pi} \left\| \widetilde{\mu}_{0.5}(\omega) - \begin{pmatrix} 1 & \overline{H(\omega)} \\ H(\omega) & |H(\omega)|^2 \end{pmatrix} \right\|_{F}^{2} d\omega \tag{6.4}$$

subject to
$$\int_{-\pi}^{\pi} \operatorname{tr} \begin{pmatrix} 1 & \overline{H(\omega)} \\ H(\omega) & |H(\omega)|^2 \end{pmatrix} d\omega = 4\pi$$
 (6.5)



whereat $\|.\|_F$ denotes the Frobenius norm. Hence, $H_{0.5}$ is the solution of another optimization problem. However, this optimization problem is not convex (e.g., $|H(\omega)|^2$ is not affine). Nevertheless, we will consider any computed solution of the optimization problem as $H_{0.5}$, although we can not ensure that the solution is not just a local minimum but also a global minimum. Furthermore, the optimization problem is not very sophisticated, therefore we can solve it in a relatively short time. We define μ_H by

$$\mu_H(\omega) := \begin{pmatrix} 1 & \overline{H_{0.5}(\omega)} \\ H_{0.5}(\omega) & |H_{0.5}(\omega)|^2 \end{pmatrix}. \tag{6.6}$$

Given the two functions $\mu_0, \mu_1 \in \mathcal{F}_{4\pi}$ (see (6.2)), we can therefore compute two different intermediate functions $\mu_{0.5}, \mu_H \in \mathcal{F}_{4\pi}$, whereat

• $\mu_{0.5}$ minimizes the sum $\mathcal{T}_{2,\lambda}(\mu_0,\mu_{0.5}) + \mathcal{T}_{2,\lambda}(\mu_{0.5},\mu_1)$, i.e., we have

$$\mathcal{T}_{2,\lambda}(\mu_0,\mu_{0.5}) + \mathcal{T}_{2,\lambda}(\mu_{0.5},\mu_1) \le \mathcal{T}_{2,\lambda}(\mu_0,\mu) + \mathcal{T}_{2,\lambda}(\mu,\mu_1)$$

for each $\mu \in \mathcal{F}_{4\pi}$. However, in general $\mu_{0.5}$ is not of form (6.3).

• μ_H is close to $\mu_{0.5}$ (with respect to (6.4)) and is of form (6.6). However, in general we

$$\mathcal{T}_{2,\lambda}(\mu_0,\mu_H) + \mathcal{T}_{2,\lambda}(\mu_H,\mu_1) > \mathcal{T}_{2,\lambda}(\mu_0,\mu_{0.5}) + \mathcal{T}_{2,\lambda}(\mu_{0.5},\mu_1).$$

In order to determine how "bad" μ_H behaves with respect to $\mathcal{T}_{2,\lambda}$, we compute the relative difference in distance, i.e.,

$$\Delta \mathcal{T}_{2,\lambda,\text{Rel}}(\mu_H, \mu_{0.5}) := \frac{\mathcal{T}_{2,\lambda}(\mu_0, \mu_H) + \mathcal{T}_{2,\lambda}(\mu_H, \mu_1)}{\mathcal{T}_{2,\lambda}(\mu_0, \mu_{0.5}) + \mathcal{T}_{2,\lambda}(\mu_{0.5}, \mu_1)} \approx 1.03696.$$

The value of $\Delta \mathcal{T}_{2,\lambda,\text{Rel}}(\mu_H,\mu_{0.5})$ appears to be close to 1, thus it seems that we have found a good approximation of $\mu_{0.5}$. However, since we have no knowledge about the reasonable interpretation of the actual values of $\mathcal{T}_{2,\lambda}$, we are not able to confidently distinguish if an approximation is good or bad.

Figure 6.3 compares $\mu_0, \mu_1, \mu_{0.5}^{-1}$ and μ_H . As before, $\mu_{0.5}$ and also μ_H seem like reasonable intermediate functions, although the height of their peaks are smaller than the height of the peaks of μ_0 and μ_1 . It seems that μ_H is the more reasonable intermediate function, since the height of the peak of $|\mu_{H,21}|$ is closer to the height of the peaks of $|\mu_{0,21}|$ and $|\mu_{1,21}|$ than the height of the peak of $|\mu_{0.5,21}|$. The reason for this lies in the fact that we have the constraint (by construction) that $|\mu_{H,21}| = \sqrt{|\mu_{H,22}|}$. Hence, it seems like the peak of $|\mu_{H,21}|$ is lifted up compared to the peak of $|\mu_{0.5,21}|$. Since all our functions are conjugate symmetric, we plot the graphs only in the interval $[0,\pi]$. In Figure 6.4, we compare the transfer functions H_0, H_1 and $H_{0.5}$.

¹In the actual $\mu_{0.5}$ there is a lot of small oscillation. For this plot, we used a small regularization term to get a smoother solution and hence a more meaningful comparison with the other functions. The value of $\Delta \mathcal{T}_{2,\lambda,\text{Rel}}(\mu_H,\mu_{0.5})$ is based on the actual $\mu_{0.5}$.



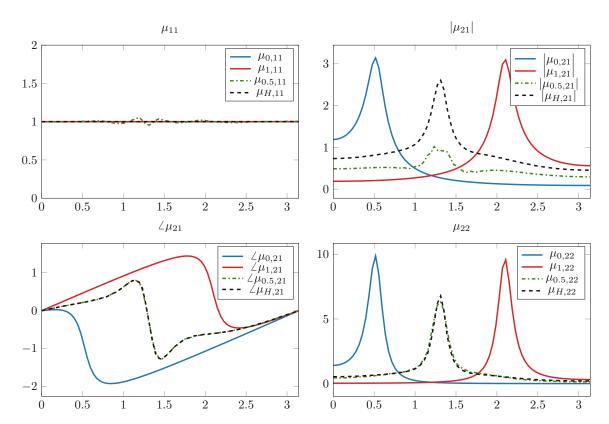


Figure 6.3: Using the same notation and arrangement of plots as in Figure 6.1, we see that both $\mu_{0.5}$ and μ_H resemble a mixture of μ_0 and μ_1 . However, the absolute values of the off-diagonal entries in μ_H seem to be more reasonable than in $\mu_{0.5}$.

6.4 Optimal mass transport for complex-valued functions

In Chapter 2, we introduced the concept of OMT for non-negative, real-valued functions $f:[a,b]\to\mathbb{R}_0^+,\ [a,b]\subseteq\mathbb{R}$. In Chapter 3, we were considering Hermitian, positive semidefinite matrix-valued functions. The matrices were subsets of $\mathbb{C}^{n\times n}$, but since the matrices were Hermitian, the diagonal entries were always real-valued. So if we consider matrices of size 1×1 , those values of our functions are not complex-valued but real-valued.

We now want to ask if it is also possible to define OMT for complex-valued functions $f:[a,b]\to\mathbb{C}$. In this case, we would expect that a corresponding transport plan is also a complex-valued function, presumably in every entry. Considering the cost functions (2.4) and (3.6), this would lead to a complex-valued cost. However, we cannot minimize complex-valued costs.

Instead, we want to recapitulate our example in Section 6.3: After talking about the theoretical setup, we considered two functions $H_0, H_1: [-\pi, \pi] \to \mathbb{C}$ and arranged them in such a way, that we could use the methods of Chapter 3. Afterwards, we extracted an intermediate function $H_{0.5}: [-\pi, \pi] \to \mathbb{C}$. Of course, we can also use this method in other situations where two complex-valued functions are given.



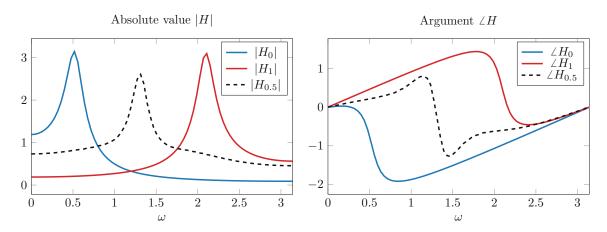


Figure 6.4: Based on the values in Figure 6.3, we use the fact that the bottom right entry of μ_H corresponds exactly to |H| and the argument of the bottom left entry of μ_H is the argument of H. Hence, we can compare H_0, H_1 and $H_{0.5}$ both in terms of absolute values and in terms of arguments, see left plot and right plot, respectively.

Let $[a, b] \subseteq \mathbb{R}$ and $f_0, f_1 : [a, b] \to \mathbb{C}$ with

$$\int_{a}^{b} |f_0(z)| \, dz = \int_{a}^{b} |f_1(z)| \, dz.$$

The functions $\mu_0, \mu_1 : [a, b] \to H^2_+$, defined by

$$\mu_0(z) = \begin{pmatrix} 1 & \overline{f_0(z)} \\ f_0(z) & |f_0(z)|^2 \end{pmatrix}, \qquad \mu_1(z) = \begin{pmatrix} 1 & \overline{f_1(z)} \\ f_1(z) & |f_1(z)|^2 \end{pmatrix},$$

are elements of \mathcal{F}_c (see (3.2)) for some $c \in (0, \infty)$. After adding the constraint $\mu_{11} = 1$, we can determine an intermediate function

$$\mu_{0.5}(z) = \begin{pmatrix} 1 & \overline{\mu_{21}} \\ \mu_{21} & \mu_{22} \end{pmatrix}.$$

Finally, we define $f_{0.5}:[a,b]\to\mathbb{C}$ as

$$f_{0.5} = \underset{f_{0.5}:[a,b]\to\mathbb{C}}{\arg\min} \int_{a}^{b} \left\| \mu_{0.5}(z) - \begin{pmatrix} 1 & \overline{f_{0.5}(z)} \\ f_{0.5}(z) & |f_{0.5}(z)|^2 \end{pmatrix} \right\|_{F}^{2} dz$$
subject to
$$\int_{a}^{b} \operatorname{tr} \begin{pmatrix} 1 & \overline{f_{0.5}(z)} \\ f_{0.5}(z) & |f_{0.5}(z)|^2 \end{pmatrix} dz = c.$$

Thus, we have found a method to determine an intermediate, complex-valued function $f_{0.5}:[a,b]\to\mathbb{C}.$



Discussion

In this thesis, we first introduced optimal mass transport in its basic form, see Chapter 2. Based on [NGT14], we provided an extension of OMT to Hermitian, positive semi-definite matrix-valued functions, see Chapter 3. In order to formulate it in a sensible way, we had to consider the tensor product space $\mathbb{C}^{n\times n}\otimes\mathbb{C}^{n\times n}$ and introduce a new transport cost. Although parts of the new formulation seem very abstract, the actual computation of an optimal transport plan can be done in a fast and effective way, since we only need to solve a convex optimization problem.

In Chapter 4 and Chapter 5, we were dealing with the theory of signals and its statistical properties. A central statement was Herglotz's theorem. We proved a multidimensional version of Herglotz's theorem and furthermore formulated and proved a statement about the positive semi-definiteness of the cross-spectral measure matrix. A corresponding corollary was later used in Chapter 6.

In Chapter 6, we used OMT of Hermitian, positive semi-definite matrix-valued functions to find intermediate signals between two multidimensional signals. For this purpose, we were not only considering the spectral density of each signal component but also the corresponding cross-spectral densities. The plots of our computed solutions revealed that OMT indeed provides realistic results for finding intermediate signals.

The first part of this thesis was understanding OMT and elaborating the paper On Matrixvalued Monge-Kantorovich Optimal Mass Transport, see [NGT14]. In particular, the partial traces and their related spaces required more precise descriptions.

The coding in MATLAB was very time-consuming, since it was not clear how to efficiently implement the optimization process. Using the CVX toolbox was the first game changer, installing the MOSEK solver finally enabled solving problems of our size. However, prior efforts with the Optimization Toolbox did not lead to any useful results.

Another challenge was introducing signals in a profound mathematical way. Most literature about this topic is dedicated to engineers and hence does not provide stringent proofs. A similar statement to one of the main theorems of this thesis, Theorem 5.8, can be found in [Lin12]. However, the given proof was not satisfying and hence we had to prove the theorem, including the required lemma, by ourselves. However, this was a very joyful task.

An exciting property of this thesis is that many different areas of mathematics come into play. The author was surprised by how many lecture notes from various courses he had to consult while working on the thesis, although the topic of the thesis seems to be quite application-oriented. In addition to basics from analysis and linear algebra, we also had to deal with more abstract objects, e.g., tensor products, complex measures and statements from functional analysis. Furthermore, stochastic processes were a central element of this thesis. Finally, optimization and numerical mathematics came into play when implementing the developed methods.

In this thesis, we have dealt with a wide variety of topics. However, there are many things that could be examined further:

- In Section 6.2 and Section 6.3, we started with functions that are mapping to the Hermitian, positive semi-definite matrices. In order to have elements of \mathcal{F}_c for some given $c \in (0, +\infty)$, we had to scale the functions, see Section 6.1. However, we did not examine the (presumably unwanted) effects of the scaling. In particular, we can ask for a way to rescale the results in order to equalize the corruption caused by the scaling.
- In the definition of the transport cost, see (3.6), we used the parameter λ , which acted as a weighting factor between the impact of distance cost and the impact of directional cost. When computing the solutions in Chapter 6, we chose $\lambda = 1/10$, since this value was also chosen in [NGT14]. However, we can consider different values of λ and compare the results.
- In Chapter 6, we applied our methods to "concrete" examples. However, the examples were still relatively theoretical¹. The plausibility of the methods was checked by evaluating the plots. In a next step, we can compare the results to real data. For example, we can consider data of Room Impulse Response generators² or set up speakers and microphones in a real room and measure the corresponding signals.
- The classical OMT deals with real-valued functions. In Section 6.4, we introduced a method of applying OMT to complex-valued functions. Next, we can look for complex-valued problems and try to solve them with our new, fruitful method.

¹Since the author is a student of Technical Mathematics, solving these examples was still one of the most applied tasks he was doing within his studies.

²An implementation of a Room Impulse Response generator based on [AB79] can be found via https: //www.audiolabs-erlangen.de/fau/professor/habets/software/rir-generator

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