On the computation of Fortet-Mourier and Dudley distances between measures: Functional analytic expressions and algorithms

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Functional analytic expressions and algorithms

Master's thesis

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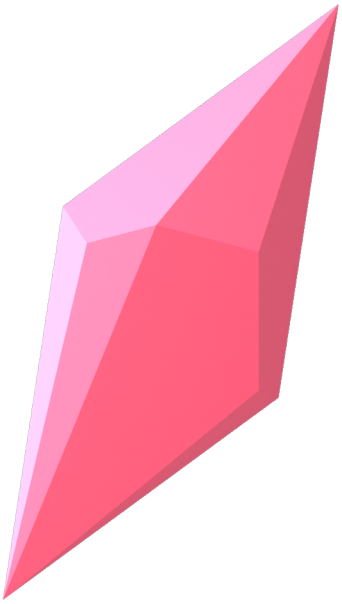

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Abstract

This master thesis is dedicated to the computation of Fortet-Mourier and Dudley norms of finite signed Borel measures on metric spaces and concepts related to it. Both norms are defined as the supremum of a convex functional on a closed unit ball in a space of bounded Lipschitz functions. Since this supremum is attained at an extreme point, we first study extreme points.

We characterize a dense subset of the extreme points of the closed unit ball in the space of bounded Lipschitz functions equipped with the norm $\|\cdot\|_{\mathrm{BL}} := \|\cdot\|_\infty + |\cdot|_L$, for any underlying connected metric space S. This is a novel result. Until now, a characterization was only known for the norm $\|\cdot\|_{\mathrm{FM}} := \max(\|\cdot\|_\infty, |\cdot|_L)$ or for the very specific space $S = [0,1]$.

After that, we derive expressions for Fortet-Mourier distances between finite positive measures ν and μ, with ν a positive linear combination of Dirac measures. We give an explicit expression for the Fortet-Mourier distance between a Dirac measure and any finite positive measure μ. Such an expression was not known in the field before, except for the distance between two Dirac measures. For ν a general positive linear combination of Dirac measures, we prove that the distance to a finite positive measure can be obtained by minimizing a convex functional over a convex and compact subset of $\mathbb{R}^n$, where n equals the number of points in the support of ν. We propose efficient numerical methods to approximate the norm.

Next, we consider the case in which ν and μ are both a linear combination of Dirac measures. We present highly efficient, exact algorithms to compute the distance between μ and ν in both the Fortet-Mourier and Dudley norm, using linear programming. Up till now, algorithms that achieve this were only known for specific cases: $S \subset \mathbb{R}$ for the Fortet-Mourier norm, or ν, μ both empirical probability measures for the Dudley norm. Our algorithms generalize substantially: they enable us to compute the distance between any two linear combinations of Dirac measures on any metric space S, in both the Fortet-Mourier and Dudley norm.

Finally, we touch upon the topic of approximation theory in a context of measures. We study approximations of finite positive measures by positive measures with a finite support consisting of at most N points. We prove an existence result for the case in which the underlying metric space is compact. For non-compact settings, we study examples and pose a conjecture.

Preface and acknowledgement

A first step towards this thesis was taken already one and a half year ago, when I was orienting on possible thesis supervisors and topics. During my studies, I had developed a big passion for the abstract side of both analysis and stochastics, and ideally, I wanted to combine both fields. In my first conversation with my supervisor, Dr. Sander Hille, it immediately became clear that our mathematical interests had a very strong overlap, and I happily made use of his offer to be my supervisor.

When I started my thesis last September, the original goal was to determine best approximations for any (fixed) probability measure with a density with respect to the Lebesgue measure, by convex or positive linear combinations of at most N Dirac measures, with $N \in \mathbb{N}$ fixed. We wanted to measure the distances between measures in Fortet-Mourier or Dudley metric since they also apply to measures with different total mass. It took some time before we came on the right track. We started by exploring articles about related approximation problems for Wasserstein distances, in the hope of finding an idea that could be applied to the Fortet-Mourier or Dudley metric as well. There were many articles about convergence rates of approximations for $N \to \infty$, but the question of a best approximation for a fixed N seemed even not to be addressed. Another attempt was to study optimal partitions for Riemann sums, but that did not provide an opening either. Therefore, we posed ourselves the question whether one can compute the distance between a probability measure and a convex combination of Dirac measures at all, and if so, how.

This question turned out to be difficult to answer. It was via functional analysis that we obtained our first essential inspiration. To me, functional analysis is one of the most delicate fields in mathematics, and the more functional analysis became involved, the more excited I became. From that point on, we kept making smaller and bigger new discoveries, deriving various new expressions and algorithms to compute Fortet-Mourier and Dudley distances between measures. It was extremely rewarding to use abstract and elegant mathematics for such a concrete goal (for mathematicians at least) as computing distances.

What I also really loved, was the fact that so many fields of mathematics turned out to be linked to our measure theoretic problems. For example, we encountered geometric problems and linear and convex programming problems. Therefore, I learned about other fields as well while working on this thesis. In the final phase, we even discovered that a very simple example of one of our original approximation problems was equivalent to a famous problem posed by Fermat four hundred years ago, in a geometric context then. Although it was somewhat intimidating that Fermat had been thinking about one of our problems, the idea also gave me joy. In this way, I felt a tiny bit connected to the great Fermat and all the other mathematicians who have been thinking about related problems.

In the end phase of my thesis, we turned back to the initial approximation questions. Even with our newly developed methods for computing distances, it remained difficult to find best approximations, even for measures of simple forms. When we accidentally discovered that one of our most simple examples was equivalent to the *Fermat-Weber problem*, we received the confirmation that finding best approximations is generally impossible. It turned out that the Fermat-Weber problem is one of the most famous problems in *location theory.* And indeed, even after several hundreds of years of mathematicians concerned with this famous problem, the problem can only be solved numerically in most cases. Then, we decided that it was time to wrap things up. Nevertheless, I sincerely hope that I will have the opportunity to study the approximation questions again as

I feel that there is more to discover yet, at least for some specific cases. The many examples we have considered revealed some interesting properties about best approximations that increased my curiosity. In the Outlook, the reader can find an outline of some new paths that might be worth exploring in the future.

Now that my school and study years are almost complete, I realize that mathematics has become very meaningful to me. As a small kid already, I loved making calculations with numbers. I got even more interested when I first learnt about the magical 'number' x, used to solve linear equations in one variable at that time. I will never forget the first time this was explained at school. While studying mathematics at university, again a new world of mathematics opened up to me, which fascinated me even more. I loved all the beautiful fields of mathematics and the clever and often elegant proofs we encountered in the courses. Also, I loved the immense power of mathematics for solving both abstract and real-world problems. In the last year, I appreciated another aspect of mathematics more than before. This was due to our troubled world, threatened by wars, political conflicts, pandemics, climate change, ecological crises and even more (but I will not depress the reader any further). It was especially comforting to do mathematics in these moments, since it is one of the only ways to have a feeling of certainty. The world can rapidly change, as we have seen in the past years. On the other hand, in mathematics, once you have proved something carefully, you can be sure that it will remain valid forever. This quality of mathematics has become more meaningful to me, especially now.

I want to thank my supervisor, Sander, a lot. The major part of the process leading to this thesis has been a true joy, and this was really due to his enthusiasm and support. Besides his knowledge and mathematical ideas, Sander's attitude towards research was really inspiring. Always relaxed (it seemed to me) and guided by a lot of curiosity. Even when I was totally stuck in mathematical problems, I felt calm after our thesis meetings and was eager to make new proving attempts. Also, the freedom and time granted for my guitar playing and conservatory exam was really appreciated. Finally, I am grateful to Sander for the very generous amount of time reserved for our discussions. I enjoyed them a lot and they made the Friday afternoons more fruitful than ever...

Esmée Suzanna Theewis
June 12, 2022

Contents

Introduction

The bulk of this master thesis is concerned with topics that can be rightfully characterized as 'fundamental mathematics'. This by no means implies that the obtained results are without application. Quite the contrary: the fundamental research has been motivated by application. We shall start introducing this connection by some examples.

The world is becoming urbanized at an ever increasing speed. In 1950, only 28.3% of the world population lived in urban areas, while in 2010, the proportion had raised to 50% ([WHL$^+$12]). It is expected that by 2050, 68% of the world population will live in urban areas. Taking global population growth into account, this means that 6.6 billion people of the global population of 9.7 billion people will be living in urban areas [SCLH20]. Urbanization gives rise to a huge amount of challenges involving interacting individuals. For example, challenges related to pedestrian and traffic flow, spread of diseases, public space planning and crowd control at large-scale events. Therefore, modeling interacting individuals is becoming more and more important.

Within mathematics, there are several fields that develop models of interacting individuals. Since the mathematical setting is abstract, it does not matter whether the modeled 'individuals' are people, animals, physical particles or anything else. The mathematical models can more or less be divided into two categories: discrete models and continuum models. In a discrete model, every individual is described separately, together with its dynamics. For example, a model can be given by a set of variables x_i representing the trait of interest of the i-th individual, together with a differential equation for each separate x_i, describing its dynamics. The equations are coupled somehow, modeling the interaction. On the other hand, in a continuum model, one represents the individuals by a (continuous) density representing the concentration of the individuals over some domain. In this case, the dynamics are described in terms of the density, for example by a partial differential equation (PDE).

Both ways of modeling have advantages and disadvantages. A discrete model contains detailed information about the separate individuals. However, when the number of individuals is large, computing the trajectory of each individual can become very inefficient. Moreover, prescribing appropriate, realistic parameter values and initial conditions for each individual separately can become cumbersome, or simply impossible.

In contrast, for continuum models, the computational efficiency is not affected by a large number of individuals, since the individuals are captured in one density anyway. Here, one describes 'the average', making it feasible to provide parameters and initial conditions. In fact, the larger the number, the more accurate the model becomes generally, provided that the individuals are somewhat 'homogeneous', in the sense that their characteristics and dynamics are not very different. A large flock of sheep could be modeled well, while the more independent behavior of a few predators (e.g., wolves) chasing the sheep could not be considered in a continuum model. Another advantage of continuum models, especially in physical contexts, is that PDEs can often be derived very naturally, e.g., from fundamental physical laws or from experimental data, while the governing dynamics of separate individuals is harder or impossible to find. In such cases, working with continuum models is convenient.

A straightforward downside of continuum models is that (deliberately) information about the separate individuals is lost. Therefore, they are foremost suitable for studying - roughly speaking - the 'mean behavior' of rather homogeneous populations of individuals. Moreover, although the theory of PDEs is far developed, most PDEs cannot be solved exactly. Therefore, one has to use numerical methods to approximate a solution. The most popular methods that achieve this (for example, finite difference methods, finite element methods and finite volume methods), require a discretization of the spatial domain of the PDE. Constructing this discretization is a huge challenge when the domain has a complicated shape, although the topic is intensively studied ([TA02],[LO80],[SS08]). Conversely, models that are discrete from the beginning are not bothered by complexly shaped domains generally.

Because of the different qualities and limitations of both types of models, it would be very beneficial if the models could be related to each other and compared in some sense. To do so, a framework in which discrete and continuum descriptions can be unified is convenient. A measure theoretic framework has this unifying property, since both discrete and continuum descriptions can be given in terms of measures.

Let us consider an example of such descriptions by measures. Suppose we want to model the spread of a virus (SARS-CoV-2, that is, ‘corona’ - why not) within a large city. Specifically, we are interested in the distribution of viral load (within the inhabitants) over the area of the city. In a discrete description, one describes the viral load of each person separately. Using measures, this could be performed as follows. Let $S \subset \mathbb{R}^2$ represent the area of a city with N inhabitants. In accordance with [Thi19] and [DGMT94], let $S \times \mathbb{R}_+$ be the state space of relevant individual characteristics. In this case, the i-th inhabitant is represented by $(x_i, \alpha_i) \in S \times \mathbb{R}_+$, where x_i is the location of this person and α_i is its viral load. The state of the population is then given by:

$$\nu_0 = \sum_{i=1}^{N} \delta_{(x_i,\alpha_i)}.$$

Often, the measure is also scaled, so that the measure becomes a probability measure: $\bar{\nu}_0 = \frac{1}{N}\sum_{i=1}^{N} \delta_{(x_i,\alpha_i)}$. A measure of the latter form is called an *empirical measure*, although this term is usually found in a context where the (x_i, α_i) are random variables. The marginal of ν_0 with respect to the first variable is defined by

$$\nu_{\mathrm{sd}}(E) := \nu_0(E \times \mathbb{R}_+), \qquad E \in \mathcal{B}(S),$$

where $\mathcal{B}(S)$ is the Borel σ-algebra of S. Hence,

$$\nu_{\mathrm{sd}} = \sum_{i=1}^{N} \delta_{x_i},$$

so the measure ν_{sd} describes the spatial distribution of the inhabitants. The distribution of viral load over the space can be captured by a measure ν_{vl} derived from ν_0:

$$\nu_{\mathrm{vl}}(E) := (\alpha d\nu_0)(E \times \mathbb{R}_+) := \int_{E\times\mathbb{R}_+} \alpha d\nu_0(x,\alpha), \qquad E \in \mathcal{B}(S).$$

Indeed, it can easily be verified that

$$\nu_{\mathrm{vl}} = \sum_{i=1}^{N} \alpha_i \delta_{x_i}, \tag{1}$$

describing exactly the viral load distribution over S. If we assume that virus is transmitted through contact only, virus can only be at the same location as individuals. This translates into the mathematical statement that ν_{vl} must be absolutely continuous with respect to ν_{sd}.

On the other hand, in a continuum description, the spatial distribution of the individuals and the viral load distribution over the space S are given by

$$\mu_{\mathrm{sd}} = f_{\mathrm{sd}} d\lambda$$

and

$$\mu_{\mathrm{vl}} = f_{\mathrm{vl}} d\lambda, \tag{2}$$

respectively, for some density functions $f_{\mathrm{sd}}, f_{\mathrm{vl}} \in L^1(\lambda)$. Recall that we are interested in the state of the viral load distribution over the city. We can now either choose (1) or (2) as a representation for this state, corresponding to a discrete and a continuum model, respectively. The convenience is that both representations are measures, enabling us to relate and compare them to each other.

Besides the unification of discrete and continuum descriptions, the measure theoretic framework has even more advantages. In some continuum models, densities converge to something which is no longer a density when time evolves. For example, this can happen if the individuals are represented by a trait x_i and in the long term, every member of the population has the same trait. In that case, the concentration is 'infinite' for that trait and zero at all other traits, so it can no longer be seen as a density function. In the measure theoretic framework, the limit state can simply be represented by a Dirac measure, solving the issue. Examples of models where densities converge to Dirac measures can be found in [AMHF99] and [AFT05], in the context of population dynamics. Another model with such a phenomenon is the *Patlak-Keller-Segel model* (also: *Keller-Segel model*). This is a model for *chemotaxis*, the movement of organisms (e.g., bacteria) caused by (different concentrations of) chemicals in their environment. In [HV97], it is proved that the solution of the classical model develops a 'Dirac-delta type' singularity in finite time. That is, at some time T, all cells have moved to a finite number of *aggregation points*. After time T, the cells stay concentrated in these aggregation points, but the points start to move, according to the dynamics described in [Vel04] and [DS09]. The solution before time T is a density relative to the Lebesgue measure, while after T, the solution can be viewed as a linear combination of Dirac measures. In [HV97], it is not explicitly put in that way yet, as the authors are not working with measure-valued solutions. However, in [DS09], measure-valued solutions are introduced and in [Bla12], the model is also studied in a measure framework. In particular, [Bla12, Theorem 1] shows that the solutions of the model are first densities but converge to a non-density. The model is still of interest. For example, in [BLM20], a discretized version of the model is presented and it is shown that the classical Patlak-Keller-Segel model is a continuum limit of this discrete version.

Since measures are abstract objects, they can describe any system of interacting individuals. Related to urbanization challenges, we already mentioned some examples of applications of logistic, biological and social nature. One can think of other relevant systems of individuals in the world of today: for example, the recent congestions at Schiphol airport, the spread of the corona virus and disappearing animal species. These systems all concern interacting living individuals. Besides that, there exist many systems of non-living interacting individuals that are studied in various sciences. In physics for instance, interacting particles, molecules, and magnetic fields are intensively studied. Here, discrete models (e.g., multi-particle models) and continuum models (e.g., as appearing in continuum mechanics) exist next to each other. Relating these models using measures is another challenging, but meaningful goal. It is worth mentioning that discrete and continuum models which are not deterministic but (partly) stochastic can be described by measures as well. This is yet another advantage of measures.

We hope the reader is by now convinced of benefits of a measure theoretic framework for modeling. Once we have a discrete and continuum model in terms of measures, we can consider distances between predictions made by these models. Distances enable us to to quantify the difference between these predictions, now measures. The main topic of this thesis, namely, computing distances between measures ν and μ, where ν is of the form (1) and μ is a finite positive measure (for instance, of the form (2)), is thus an essential tool when comparing models within a measure framework.

To measure distances, one first needs suitable metrics for measures. The so-called *Wasserstein distances* W_p, for $p \geq 1$, are a popular family of metrics on measures. However, these metrics are only defined for measures with the same total mass, which is very limiting when considering measures with dynamics ([PR13]). Measures modeling the earlier mentioned situations, typically do not have preservation of mass. For example, when modeling the spread of a virus via (1), the total mass $|\nu_{\mathrm{vl}}|(S) = \sum_{i=1}^{N} \alpha_i$ represents the total presence of virus in the N individuals. However, when time evolves and the people meet and get infected by each other, the total viral load can increase. Conversely, the load can decrease when more people have overcome an infection. So the total mass of the measures representing the states of the system varies and Wasserstein metrics are not suitable in these settings. Therefore, we consider other distances in this thesis. Some that do apply to measures of different total mass.

Luckily, there exist several alternative metrics for measures with different total mass. Rather recently, new metrics were proposed in [PR13]. In this thesis, we will be working with distances that have a longer tradition but have not been studied as much as Wasserstein distances. We measure distances between measures in the *Fortet-Mourier norm* $\|\cdot\|^*_{\mathrm{FM}}$ and *Dudley* or *bounded Lipschitz norm* $\|\cdot\|^*_{\mathrm{BL}}$. These norms are given by

$$\|\mu\|^*_{\mathrm{FM}} := \sup\{\int_S f\,d\mu : f \text{ bounded Lipschitz, } \|f\|_\infty \leq 1, |f|_L \leq 1\}$$

and

$$\|\mu\|^*_{\mathrm{BL}} := \sup\{\int_S f\,d\mu : f \text{ bounded Lipschitz, } \|f\|_\infty + |f|_L \leq 1\},$$

where $\|\cdot\|_\infty$ and $|\cdot|_L$ denote the supremum norm and Lipschitz constant, respectively. In fact, both norms are dual norms, that are defined in a natural way when one embeds the measures into duals of spaces of bounded Lipschitz functions. This will be discussed in detail in Chapter 1. Besides the fact that these norms operate on the whole space of finite signed measures, they have other pleasant properties. To mention one, they metrize the weak topology on finite positive measures (Theorem 1.2.13). Therefore, convergence in one of our studied norms automatically implies weak convergence.

The main part of this thesis is devoted to the computation of distances of the form

$$||\nu - \mu||^*_\bullet, \qquad \nu = \sum_{i=1}^N \alpha_i \delta_{x_i},\ x_i \in S,\ \alpha_i \geq 0,\ \mu \in \mathcal{M}^+(S), \qquad \bullet = \mathrm{FM}, \mathrm{BL}\,. \tag{3}$$

Here, S can be any metric space and $\mathcal{M}^+(S)$ denotes the set of finite positive Borel measures on S. In particular, the results can be applied to distances between the measures ν_{vl} and μ_{vl} given in (1) and (2), where ν_{vl} appeared in a discrete description and μ_{vl} was part of a continuum description.

Until now, very few results have been known about distances as in (3). The only exact, explicit expressions for such distances that are stated in the literature, are for distances between two Dirac measures:

$$\|\delta_x - \delta_y\|^*_{\mathrm{FM}} = \min(2, d(x,y)), \qquad \|\delta_x - \delta_y\|^*_{\mathrm{BL}} = \frac{d(x,y)}{2 + d(x,y)},$$

as can be found in [HW09, Lemma 3.5 and Remark], for example. Also, there exist some estimates and upper bounds on (3), but mostly for more specific cases. For instance, it is possible to estimate (3) for $\bullet = \mathrm{BL}$ when both ν and μ are probability measures, using random samples drawn from ν and μ. In [SFG⁺12], it is shown that such ‘empirical estimators’ converge to the exact distance. However, one should be cautious when consulting the literature, since there exist many different names for metrics on measures, and the same names may refer to different metrics. For instance, the Fortet-Mourier metric in [SFG⁺12] is different from the one defined in this thesis, so only the results for the Dudley metric ($\bullet = \mathrm{BL}$) apply.

In this thesis, the knowledge on distances as in (3) is extended. We derive several new expressions that can be applied to compute distances. Let us highlight a few of the new results.

In Propositions 3.1.2 and 4.1.2, we derive an expression for

$$\|\delta_x - \mu\|^*_{\mathrm{FM}}, \qquad x \in S, \mu \in \mathcal{M}^+(S).$$

This is a considerable generalization compared to the only case $\mu = \delta_y$ for which an explicit expression was known.

Secondly, in Section 4.4, we present an exact algorithm for computing

$$\|\nu - \mu\|^*_\bullet, \qquad \nu = \sum_{i=1}^n \alpha_i \delta_{x_i},\ \mu = \sum_{i=1}^m \beta_j \delta_{y_j},\ \alpha_i, \beta_j \in \mathbb{R},\ x_i, y_j \in S,\ n, m \in \mathbb{N}, \qquad \bullet = \mathrm{FM}, \mathrm{BL}\,. \tag{4}$$

The problem of computing such distances has been considered before, in [JMC13] and by others. Thus far, methods only applied to specific cases. For the case in which ν and μ are both empirical probability measures (that is, $\alpha_i = \frac{1}{n}$, $\beta_j = \frac{1}{m}$ for all i and j) and $\bullet = \mathrm{BL}$, a method can be found in [SFG+12, Theorem 2.3]. On the other hand, for general $\alpha_i, \beta_j \in \mathbb{R}$, but in the specific setting $\bullet = \mathrm{FM}$ and $S = [a, b] \subset \mathbb{R}$ an interval, or $S = \mathbb{R}$, a rather complicated algorithm was obtained in [JMC13, §3.3]. The total ordering on $\mathbb{R}$ was exploited in an essential way in the algorithm proposed in this paper. The general metric space setting causes more difficulties, since one cannot use a natural total ordering on S such as '$\leq$' on $\mathbb{R}$. However, by using a functional analytic perspective, we bypass this problem. Our algorithm thus generalizes the algorithm in [JMC13] in two directions: it can be applied to all metric spaces S and to both the Fortet-Mourier and Dudley distance.

Lastly, we would like to emphasize the novel result in Theorem 2.5.10, which we find beautiful in itself, although not immediately applicable to the computation of norms. This theorem provides a characterization of a dense subset of the extreme points of the closed unit ball in the space of bounded Lipschitz functions, equipped with the norm $\|\cdot\|_{\mathrm{BL}} = \|\cdot\|_\infty + |\cdot|_L$. In our result, the underlying metric space S is only assumed to be connected. Until now, such a dense subset for general metric spaces S was only known for the norm $\max(\|\cdot\|_\infty, |\cdot|_L)$ and for S connected and compact, a result by [Joh75]. Establishing a proof of Theorem 2.5.10 was a considerable challenge and required several non-trivial preliminary results.

In Chapter 5, we consider a different challenge than computing norms. Namely, we study some approximation problems that came up naturally while considering the following. Suppose we have a continuum model with some density solution $fd\lambda$. Furthermore, suppose it is given that the density models a system of N interacting individuals (with weights) for some $N \in \mathbb{N}$. Then, two questions arise: first, how can one replace the initial condition in the continuum description, say $\mu_0 = f_0 d\lambda$, by a configuration of a weighted sum of N Dirac measures with the least error? Next, one would like to estimate the change in error when the two types of solutions evolve. Therefore, one needs to be able to compute or estimate norms of the form $\|\nu - fd\lambda\|_\bullet^*$ ($\bullet = \mathrm{FM}, \mathrm{BL}$), where ν is a positive sum of at most N Dirac measures, for example. It is natural to desire that this error remains as small as possible. So again, one can wonder: which discrete description of the form (1) (with N fixed) is closest to the density description $fd\lambda$? And before that, does such a closest discrete description exist? It is well known that $fd\lambda$ can be approximated arbitrarily well by linear combinations of Dirac measures in Fortet-Mourier and Dudley norm, as long as N is allowed to increase to ∞ (see Theorem 1.2.18). However, little can be found on best approximations.

The approximation problem mentioned also seems related to problems in numerical analysis, in some way. Many numerical analytic methods require a discretization of a domain, after which a 'target function' (for instance, the solution of a PDE) is approximated by a piecewise polynomial that is determined by its values at these mesh points. It is rather natural to fix a maximal number of mesh points N to limit the computational cost. Then, one can wonder which locations of N mesh points will lead to best approximations of the target function. This resembles our approximation problem for measures slightly.

We conclude with an outline of this thesis.

Outline

Before we derive new expressions for distances between measures, we properly introduce all spaces and metrics involved and we study some results from measure theory. These matters form the main contents of Chapter 1.

In Chapter 2, we present a thorough study of the closed unit balls in spaces of bounded Lipschitz functions. We demonstrate that Fortet-Mourier and Dudley distances between measures can be expressed in terms of the extreme points of closed unit balls in Lipschitz spaces. Therefore, we proceed by studying the extreme points of these balls. For the norm $\max(\|\cdot\|_\infty, |\cdot|_L)$ on bounded Lipschitz functions, [Joh75] already presented a characterization of a dense subset of the extreme points in a general compact, connected metric space setting (see Theorem 2.4.7). We discuss and prove this theorem and extend it to non-compact connected metric spaces. In contrast, for the norm $\|\cdot\|_{\mathrm{BL}} := \|\cdot\|_\infty + |\cdot|_L$, a similar characterization was not known yet (only for $S = [0,1]$, in [RR70]). We present and prove a dense subset for the norm $\|\cdot\|_{\mathrm{BL}}$ in Theorem 2.5.10. The norm $\|\cdot\|_{\mathrm{BL}}$ is more complicated to work with than the norm $\|\cdot\|_{\mathrm{FM}}$. Therefore, the preparations for proving Theorem 2.5.10 occupy a considerable part of the chapter. We conclude by showing that the established dense subsets are sufficient for defining the Fortet-Mourier and Dudley norm of any finite signed measure.

In Chapter 3, we start computing distances explicitly. Here, we turn our attention to computing distances when both ν and μ are probability measures, with ν a convex combination of Dirac measures. In the proofs of the expressions that we derive, we encounter many of the extreme points described in Chapter 2. However, the proofs are independent of the results in the latter chapter. Thus, the results from Chapter 3 are proved in large generality: we do not impose any condition on the underlying metric space. A novel result is Theorem 3.1.2, which gives an explicit expression for the Fortet-Mourier distance between a Dirac measure and any probability measure.

In Chapter 4, we generalize to distances between measures with different total mass. Theorem 4.1 provides an expression for the Fortet-Mourier distance between a Dirac measure and any finite positive measure. After that, we consider the case in which both ν and μ are a linear combination of Dirac measures. In Section 4.4, we present our already mentioned new algorithm that computes the distance between linear combinations of Dirac measures on any metric space, in both the Fortet-Mourier and Dudley norm, generalizing the result in [JMC13] considerably. Section 4.5 discusses an alternative approach to computing the distances. The approach is of limited practical use, but it offers an insightful geometric picture for the problem. We conclude the chapter by considering again our most general setting, with μ any finite positive measure. We show that the distances $\|\nu-\mu\|_\bullet^*$ can be obtained by minimizing a convex and Lipschitz continuous functional and give examples to do so numerically.

In Chapter 5, we consider approximation problems for measures of a specific form: given a probability measure μ, does there exist a best approximation within the set of all measures of the form (1)? That is, within the set of all positive linear combinations of at most N Dirac measures. Here, 'best' is meant as 'closest' with respect to the Fortet-Mourier or Dudley distance. For compact Polish spaces S, we establish a proof for the affirmative. For non-compact spaces, we formulate a conjecture, which is still an open problem. To get more insights, we study some simple examples of our approximation problems, for which we can explicitly find best approximations using the new expressions obtained in the previous chapters. In Section 5.3, we prove that finding a best approximation for one of our simplest examples is equivalent to the - not at all trivial - *Fermat-Weber problem.* In Section 5.4, we sketch some possible strategies for proving our existence conjecture and outline the obstacles that have to be overcome. We suggest some ideas that could help to achieve this.

The thesis concludes with an outlook in which we give some recommendations for further research, based on our results.

Chapter 1

Preliminaries

In this chapter, we introduce normed spaces of bounded Lipschitz functions and we describe how measures can be viewed naturally as elements of their dual space. Furthermore, we introduce molecular measures, which will play an important role in Chapter 2. Finally, we relate the several topologies on spaces of measures that are used in this thesis. The material in this chapter is mainly based on [Dud66], [Bog07] and [HW09].

In what follows, we assume that (S, d) is a metric space.

1.1 Bounded Lipschitz functions

Definition 1.1.1. We denote the linear space of real-valued bounded Lipschitz functions on S by $\mathrm{BL}(S) := \mathrm{BL}_{\mathbb{R}}(S, d)$. We will be working with two different norms on this space. The first one is the *Fortet-Mourier norm* $\|\cdot\|_{\mathrm{FM}}$, given by

$$\|f\|_{\mathrm{FM}} := \max(\|f\|_\infty, |f|_L),$$

where

$$\|f\|_\infty := \sup_{s\in S} |f(s)|, \qquad |f|_L := \sup_{x\neq y, x,y\in S} \frac{|f(x)-f(y)|}{d(x,y)}.$$

The value $|f|_L$ is known as the *Lipschitz constant* of f. The name 'Fortet-Mourier norm' usually refers to a related norm on measures that we encounter later. However, we choose to use the same term for the norm on $\mathrm{BL}(S)$ above.

The second norm is the *bounded Lipschitz norm* $\|\cdot\|_{\mathrm{BL}}$, given by

$$\|f\|_{\mathrm{BL}} = \|f\|_\infty + |f|_L.$$

We call the metrics induced by $\|\cdot\|_{\mathrm{FM}}$ and $\|\cdot\|_{\mathrm{BL}}$ the *Fortet-Mourier distance* and the *bounded Lipschitz distance*, respectively. We abbreviate 'Fortet-Mourier' by 'FM' and 'bounded Lipschitz' by 'BL'.

To make clear with what norm we are working, we write $\mathrm{BL}(S)_{\mathrm{FM}} := (\mathrm{BL}(S), \|\cdot\|_{\mathrm{FM}})$ and $\mathrm{BL}(S)_{\mathrm{BL}} := (\mathrm{BL}(S), \|\cdot\|_{\mathrm{BL}})$. We denote the closed unit balls in these spaces by

$$\mathrm{B}_\bullet := \{f \in \mathrm{BL}(S) : \|f\|_\bullet \leq 1\}, \qquad \bullet = \mathrm{FM}, \mathrm{BL}.$$

Lemma 1.1.2. *The norms* $\|\cdot\|_{\mathrm{FM}}$ *and* $\|\cdot\|_{\mathrm{BL}}$ *are equivalent on* $\mathrm{BL}(S)$.

Proof. For any $f \in \mathrm{BL}(S)$, we have

$$\frac{1}{2}(\|f\|_\infty + |f|_L) \leq \max(\|f\|_\infty, |f|_L) \leq \|f\|_\infty + |f|_L,$$

giving the result. □

Proposition 1.1.3. $\mathrm{BL}(S)_{\mathrm{FM}}$ *and* $\mathrm{BL}(S)_{\mathrm{BL}}$ *are Banach spaces.*

Proof. We prove the statement for $\mathrm{BL}(S)_{\mathrm{FM}}$. From Lemma 1.1.2, it then follows that $\mathrm{BL}(S)_{\mathrm{BL}}$ is a Banach space too.

Let $(f_n) \subset \mathrm{BL}(S)$ be a Cauchy sequence in $\mathrm{BL}(S)_{\mathrm{FM}}$. Then, we have for all $x \in S$ and $n, m \in \mathbb{N}$:

$$|f_n(x) - f_m(x)| \leq \|f_n - f_m\|_\infty \leq \|f_n - f_m\|_{\mathrm{FM}}.$$

So $(f_n(x)) \subset \mathbb{R}$ is a Cauchy sequence for each $x \in S$ and has a limit, which we denote by $f(x) := \lim_{n\to\infty} f_n(x)$. We show that $f \in \mathrm{BL}(S)$ and $f_n \to f$ in $\mathrm{BL}(S)_{\mathrm{FM}}$.

To see that f is bounded, note that

$$\big|\|f_n\|_\infty - \|f_m\|_\infty\big| \leq \|f_n - f_m\|_\infty \leq \|f_n - f_m\|_{\mathrm{FM}},$$

so $(\|f_n\|_\infty) \subset \mathbb{R}$ is Cauchy, thus convergent. In particular, it is bounded, so there exists $M \in \mathbb{R}$ with $\|f_n\|_\infty \leq M$ for all $n \in \mathbb{N}$. Then, $|f(x)| = \lim_{n\to\infty} |f_n(x)| \leq \limsup_{n\to\infty} \|f_n\|_\infty \leq M$ for all $x \in S$, so $\|f\|_\infty \leq M$.

Let $\varepsilon > 0$ and let $N \in \mathbb{N}$ be such that $\|f_n - f_m\|_{\mathrm{FM}} < \varepsilon$ for all $n, m > N$. For all $n > N$ and $x, y \in S$, we have

$$\begin{aligned}|(f_n - f)(x) - (f_n - f)(y)| = \lim_{m\to\infty} |(f_n - f_m)(x) - (f_n - f_m)(y)| &\leq \limsup_{m\to\infty} |f_n - f_m|_L d(x,y)\\ &\leq \limsup_{m\to\infty} \|f_n - f_m\|_{\mathrm{FM}} d(x,y)\\ &\leq \varepsilon\, d(x,y),\end{aligned}$$

so

$$|f_n - f|_L = \sup_{x,y\in S, x\neq y} \frac{|(f_n - f)(x) - (f_n - f)(y)|}{d(x,y)} \leq \varepsilon\,.$$

This proves that $f = f_n - (f_n - f)$ is Lipschitz continuous, as it is the difference between two Lipschitz continuous functions. Since f was also bounded, this gives $f \in \mathrm{BL}(S)$.

Finally, for $n > N$ and for all $x \in S$, we have

$$|f_n(x) - f(x)| = \lim_{m\to\infty} |f_n(x) - f_m(x)| \leq \limsup_{m\to\infty} \|f_n - f_m\|_\infty \leq \limsup_{m\to\infty} \|f_n - f_m\|_{\mathrm{FM}} \leq \varepsilon,$$

so $\|f_n - f\|_\infty \leq \varepsilon$. Therefore, $\|f_n - f\|_{\mathrm{FM}} \leq \varepsilon$ for $n > N$. This proves that $\|f_n - f\|_{\mathrm{FM}} \to 0$, with $f \in \mathrm{BL}(S)$. We conclude that $\mathrm{BL}(S)_{\mathrm{FM}}$ is complete. □

We continue with some useful results on bounded Lipschitz functions.

Lemma 1.1.4. *Let* $f_1, \dots, f_n \in \mathrm{BL}(S)$*. It holds that* $f_{\min}, f_{\max} \in \mathrm{BL}(S)$*, where*

$$f_{\min} = \min(f_1, \dots, f_n), \quad f_{\max} = \max(f_1, \dots, f_n),$$

and

$$|f_{\min}|_L, |f_{\max}|_L \leq \max_{1\leq i\leq n} |f_i|_L.$$

Proof. See [Dud66, Lemma 4]. □

The following proposition is also known as the *Tietze Extension Theorem* for Lipschitz functions.

Proposition 1.1.5. *Let* P *be a non-empty subset of* S *and let* $f^* \in \mathrm{BL}(P)$ *with* $\|f^*\|_\infty = M$ *and* $|f^*|_L = C$*. Then there exists* $f \in \mathrm{BL}(S)$ *with* $f|_P = f^*$*,* $\|f\|_\infty = M$ *and* $|f|_L = C$*.*

Proof. Define

$$f_0 : S \to \mathbb{R} : s \mapsto \sup\{f^*(t) - Cd(t,s) : t \in P\}$$

and

$$f : S \to \mathbb{R} : s \mapsto \max(f_0(s), -M).$$

For any $s \in S$ and $t \in P$, it holds that $f^*(t) - Cd(t,s) \leq f^*(t) \leq \|f^*\|_\infty = M$, so $f_0 \leq M$. From the definition of f, it follows that $-M \leq f \leq M$, i.e., $\|f\|_\infty \leq M$.

Now, we show that $f = f_0 = f^*$ on P. Let $t_0 \in P$. Recall that $|f^*|_L = C$, so for any $t \in P$, we have

$$f^*(t) - f^*(t_0) \leq |f^*(t) - f^*(t_0)| \leq Cd(t,t_0).$$

This yields for all $t \in P$:

$$f^*(t) - Cd(t,t_0) \leq f^*(t) - (f^*(t) - f^*(t_0)) = f^*(t_0) = f^*(t_0) - Cd(t_0,t_0).$$

Hence, $f_0(t_0) = f^*(t_0)$. Also, $f^*(t_0) \geq -\|f^*\|_\infty = -M$. So $f(t_0) = \max(f_0(t_0), -M) = f_0(t_0) = f^*(t_0)$. As $t_0 \in P$ was arbitrary, we conclude that $f = f_0 = f^*$ on P.

As an immediate consequence of the fact that $f|_P = f^*$, we have $\|f\|_\infty \geq \|f^*\|_\infty = M$ and $|f|_L \geq |f^*|_L = C$, provided that f is Lipschitz continuous. Since we already proved that $\|f\|_\infty \leq M$, we conclude that $\|f\|_\infty = M$ and it only remains to show that f is Lipschitz continuous with $|f|_L \leq C$.

To this end, we first show that f_0 is Lipschitz continuous with $|f_0|_L \leq C$. Let $s_1, s_2 \in S$. Applying the triangle inequality twice yields

$$f^*(t) - Cd(t,s_2) - Cd(s_1,s_2) \leq f^*(t) - Cd(t,s_1) \leq f^*(t) - Cd(t,s_2) + Cd(s_1,s_2),$$

for all $t \in P$. Taking the supremum over $t \in P$, it follows that

$$f_0(s_2) - Cd(s_1,s_2) \leq f_0(s_1) \leq f_0(s_2) + Cd(s_1,s_2).$$

Therefore, $|f_0(s_1) - f_0(s_2)| \leq Cd(s_1,s_2)$ and f_0 is Lipschitz continuous. From Lemma 1.1.4 it follows that f is Lipschitz continuous and $|f|_L \leq \max(|f_0|_L, |-M|_L) \leq \max(C,0) = C$. Since we already proved the other inequality, we conclude that $|f|_L = C$. ☐

In future chapters, we consider restrictions of functions to subsets and norms on these. To omit confusion, we sometimes stress the underlying subset in our notation.

Definition 1.1.6. Let $\emptyset \neq P \subset S$. We let P inherit the metric d from S, so that we can consider $\mathrm{BL}(P)$, equipped with the norm

$$\|\cdot\|_{\bullet,P} := \max(\|\cdot\|_{\infty,P}, |\cdot|_{L,P}), \qquad \bullet = \mathrm{FM},\ \mathrm{BL},$$

where for $f \in \mathrm{BL}(S)$,

$$\|f\|_{\infty,P} := \sup_{s\in P} |f(s)|, \qquad |f|_{L,P} := \sup_{x\neq y, x,y\in P} \frac{|f(x)-f(y)|}{d(x,y)}.$$

We write $\mathrm{B}_\bullet^P$ for the closed unit ball in $\mathrm{BL}(P)$ with respect to the $\|\cdot\|_{\bullet,P}$-norm.

For $\bullet = \mathrm{FM}, \mathrm{BL}$, the notations $\|\cdot\|_\bullet$ and $\mathrm{B}_\bullet$ without the extra subscripts will always refer to $\|\cdot\|_{\bullet,S}$ and $\mathrm{B}_\bullet^S$, respectively. The latter notations are sometimes also used, to make a clearer distinction between the whole space S and its subset P.

On the other hand, to improve readability, we will sometimes omit the subscript P in $\|f\|_{\infty,P}$ and $|f|_{L,P}$ when $f \in \mathrm{BL}(P)$. Since the domain of f is P, it should automatically be clear that $\|f\|_\infty$ and $|f|_L$ refer to $\|f\|_{\infty,P}$ and $|f|_{L,P}$, respectively.

Corollary 1.1.7. *Let $\emptyset \neq P \subset S$. The restriction map $R_P : \mathrm{BL}(S)_\bullet \to \mathrm{BL}(P)_\bullet : g \mapsto g|_P$ maps $\mathrm{B}_\bullet^S$ onto $\mathrm{B}_\bullet^P$ for $\bullet = \mathrm{FM}, \mathrm{BL}$.*

Proof. Well-definedness is trivial. Let $f \in \mathrm{B}_\bullet^P$ and let g be its extension to S as constructed in Proposition 1.1.5. Then $g \in \mathrm{B}_\bullet^S$, $R_P(g) = f$ and $\|g\|_\bullet = \|f\|_{\bullet,P}$, so $\mathrm{B}_\bullet^P \subset R_P(\mathrm{B}_\bullet^S)$. On the other hand, from the definition of $\|\cdot\|_{\bullet,P}$ it is immediate that $\|R_P(g)\|_{\bullet,P} \leq \|g\|_\bullet$ for all $g \in \mathrm{B}_\bullet^S$, yielding $R_P(\mathrm{B}_\bullet^S) \subset \mathrm{B}_\bullet^P$. We conclude that $\mathrm{B}_\bullet^P = R_P(\mathrm{B}_\bullet^S)$. ☐

1.2 Embeddings of measures in dual Lipschitz spaces

As a consequence of Lemma 1.1.2, the dual spaces of $\mathrm{BL}(S)_{\mathrm{FM}}$ and $\mathrm{BL}(S)_{\mathrm{BL}}$ are the same as sets, and we denote this set by $\mathrm{BL}(S)^*$. However, the dual norm on $\mathrm{BL}(S)^*$ will depend on the norm we choose on $\mathrm{BL}(S)$. Therefore, we have two different (normed) dual spaces.

Definition 1.2.1. We denote the dual spaces of $\mathrm{BL}(S)_{\mathrm{FM}}$ and $\mathrm{BL}(S)_{\mathrm{BL}}$ by

$$\mathrm{BL}(S)^*_{\mathrm{FM}} = (\mathrm{BL}(S)^*, \|\cdot\|^*_{\mathrm{FM}}), \qquad \mathrm{BL}(S)^*_{\mathrm{BL}} = (\mathrm{BL}(S)^*, \|\cdot\|^*_{\mathrm{BL}}),$$

respectively. Here, the dual norms are given by

$$\|\phi\|^*_{\mathrm{FM}} := \sup\{\phi(f) : f \in \mathrm{B}_{\mathrm{FM}}\}, \qquad \|\phi\|^*_{\mathrm{BL}} := \sup\{\phi(f) : f \in \mathrm{B}_{\mathrm{BL}}\}.$$

Although the dual norms defined above are different, the topology they induce is the same, as a result of the next lemma.

Lemma 1.2.2. *The norms* $\|\cdot\|^*_{\mathrm{FM}}$ *and* $\|\cdot\|^*_{\mathrm{BL}}$ *are equivalent on* $\mathrm{BL}(S)^*$.

Proof. By Lemma 1.1.2, we have $\frac{1}{2}\|\cdot\|_{\mathrm{BL}} \leq \|\cdot\|_{\mathrm{FM}} \leq \|\cdot\|_{\mathrm{BL}}$, so $\mathrm{B}_{\mathrm{BL}} \subset \mathrm{B}_{\mathrm{FM}} \subset 2\cdot \mathrm{B}_{\mathrm{BL}}$. Hence, for any $\phi \in \mathrm{BL}(S)^*$, we have

$$\begin{aligned}
\|\phi\|^*_{\mathrm{BL}} = \sup\{\phi(f) : f \in \mathrm{B}_{\mathrm{BL}}\} &\leq \sup\{\phi(f) : f \in \mathrm{B}_{\mathrm{FM}}\} = \|f\|^*_{\mathrm{FM}} \\
&\leq \sup\{\phi(f) : f \in 2\cdot \mathrm{B}_{\mathrm{BL}}\} \\
&= \sup\{\phi(2f) : f \in \mathrm{B}_{\mathrm{BL}}\} \\
&= \sup\{2\phi(f) : f \in \mathrm{B}_{\mathrm{BL}}\} \\
&= 2\|\phi\|^*_{\mathrm{BL}}.
\end{aligned}$$

□

We now turn our attention to measures. Using the upcoming Lemma 1.2.7, we will demonstrate how measures can be viewed as elements of $\mathrm{BL}(S)^*$. But first, we give some notations and introduce the subspace of *molecular measures*, consisting of linear combinations of Dirac measures. Moreover, we prove two lemmas about the support of a measure. These will be convenient for the material in Chapter 5.

Definition 1.2.3. We denote the space of finite signed measures on a measurable space (S, Σ) by $\mathcal{M}(S, \Sigma)$. In this thesis, we only work with topological (metric) spaces S, and we always let $\Sigma := \mathcal{B}(S)$ be the Borel σ-algebra, i.e., the σ-algebra generated by all open subsets of S. Therefore, we reserve the shorter notation $\mathcal{M}(S) := \mathcal{M}(S, \mathcal{B}(S))$ for the set of all finite signed Borel measures.

We define the subspace of *molecular measures* by

$$\mathrm{Mol}(S) := \mathrm{span}\{\delta_x : x \in S\}.$$

We let $\mathcal{M}^+(S) \subset \mathcal{M}(S)$ be the cone of positive measures and let $\mathcal{P}(S) \subset \mathcal{M}^+(S)$ be the subset of probability measures.

For $\mu \in \mathcal{M}(S)$, $|\mu| := \mu^+ + \mu^-$ denotes the total variation measure of μ. Here, μ^+ and μ^- denote the positive and negative parts of μ, respectively. If the reader is not familiar with these measures, we refer to [Bog07, I, Theorem 3.1.1, Corollary 3.1.2, Definition 3.1.4] for the construction of these and some useful properties.

Finally, the *support* of $\mu \in \mathcal{M}(S)$ is defined by

$$\mathrm{supp}(\mu) := \bigcap\{F \subset S : F \text{ is closed }, |\mu|(S \setminus F) = 0\}. \tag{1.1}$$

If $\#\,\mathrm{supp}(\mu) < \infty$, then μ is called *finitely supported.*

Lemma 1.2.4. *Let* (S, d) *be a separable metric space and let* $\mu \in \mathcal{M}(S)$. *Then, the following statements hold:*

(i) $|\mu|(\operatorname{supp}(\mu)) = |\mu|(S)$.

(ii) $|\mu|(E) = |\mu|(E \cap \operatorname{supp}(\mu))$ *for all* $E \in \mathcal{B}(S)$.

(iii) For any open $A \subset S$, *it holds that* $|\mu|(A) = 0$ *if and only if* $\operatorname{supp}(\mu) \cap A = \emptyset$.

Proof. A proof of (i) can be found in [Bog07, II, Proposition 7.2.9]. For (ii), note that $0 \leq |\mu|(E \cap \operatorname{supp}(\mu)^c) \leq |\mu|(\operatorname{supp}(\mu)^c)) = |\mu|(S) - |\mu|(\operatorname{supp}(\mu) = 0$, so $|\mu|(E \cap \operatorname{supp}(\mu)^c) = 0$. Consequently, $|\mu|(E) = |\mu|(E) - |\mu|(E \cap \operatorname{supp}(\mu)^c) = |\mu|(E \cap \operatorname{supp}(\mu))$. Finally, for (iii), assume that $|\mu|(A) = 0$. Then $|\mu|(A \cap \operatorname{supp}(\mu)) = |\mu|(A) = 0$ by (ii). Hence, $|\mu|(\operatorname{supp}(\mu) \cap A^c) = |\mu|(\operatorname{supp}(\mu)) - |\mu|(A \cap \operatorname{supp}(\mu)) = |\mu|(\operatorname{supp}(\mu)) = |\mu|(S)$. Now, if $\operatorname{supp}(\mu) \cap A \neq \emptyset$, then $\operatorname{supp}(\mu) \cap A^c$ is a closed set that is strictly contained in $\operatorname{supp}(\mu)$, with $|\mu|(S \setminus (\operatorname{supp}(\mu) \cap A^c)) = 0$, contradicting (1.1). For the reverse implication, suppose that $\operatorname{supp}(\mu) \cap A = \emptyset$. By (ii), we have $|\mu(A)| = |\mu|(A \cap \operatorname{supp}(\mu)) = |\mu|(\emptyset) = 0$. ☐

Lemma 1.2.5. *Let* (S, d) *be a separable metric space and let* $\mu \in \mathcal{M}^+(S)$. *Then for any* $N \in \mathbb{N}$, μ *is a finitely supported measure with* $\# \operatorname{supp}(\mu) \leq N$ *if and only if* $\mu = \sum_{i=1}^N \alpha_i \delta_{x_i}$ *for some* $x_i \in S$ *and* $\alpha_i \geq 0$.

Proof. Suppose that $\mu \in \mathcal{M}^+(S)$ and $k := \# \operatorname{supp}(\mu) \leq N$. Write $\operatorname{supp}(\mu) = \{x_1, \ldots, x_k\}$ and define $x_j = x_1$ for $k < j \leq N$. Let $\alpha_i = \mu(\{x_i\})$ for $1 \leq i \leq k$ and put $\alpha_i = 0$ for $k < i \leq N$. Note that $\alpha_i \geq 0$ for all i, since $\mu \in \mathcal{M}^+(S)$. Define $\nu = \sum_{i=1}^N \alpha_i \delta_{x_i}$. We show that $\mu = \nu$. Since S is a separable metric space, for all $E \in \mathcal{B}(S)$, we have by Lemma 1.2.4 (ii):

$$\mu(E) = \mu(E \cap \operatorname{supp}(\mu)) = \mu(E \cap \{x_1, \ldots, x_n\}) = \sum_{i=1}^k \mu(\{x_i\}) \, \mathbb{1}_E(x_i) = \sum_{i=1}^k \alpha_i \, \mathbb{1}_E(x_i) = \nu(E),$$

i.e., $\mu = \nu$.

For the other implication, let $\mu = \sum_{i=1}^N \alpha_i \delta_{x_i}$ for some $x_i \in S$ and $\alpha_i \geq 0$. Clearly, $\mu \in \mathcal{M}^+(S)$. Also, $\mu(S \setminus \{x_1, \ldots, x_N\}) = 0$ and $\{x_1, \ldots, x_N\}$ is a closed set, so by Definition 1.2.3, $\operatorname{supp}(\mu) \subset \{x_1, \ldots, x_N\}$. In particular, $\# \operatorname{supp}(\mu) \leq N$, concluding the proof. ☐

Remark 1.2.6. *A main reference used in the upcoming results is Dudley's article [Dud66]. There,* $\mathcal{M}(S)$ *denotes the finite signed Baire measures* $\mathcal{M}(S, \mathcal{B}a(S))$. *However, for metric spaces* S *it holds that* $\mathcal{B}a(S) = \mathcal{B}(S)$ *([HW09, p.6]). So the results in [Dud66] also apply to the setting in this thesis.*

The following lemma gives embeddings of $\mathcal{M}(S)$ into $\mathrm{BL}(S)^*$ and $C_b(S)^*$. Consequently, we can naturally view $\mathcal{M}(S)$ as a subspace of $\mathrm{BL}(S)^*$ and $C_b(S)^*$.

Lemma 1.2.7. *The maps*

$$\iota : \mathcal{M}(S) \to \mathrm{BL}(S)^*, \ \iota(\mu)(f) := \int_S f \, d\mu, \quad \iota_2 : \mathcal{M}(S) \to C_b(S)^*, \ \iota_2(\mu)(f) := \int_S f \, d\mu$$

are well-defined and injective.

Proof. It is easy to check that $\iota(\mu)$ and $\iota_2(\mu)$ are elements of $\mathrm{BL}(S)^*$ and $C_b(S)^*$, respectively, for any $\mu \in \mathcal{M}(S)$. So ι and ι_2 are well-defined. Injectivity of ι is an immediate consequence of [Dud66, Lemma 6]. For injectivity of ι_2, note that $\mathrm{BL}(S) \subset C_b(S)$ and note that for all $\mu \in \mathcal{M}(S) \setminus \{0\}$, there exists $f \in \mathrm{BL}(S) \subset C_b(S)$ with $\iota_2(\mu)(f) = \iota(\mu)(f) \neq 0$, which also proves injectivity of ι_2. ☐

Definition 1.2.8. Using the embedding ι from Lemma 1.2.7, we can define the spaces $\mathcal{M}(S)_{\mathrm{FM}} := (\mathcal{M}(S), \| \cdot \|_{\mathrm{FM}}^*)$ and $\mathcal{M}(S)_{\mathrm{BL}} := (\mathcal{M}(S), \| \cdot \|_{\mathrm{BL}}^*)$. Here ,

$$\|\mu\|_\bullet^* := \|\iota(\mu)\|_\bullet^* = \sup\{ | \langle \mu, f \rangle | : f \in \mathrm{B}_\bullet \}, \qquad \bullet = \mathrm{FM}, \mathrm{BL},$$

where we use the notation

$$\langle \mu, f \rangle := \iota(\mu)(f) = \int_S f \, d\mu, \qquad \mu \in \mathcal{M}(S), f \in \mathrm{BL}(S).$$

By definition of $\|\cdot\|_{\mathrm{FM}}^*$ and $\|\cdot\|_{\mathrm{BL}}^*$ and by Lemma 1.2.7, we trivially have $\mathcal{M}(S)_{\mathrm{FM}} \cong \iota(\mathcal{M}(S)_{\mathrm{FM}})$ and $\mathcal{M}(S)_{\mathrm{BL}} \cong \iota(\mathcal{M}(S)_{\mathrm{BL}})$ as topological spaces.

For finite signed measures, we call $\|\cdot\|_{\mathrm{FM}}^*$ the *Fortet-Mourier norm* and $\|\cdot\|_{\mathrm{BL}}^*$ the *bounded Lipschitz norm*, respectively. Recall that we use the same names for $\|\cdot\|_{\mathrm{FM}}$ and $\|\cdot\|_{\mathrm{BL}}$. It will always be clear from the context whether we refer to a norm for bounded Lipschitz functions or to a dual norm for measures.

The spaces $\iota(\mathcal{M}(S)_{\mathrm{FM}})$ and $\iota(\mathcal{M}(S)_{\mathrm{BL}})$ are generally not closed in $\mathrm{BL}(S)_{\mathrm{FM}}^*$ and $\mathrm{BL}(S)_{\mathrm{BL}}^*$, respectively (see [HW09, Theorem 3.11] and Lemma 1.2.2). However, we can define their closure:

$$\overline{\mathcal{M}}(S)_\bullet := \left(\overline{\iota(\mathcal{M}(S))}^{\|\cdot\|_\bullet^*}, \|\cdot\|_\bullet^*\right) \subset \mathrm{BL}(S)_\bullet^*, \qquad \bullet = \mathrm{FM}, \mathrm{BL}.$$

Likewise, we define for the molecular measures:

$$\overline{\mathrm{Mol}}(S)_\bullet := \left(\overline{\iota(\mathrm{Mol}(S))}^{\|\cdot\|_\bullet^*}, \|\cdot\|_\bullet^*\right) \subset \mathrm{BL}(S)_\bullet^*.$$

Remark 1.2.9. *In the literature, many different names are used for dual norms on measures. For example,* $\|\cdot\|_{\mathrm{BL}}^*$ *is also referred to as the* Dudley norm, *the* dual bounded Lipschitz norm *and the* flat norm. *To make things more confusing, the norm* $\|\cdot\|_{\mathrm{FM}}^*$ *is also called the flat norm occasionally. In [Bog07, II],* $\|\cdot\|_{\mathrm{FM}}^*$ *is called the* Kantorovich-Rubinshtein norm, *whilst incorrect. The Kantorovich-Rubinshtein norm was originally invented in the context of optimal transport problems, and is given by* $\|\mu\|_{\mathrm{KR}} = \sup\{|\langle \mu, f \rangle| : f \in \mathrm{Lip}(S), |f|_L \le 1\}$. *We choose to adopt the terminology 'Fortet-Mourier norm' from Lasota and Szarek (see [LMS02]), for the reason that it is commonly used. Ironically, Fortet and Mourier only define* $\|\cdot\|_{\mathrm{BL}}^*$ *in their original paper [FM53, p. 277]. We hope the reader will be forgiving.*

Another well-known topology on $\mathcal{M}(S)$ is the *weak topology*, which is defined using the second embedding in Lemma 1.2.7.

Definition 1.2.10. The *weak topology* on $\mathcal{M}(S)$ is defined as the $\sigma(\mathcal{M}(S), C_b(S))$-topology, where $\mathcal{M}(S)$ is identified with $\iota_2(\mathcal{M}(S)) \subset C_b(S)^*$ as in Lemma 1.2.7.

Strictly speaking, the term 'weak topology' is incorrect in Definition 1.2.10, as the indicated topology is actually the weak* topology on $C_b(S)^*$ restricted to $\mathcal{M}(S)$. In the literature, it is sometimes also referred to as the weak* topology, e.g. in [Dud66]. However, 'weak topology' is the most commonly used terminology and for that reason, we use it here.

A very important characterization for weak convergence of positive measures is given by *Alexandrov's Theorem*, also known as the *Portmanteau Theorem*. We state it now.

Theorem 1.2.11. *Let* $(\mu_a)_{a\in A}$ *be a net in* $\mathcal{P}(S)$ *and* $\mu \in \mathcal{P}(S)$. *Then the following are equivalent:*

(i) (μ_a) *converges weakly to* μ.

(ii) For every closed set $F \subset S$, $\limsup_a \mu_a(F) \le \mu(F)$.

(iii) For every open set $U \subset S$, $\liminf_a \mu_a(U) \ge \mu(U)$.

In case $\mu_a, \mu \in \mathcal{M}^+(S)$ *and* $\lim_a \mu_a(S) = \mu(S)$, *then still (i), (ii) and (iii) are equivalent.*

Proof. See [Bog07, II, Theorem 8.2.3]. ☐

In this thesis, specifically, in Chapters 2 and 5, we will work with so-called *Polish spaces*, which we define now.

Definition 1.2.12. A *Polish space* is a separable topological space S that is metrizable by a metric d, such that (S,d) is complete. If a metric d on S metrizes the original topology on S and (S,d) is complete, then d is called *admissible.*

Whenever we state that (S,d) is a Polish space, we assume that d is an admissible metric.

The next theorem tells us that for the finite positive Borel measures on a Polish space, the weak topology coincides with the norm topology induced by $\|\cdot\|_{\mathrm{BL}}^*$ or $\|\cdot\|_{\mathrm{FM}}^*$.

Theorem 1.2.13. *Let (S,d) be a Polish space and let $(\mu_n) \subset \mathcal{M}^+(S)$, $\mu \in \mathcal{M}^+(S)$. Then, $\mu_n \to \mu$ weakly if and only if $\mu_n \to \mu$ in $\|\cdot\|_{\mathrm{BL}}^*$ or $\|\cdot\|_{\mathrm{FM}}^*$.*

Proof. See [Dud66, Theorem 6, Theorem 8] and Lemma 1.2.2. ☐

Proposition 1.2.14. *Let (S,d) be a Polish space. The sets $\mathcal{M}^+(S)$ and $\mathcal{P}(S)$ are weakly closed in $\mathcal{M}(S)$.*

Proof. By [Dud66, Theorem 9], it holds that $\mathcal{M}^+(S)$ is $\|\cdot\|_{\mathrm{BL}}^*$-closed (note that S is complete and separable). From Theorem 1.2.13, it follows that $\mathcal{M}^+(S)$ is also weakly closed.

Now we show that $\mathcal{P}(S)$ is weakly closed. Let $(\mu_a) \subset \mathcal{P}(S)$ be a net and $\mu_a \to \mu$ weakly in $\mathcal{M}(S)$. By the weak closedness of $\mathcal{M}^+(S) \supset \mathcal{P}(S)$, $\mu \in \mathcal{M}^+(S)$. Moreover, since $1 \in C_b(S)$, we have $\mu(S) = \langle \mu, 1 \rangle = \lim_a \langle \mu_a, 1 \rangle = \lim_a \mu_a(S) = \lim_a 1 = 1$, so $\mu \in \mathcal{P}(S)$. ☐

Definition 1.2.15. A finite signed Borel measure $\mu \in \mathcal{M}(S)$ is *tight*, if for all $\varepsilon > 0$, there exists a compact set $K_\varepsilon \subset S$ such that $|\mu|(S \setminus K_\varepsilon) < \varepsilon$.

A finite signed Borel measure $\mu \in \mathcal{M}(S)$ is *Radon*, if for all $A \in \mathcal{B}(S)$ and for all $\varepsilon > 0$, there exists a compact set $K_\varepsilon \subset S$ such that $|\mu|(A \setminus K_\varepsilon) < \varepsilon$. Another definition is used for positive (possibly infinite) measures, e.g., see [Fol99, Chapter 7]. The definition we have given is as it appears in [Bog07, II, Definition 7.1.1].

Proposition 1.2.16. *If (S,d) is a Polish space, then any $\mu \in \mathcal{M}(S)$ is Radon. In particular, any $\mu \in \mathcal{M}(S)$ is tight.*

Proof. See [Bog07, II, Theorem 7.1.7]. ☐

Our next aim is to show that any finite signed measure μ is the limit of a sequence of molecular measures. In Theorem 1.2.18, we prove this for the weak topology, when $\mu \in \mathcal{P}(S)$. After that, we extend the result for $\mu \in \mathcal{M}(S)$ and for the $\|\cdot\|_{\mathrm{FM}}^*$- and $\|\cdot\|_{\mathrm{BL}}^*$-topology. We first need a lemma.

Lemma 1.2.17. *Let (S,d) be a Polish space and let $\mu \in \mathcal{P}(S)$. Then there exists a probability space $(\Omega, \mathcal{F}, \mathbb{P})$ and an i.i.d. sequence of random variables (X_n), such that each $X_n : (\Omega, \mathcal{F}) \to (S, \mathcal{B}(S))$ is μ-distributed.*

Proof. A proof of the existence of one μ-distributed random variable can be found in multiple sources, e.g., in [BD83]. Then, via a standard procedure, one can construct an i.i.d. sequence of μ-distributed random variables on the product space $(\tilde{\Omega}^{\mathbb{N}}, \mathcal{F}^{\mathbb{N}}, \tilde{\mathbb{P}}^{\mathbb{N}})$. For the construction of the infinite product of measures, see [Bog07, I, §3.5].

Let $\tilde{X}$ be a μ-distributed random variable and let $(\Omega, \mathcal{F}, \mathbb{P}) := (\tilde{\Omega}^{\mathbb{N}}, \mathcal{F}^{\mathbb{N}}, \tilde{\mathbb{P}}^{\mathbb{N}})$. Define random variables $X_n : (\tilde{\Omega}^{\mathbb{N}}, \mathcal{F}^{\mathbb{N}}) \to (S, \mathcal{B}(S)) : X_n(\omega_1, \omega_2, \ldots) = \tilde{X}(\omega_n)$. The X_n are i.i.d. and μ-distributed, since:

$$\begin{aligned}
\mathbb{P}(X_n \in B) = \tilde{\mathbb{P}}^{\mathbb{N}}(\tilde{\Omega} \times \ldots \times \tilde{\Omega} \times \tilde{X}^{-1}(B) \times \tilde{\Omega} \times \ldots \times \tilde{\Omega}) &= \prod_{i \in \mathbb{N}, i \neq n} \tilde{\mathbb{P}}(\tilde{\Omega}) \cdot \tilde{\mathbb{P}}(\tilde{X}^{-1}(B)) \\
&= \prod_{i \in \mathbb{N}, i \neq n} 1 \cdot \mu(B) \\
&= \mu(B).
\end{aligned}$$

The independency of the X_n follows immediately from the product measure property of $\tilde{\mathbb{P}}^{\mathbb{N}}$. ☐

The following theorem shows that any element of $\mathcal{P}(S)$ is the weak limit of a sequence in $\mathrm{Mol}(S)$. An alternative proof can be found in [Bog07, II, Example 8.1.6(i)].

Theorem 1.2.18. *Let* (S, d) *be a Polish space and let* $\mu \in \mathcal{P}(S)$*. Then there exists a sequence* $(\tilde{\mu}_n) \subset \mathrm{Mol}(S)$ *that converges weakly to* μ *as* $n \to \infty$*.*

The $\tilde{\mu}_n$ *can be chosen as* empirical measures, *meaning that* $\tilde{\mu}_n = \frac{1}{n}\sum_{i=1}^n \delta_{x_i} \in \mathcal{P}(S) \cap \mathrm{Mol}(S)$ *for a sequence* $(x_i) \subset S$*.*

Proof. Take a sequence (X_n) of i.i.d. and μ-distributed random variables on a probability space $(\Omega, \mathcal{F}, \mathbb{P})$. Such a sequence exists by Lemma 1.2.17. Define $\mu_n : \Omega \to \mathcal{P}(S) : \omega \mapsto \frac{1}{n}\sum_{i=1}^n \delta_{X_i(\omega)}$.

First of all, for any bounded, measurable $h : S \to \mathbb{R}$, for all $\omega \in \Omega$ and $n \in \mathbb{N}$, we have

$$\int h \, d\mu_n(\omega) = \frac{1}{n}\sum_{i=1}^n \int h \, d\delta_{X_i(\omega)} = \frac{1}{n}\sum_{i=1}^n h(X_i(\omega)).$$

Note that the $h(X_n)$ are i.i.d. random variables and integrable, since they are bounded and μ is finite. By the Strong Law of Large Numbers ([Fol99, Theorem 10.12]), we thus obtain:

$$\int h \, d\mu_n = \frac{1}{n}\sum_{i=1}^n h(X_i) \overset{\mathbb{P}\text{−a.s.}}{\to} \mathbb{E}(h(X_1)) = \int h \, d\mu. \tag{1.2}$$

Since S is Polish, μ is tight by Proposition 1.2.16. So for all $m \in \mathbb{N}$, there exists a compact set $K_m \subset S$ with $\mu(S \setminus K_m) < \frac{1}{m}$. Since $C_b(K_m)$ is separable, it has a countable dense subset $\{g_1^m, g_2^m, \ldots\}$. By the Tietze Extension Theorem ([Fol99, Theorem 4.16], note that K_m is closed), there exists an extension $G_j^m \in C_b(S)$ of g_j^m for each $j, m \in \mathbb{N}$, with $\|G_j^m\|_{\infty,S} = \|g_j^m\|_{\infty,K_m}$.

Define for $j, m \in \mathbb{N}$:

$$\begin{aligned} F^m &:= \{\omega \in \Omega : \lim_{n\to\infty} \mu_n(\omega)(S \setminus K_m) = \mu(S \setminus K_m)\}, \\ A_j^m &:= \{\omega \in \Omega : \lim_{n\to\infty} \int G_j^m \, d\mu_n(\omega) = \int G_j^m \, d\mu\}. \end{aligned}$$

By (1.2) applied to $h = \mathbb{1}_{S\setminus K_m}$, it holds that $\mathbb{P}(F^m) = 1$ for all $m \in \mathbb{N}$. Likewise, taking $h = G_j^m$, we obtain $\mathbb{P}(A_j^m) = 1$ for all $j, m \in \mathbb{N}$. Therefore, for the countable intersection $C := \bigcap_{j,m=1}^\infty A_j^m \cap \bigcap_{m=1}^\infty F^m$, we also have $\mathbb{P}(C) = 1$. In particular, $C \neq \emptyset$, so we can pick $\omega \in C$. We will show that $\mu_n(\omega) \to \mu$ weakly.

Let $f \in C_b(S)$. We have to show that $\lim_{n\to\infty} \int f \, d\mu_n(\omega) = \int f \, d\mu$. Let $\varepsilon \in (0, 1)$ and pick $m > \frac{9(1+2\|f\|_\infty)}{\varepsilon}$. Since $f|_{K_m} \in C_b(K_m)$ and since $\{g_1^m, g_2^m, \ldots\}$ is dense, there exists $j \in \mathbb{N}$ such that $\|g_j^m - f\|_{\infty,K_m} < \frac{\varepsilon}{6}$. Now,

$$\|G_j^m\|_{\infty,S} = \|g_j^m\|_{\infty,K_m} \le \|g_j^m - f\|_{\infty,K_m} + \|f\|_{\infty,K_m} < \frac{\varepsilon}{6} + \|f\|_\infty < 1 + \|f\|_\infty.$$

Moreover, $\omega \in C$, so we have $\omega \in A_j^m$ and $\omega \in F^m$. Thus, we can pick n large enough such that $|\langle \mu_n(\omega) - \mu, G_j^m\rangle| < \frac{\varepsilon}{3}$ and $|\mu_n(\omega)(S \setminus K_m) - \mu(S \setminus K_m)| < \frac{1}{m}$. Then,

$$\begin{aligned} |\langle \mu_n(\omega) - \mu, f\rangle| &\le |\langle \mu_n(\omega) - \mu, G_j^m\rangle| + |\langle \mu_n(\omega) - \mu, f - G_j^m\rangle| \\ &< \frac{\varepsilon}{3} + \langle |\mu_n(\omega) - \mu|, |f - G_j^m| 1_{K_m}\rangle + \langle |\mu_n(\omega) - \mu|, |f - G_j^m| 1_{S\setminus K_m}\rangle \\ &\le \frac{\varepsilon}{3} + \|f - G_j^m\|_{\infty,K_m} |\mu_n(\omega) - \mu|(S) + \|f - G_j^m\|_\infty |\mu_n(\omega) - \mu|(S \setminus K_m) \\ &\le \frac{\varepsilon}{3} + \|f - g_j^m\|_{\infty,K_m} \cdot 2 + (\|f\|_\infty + \|G_j^m\|_\infty)\frac{3}{m} \\ &< \frac{\varepsilon}{3} + \frac{\varepsilon}{6} \cdot 2 + (2\|f\|_\infty + 1)\frac{3\,\varepsilon}{9(1 + 2\|f\|_\infty)} \\ &= \varepsilon\,. \end{aligned}$$

In the fourth inequality, we used that $|\mu_n(\omega) - \mu|(S) \leq \mu_n(\omega)(S) + \mu(S) = 2$ and

$$\begin{aligned}|\mu_n(\omega) - \mu|(S \setminus K_m) &\leq \mu_n(\omega)(S \setminus K_m) + \mu(S \setminus K_m)\\ &\leq |\mu_n(\omega)(S \setminus K_m) - \mu(S \setminus K_m)| + \mu(S \setminus K_m) + \mu(S \setminus K_m)\\ &< \frac{1}{m} + \frac{1}{m} + \frac{1}{m} = \frac{3}{m}.\end{aligned}$$

We now define $x_i := X_i(\omega)$. Then it holds that $\tilde{\mu}_n = \mu_n(\omega)$, and we are done. □

Remark 1.2.19. *The tightness of μ is vital in the above proof. In a general metric space, $\mu \in \mathcal{P}(S)$ is not necessarily tight, and the proof does not work. However, the first statement of Theorem 1.2.18 can be proved when (S, d) is a separable (not necessarily Polish) metric space.*

Via Bochner integration theory, in [HW09, Theorem 3.9], it is proved that any separable, *finite positive measure μ is the weak limit of a sequence of positive molecular measures. Here, μ is called* separable *if it is concentrated on a separable Borel subset of S. When S is separable, any $\mu \in \mathcal{P}(S)$ is trivially concentrated on the separable Borel set S itself, hence separable. Now, [HW09, Theorem 3.9] immediately yields the first statement of Theorem 1.2.18.*

We note that the separability condition is needed to apply the Pettis Measurability Theorem for strong μ-measurability of $\delta : S \to \mathcal{S}_{\mathrm{BL}}^* : x \mapsto \delta_x$ in the proof of [HW09, Theorem 3.9] (consult [HW09] for notations). The remainder of the proof relies mainly on [DU77, Corollary II.8]. For a more constructive approach, one can alternatively use [Coh80, Proposition E.2]. By this proposition, the map δ can then be approximated by simple functions with coefficients in $\mathbb{Q}\cdot\delta(S) := \{q\delta_x : q \in \mathbb{Q}, x \in S\}$, as follows from the proof in [Coh80]. That is, there exists $(f_n) \subset \mathcal{M}(S)$,

$$f_n(x) = \sum_{k=1}^{n} q_k^{(n)} \delta_{x_k^{(n)}} \mathbb{1}_{E_k^{(n)}}(x), \qquad q_k^{(n)} \in \mathbb{Q}, x_k^{(n)} \in S, E_k^{(n)} \in \mathcal{B}(S)$$

with $\|f_n(x) - \delta_x\|_{\mathrm{BL}}^* \to 0$ as $n \to \infty$, for μ - a.e. $x \in S$. Using Bochner integration and the Dominated Convergence Theorem, one can estimate

$$\|\mu - \sum_{k=1}^{n} q_k^{(n)} \delta_{x_k^{(n)}} \mu(E_k^{(n)})\|_{\mathrm{BL}}^* \leq \int_S \|\delta_x - \sum_{k=1}^{n} q_k^{(n)} \delta_{x_k^{(n)}} \mathbb{1}_{E_k^{(n)}}(x)\|_{\mathrm{BL}}^* d\mu(x) \to 0.$$

Thus, $\sum_{k=1}^n q_k^{(n)} \mu(E_k^{(n)}) \delta_{x_k^{(n)}} \to \mu$ weakly.

Corollary 1.2.20. *Let (S, d) be a Polish space. Then $\mathrm{Mol}(S)$ is dense in $\mathcal{M}(S)$ with respect to $\|\cdot\|_{\mathrm{FM}}^*$ and $\|\cdot\|_{\mathrm{BL}}^*$. Moreover, $\overline{\mathcal{M}}(S)_{\mathrm{FM}} = \overline{\mathrm{Mol}}(S)_{\mathrm{FM}} = \overline{\mathrm{Mol}}(S)_{\mathrm{BL}} = \overline{\mathcal{M}}(S)_{\mathrm{BL}}$.*

Proof. Let $\mu \in \mathcal{M}(S)$. An application of Theorem 1.2.18 to $\nu^+ := \frac{1}{\mu^+(S)}\mu^+ \in \mathcal{P}(S)$ and $\nu^- := \frac{1}{\mu^-(S)}\mu^- \in \mathcal{P}(S)$ yields sequences $(\nu_n^+), (\nu_n^-) \subset \mathrm{Mol}(S)$ with $\nu_n^+ \to \nu^+$ weakly and $\nu_n^- \to \nu^-$ weakly. By Theorem 1.2.13 we also have convergence with respect to $\|\cdot\|_{\mathrm{FM}}^*$ and $\|\cdot\|_{\mathrm{BL}}^*$. Next, it follows that $\mu^+(S)\nu_n^+ \to \mu^+(S)\nu^+ = \mu^+$ and $\mu^-(S)\nu_n^- \to \mu^-(S)\nu^- = \mu^-$ with respect to $\|\cdot\|_{\mathrm{FM}}^*$ and $\|\cdot\|_{\mathrm{BL}}^*$. Hence, in these norms we also have

$$\mu^+(S)\nu_n^+ - \mu^-(S)\nu_n^- \to \mu^+ - \mu^- = \mu.$$

As $\mu^+(S)\nu_n^+ - \mu^-(S)\nu_n^- \in \mathrm{Mol}(S)$, we conclude that $\mathrm{Mol}(S)$ is dense in $\mathcal{M}(S)$.

For the second statement, let $\phi \in \overline{\mathcal{M}}(S)_{\mathrm{FM}}$. By definition, there exists a sequence $(\mu_n) \subset \mathcal{M}(S)$ such that $\lim_{n\to\infty} \|\iota(\mu_n) - \phi\|_{\mathrm{FM}}^* = 0$. By the first part of this corollary, we can pick $\nu_n \in \mathrm{Mol}(S)$ such that $\|\nu_n - \mu_n\|_{\mathrm{FM}}^* < \frac{1}{n}$ for each $n \in \mathbb{N}$. Now, let $\varepsilon > 0$. Pick $N \in \mathbb{N}$ such that $N > \frac{2}{\varepsilon}$ and $\|\iota(\mu_n) - \phi\|_{\mathrm{FM}}^* < \frac{\varepsilon}{2}$ for all $n > N$. Then

$$\|\iota(\nu_n) - \phi\|_{\mathrm{FM}}^* \leq \|\iota(\nu_n) - \iota(\mu_n)\|_{\mathrm{FM}}^* + \|\iota(\mu_n) - \phi\|_{\mathrm{FM}}^* = \|\nu_n - \mu_n\|_{\mathrm{FM}}^* + \|\iota(\mu_n) - \phi\|_{\mathrm{FM}}^* < \frac{1}{n} + \frac{\varepsilon}{2} < \varepsilon\,.$$

As $(\iota(\nu_n)) \subset \iota(\mathrm{Mol}(S))$, we conclude that $\phi \in \overline{\mathrm{Mol}}(S)_{\mathrm{FM}}$, hence $\overline{\mathcal{M}}(S)_{\mathrm{FM}} \subset \overline{\mathrm{Mol}}(S)_{\mathrm{FM}}$.

The inclusion $\overline{\mathcal{M}}(S)_{\mathrm{FM}} \supset \overline{\mathrm{Mol}}(S)_{\mathrm{FM}}$ is immediate from the definitions and the fact that $\mathcal{M}(S) \supset \mathrm{Mol}(S)$, so $\overline{\mathcal{M}}(S)_{\mathrm{FM}} = \overline{\mathrm{Mol}}(S)_{\mathrm{FM}}$. The proof for the BL-norm can be given completely analogously.

It remains to show that $\overline{\mathrm{Mol}}(S)_{\mathrm{FM}} = \overline{\mathrm{Mol}}(S)_{\mathrm{BL}}$. But this is almost trivial. By Lemma 1.2.2, $\|\cdot\|_{\mathrm{FM}}$ and $\|\cdot\|_{\mathrm{BL}}$ are equivalent on $BL(S)^*$. So the convergent sequences consisting of elements in $\iota(\mathrm{Mol}(S))$ are the same for both norms, and so is their limit. Therefore, the closure of $\iota(\mathrm{Mol}(S))$ in $\mathrm{BL}(S)^*$ is the same for both norms. $\square$

Chapter 2

Structure of unit balls in Banach spaces of Lipschitz functions

In this chapter, we study the closed unit balls of the spaces $\mathrm{BL}(S)_{\mathrm{FM}}$ and $\mathrm{BL}(S)_{\mathrm{BL}}$. In Section 2.1, we prove some elementary properties of B_{FM} which will be of great use in Section 2.4 and in later chapters. The other sections in this chapter are devoted to the study of the extreme points of the unit balls B_{FM} and B_{BL}. As mentioned in the introduction to this thesis, our main goal is to compute distances between measures, measured in the Fortet-Mourier and Dudley metric. With that goal in mind, our motivation for studying extreme points will become clear from the upcoming Proposition 2.3.3. There, we see that $\|\nu-\mu\|_{\bullet}^{*}=\langle\,\nu-\mu,g\,\rangle$ for some extreme point g of the closed unit ball in $\mathrm{BL}(S)_{\bullet}$ ($\bullet=\mathrm{FM},\mathrm{BL}$). Therefore, a better understanding of the extreme points, will help us find ways to compute $\|\nu-\mu\|_{\bullet}^{*}$ for measures ν and μ.

As before, unless we explicitly state otherwise, we only assume that (S,d) is a metric space. No completeness or separability assumption is required. From now on, we will regularly use symbolic notations for maxima and minima of real numbers. Let us introduce these notations.

Definition 2.0.1. For $a,b,a_1,\dots,a_n\in\mathbb{R}$, we define

$$a\vee b:=\max(a,b),\quad a\wedge b:=\min(a,b),\quad \bigvee_{i=1}^{n}a_i:=\max(a_1,\dots,a_n).$$

2.1 Elementary properties of the unit ball for the FM-norm

We begin this chapter with a few lemmas about B_{FM}. These lemmas contain examples of elements of B_{FM} that will be useful when computing Fortet-Mourier distances between measures in Chapters 3 and 4.

Lemma 2.1.1. *Let* $\{x_1\dots,x_N\}\subset S$ *and let* $\theta_1,\dots,\theta_N\in[-1,1]$ *for some* $N\in\mathbb{N}$. *Then, for* $h_{\theta_1,\dots,\theta_N}:=(-1)\vee\bigvee_{i=1}^{N}(\theta_i-d(x_i,\cdot))$, *it holds that* $h_{\theta_1,\dots,\theta_N}\in\mathrm{B}_{\mathrm{FM}}$.

Proof. By construction, $-1\le h_{\theta_1,\dots,\theta_N}\le 1$. Also, by Lemma 1.1.4 we have $|h_{\theta_1,\dots,\theta_N}|_L\le\max_{1\le i\le N}(|-1|_L,|\theta_i-d(x_i,\cdot)|_L)$. Using the reverse triangle inequality, we have for all $i\in\{1,\dots,N\}$:

$$|\theta_i-d(x_i,s)-(\theta_i-d(x_i,t))|=|d(x_i,s)-d(x_i,t)|\le d(s,t),\tag{2.1}$$

so $|\theta_i-d(x_i,\cdot)|_L\le 1$. Therefore, $|h_{\theta_1,\dots,\theta_N}|_L\le 1$ and $h_{\theta_1,\dots,\theta_N}\in\mathrm{B}_{\mathrm{FM}}$. □

Lemma 2.1.2. *Let* $g\in\mathrm{B}_{\mathrm{FM}}$ *and define* $h:=g(\cdot)\vee(1-d(x,\cdot))$. *Then* $h\in\mathrm{B}_{\mathrm{FM}}$, $h(x)=1$ *and* $|g-h|=h-g\le 1-g(x)$ *on* S.

Proof. Clearly, $h(x) = 1$. We show that $h \in \mathrm{B}_{\mathrm{FM}}$. For all $s \in S$, we have $h(s) \geq g(s) \geq -1$. Also, $1 - d(x,s) \leq 1$, so $h \leq \max(\|g\|_\infty, 1) = 1$. Therefore, $\|h\|_\infty = 1$. By Lemma 1.1.4 and (2.1), h is Lipschitz continuous with $|h|_L \leq \max(|g|_L, |1 - d(x,\cdot)|_L) \leq \max(|g|_L, 1) = 1$. So $h \in \mathrm{B}_{\mathrm{FM}}$.

Next, we show that $|g - h| \leq 1 - g(x)$. Note that $h \geq g$ by construction, so $|g - h| = h - g$. Let $s \in S$ and consider two cases. If $g(s) \geq 1 - d(x,s)$, then $h(s) = g(s)$, so $h(s) - g(s) = 0 \leq 1 - g(x)$. For the case $g(s) < 1 - d(x,s)$, we note that $|g|_L \leq 1$, so $-d(x,s) \leq g(s) - g(x) \leq d(x,s)$. Hence, $-d(x,s) - g(s) \leq -g(x)$. This yields

$$h(s) - g(s) = 1 - d(x,s) - g(s) \leq 1 - g(x).$$

So indeed, $|g - h| = h - g \leq 1 - g(x)$.

□

Lemma 2.1.3. *Let $x \in S$ and define $\tilde{g} := (1 - d(x,\cdot)) \vee (-1)$. Then, $\tilde{g} \in \mathrm{B}_{\mathrm{FM}}$, $\tilde{g}(x) = 1$ and every $g \in \mathrm{B}_{\mathrm{FM}}$ with $g(x) = 1$ satisfies $\tilde{g} \leq g$.*

Proof. By construction, $-1 \leq \tilde{g} \leq 1$ and $\tilde{g}(x) = 1$, so $\|\tilde{g}\|_\infty = 1$. By Lemma 1.1.4 and (2.1), $|\tilde{g}|_L \leq \max(|1 - d(x,\cdot)|_L, |-1|_L) \leq \max(1, 0) = 1$. Hence, $\tilde{g} \in \mathrm{B}_{\mathrm{FM}}$.

Now suppose that $g \in \mathrm{B}_{\mathrm{FM}}$ and $g(x) = 1$. We have $\|g\|_\infty \leq \|g\|_{\mathrm{FM}} \leq 1$, so $g \geq -1$. Also, $|g|_L \leq \|g\|_{\mathrm{FM}} \leq 1$. For all $s \in S$, this gives $1 - g(s) = g(x) - g(s) \leq |g|_L d(x,s) \leq d(x,s)$, so $g(s) \geq 1 - d(x,s)$. We conclude that $g(s) \geq (1 - d(x,s)) \vee (-1) = \tilde{g}(s)$. □

Lemma 2.1.4. *Let $P = \{x_1, \ldots, x_N\} \subset S$ for some $N \in \mathbb{N}$ and let $g \in \mathrm{B}_{\mathrm{FM}}$. Then,*

$$h := (-1) \vee \bigvee_{i=1}^{N} (g(x_i) - d(x_i, \cdot))$$

satisfies $h \in \mathrm{B}_{\mathrm{FM}}$, $h \leq g$ on S and $h|_P = g|_P$.

Proof. With the notation of Lemma 2.1.1, we have $h = h_{g(x_1),\ldots,g(x_N)}$, and $g(x_i) \in [-1, 1]$. So by Lemma 2.1.1, $h \in \mathrm{B}_{\mathrm{FM}}$.

Now we show that $h \leq g$. For any $s \in S$, we have $h(s) = -1$ or $h(s) = g(x_i) - d(x_i, s)$ for some $i \in \{1, \ldots, N\}$. In the first case, we trivially have $h(s) = -1 \leq -\|g\|_\infty \leq g(s)$. In the second case, we have $g(x_i) - g(s) \leq |g(x_i) - g(s)| \leq d(x_i, s)$, so $h(s) = g(x_i) - d(x_i, s) \leq g(s)$. So indeed, $h \leq g$.

Finally, by the definition of h, we have for all $i \in \{1, \ldots, N\}$: $h(x_i) \geq g(x_i) - d(x_i, x_i) = g(x_i)$, hence $h(x_i) = g(x_i)$. □

Lemma 2.1.5. *Let $P = \{x_1, \ldots, x_N\} \subset S$ for some $N \in \mathbb{N}$ and let $f^* \in \mathrm{B}_{\mathrm{FM}}^P$. Then,*

$$h := (-1) \vee \bigvee_{i=1}^{N} (f^*(x_i) - d(x_i, \cdot))$$

satisfies $h \in \mathrm{B}_{\mathrm{FM}}$ and $h|_P = f^*$.

Proof. Let g be the extension of f^* as constructed in Proposition 1.1.5. Then $\|g\|_{\mathrm{FM}} = \|f^*\|_{\mathrm{FM},P}$, so $g \in \mathrm{B}_{\mathrm{FM}}$. Also, $g(x_i) = f^*(x_i)$ for all $i \in \{1, \ldots, N\}$. Thus, Lemma 2.1.4 gives $h \in \mathrm{B}_{\mathrm{FM}}$ and $h|_P = g|_P$. □

Lemma 2.1.6. *Let $g \in \mathrm{B}_{\mathrm{FM}}$ and let $P = \{x_1, \ldots, x_N\} \subset S$ for some $N \in \mathbb{N}$. Define*

$$\varepsilon := \min_{i=1,\ldots,N} (1 - g(x_i)), \qquad h := (-1) \vee \bigvee_{i=1}^{N} (g(x_i) + \varepsilon - d(x_i, \cdot)).$$

Then h satisfies $h \in \mathrm{B}_{\mathrm{FM}}$, $h \leq g + \varepsilon$ on S, $h|_P = g|_P + \varepsilon$ and $\max h|_P = 1$.

Proof. Define $\theta_i := g(x_i) + \varepsilon$ for $i = 1, \dots, N$ and note that $\theta_i \in [-1, 1]$. With the notation of Lemma 2.1.1, we have

$$h = h_{\theta_1,\dots,\theta_N}.$$

Thus, by Lemma 2.1.1, $h \in \mathrm{B}_{\mathrm{FM}}$.

Now we show that $h \le g + \varepsilon$ on S. If $h(s) = -1$, it is trivially true, since $g \ge -1$ and $\varepsilon \ge 0$. On the other hand, if $h(s) > -1$, then $h(s) = \theta_i - d(x_i, s) = g(x_i) + \varepsilon - d(x_i, s)$ for some $i \in \{1, \dots, N\}$. Recall that $|g|_L \le 1$, so

$$g(x_i) - g(s) \le |g(x_i) - g(s)| \le d(x_i, s).$$

Hence, $h(s) = g(x_i) + \varepsilon - d(x_i, s) \le g(s) + \varepsilon$ and indeed, $h \le g + \varepsilon$.

For all $i \in \{1, \dots, N\}$, we have

$$h(x_i) \ge \theta_i - d(x_i, x_i) = g(x_i) + \varepsilon\,.$$

Together with the inequality $h \le g + \varepsilon$, this gives $h|_P = g|_P + \varepsilon$.

Finally, let $k \in \{1, \dots, N\}$ be such that $1 - g(x_k) = \min_{1 \le i \le N}(1 - g(x_i))$. Then $h(x_k) = g(x_k) + \varepsilon = 1$, proving $\max h|_P = 1$. ☐

2.2 Measures as the predual of Lipschitz spaces

For our upcoming study of extreme points, we first need some results regarding the dual spaces of $\overline{\mathrm{Mol}}(S)_{\mathrm{FM}}$ and $\overline{\mathrm{Mol}}(S)_{\mathrm{BL}}$.

Analogues of the next theorem can be found in the literature for related norms. The proof of the version below is analogous to [HW09, Theorem 3.6], the isometric property excepted. To show that the linear isomorphism is isometric, a different argument is required.

Theorem 2.2.1. *Let $\overline{\mathrm{Mol}}(S)_{\mathrm{FM}} \subset \mathrm{BL}(S)^*_{\mathrm{FM}}$ be as in Definition 1.2.8.*
It holds that $\left(\overline{\mathrm{Mol}}(S)_{\mathrm{FM}}\right)^* \cong \mathrm{BL}(S)_{\mathrm{FM}}$ as topological spaces and as normed linear spaces, via a linear isometric isomorphism.

Proof. We will write $\|\cdot\|^*$ for the dual norm on $\left(\overline{\mathrm{Mol}}(S)_{\mathrm{FM}}\right)^*$. Let

$$T : \mathrm{BL}(S)_{\mathrm{FM}} \to \left(\overline{\mathrm{Mol}}(S)_{\mathrm{FM}}\right)^* : Tf(\phi) = \phi(f), \qquad f \in \mathrm{BL}(S), \phi \in \overline{\mathrm{Mol}}(S)_{\mathrm{FM}}.$$

We show that T is a well defined linear isometric isomorphism.

First of all, Tf clearly is a linear map on $\overline{\mathrm{Mol}}(S)_{\mathrm{FM}} \subset \mathrm{BL}(S)^*_{\mathrm{FM}}$, for any $f \in \mathrm{BL}(S)_{\mathrm{FM}}$. Moreover, for $\phi \in \overline{\mathrm{Mol}}(S)_{\mathrm{FM}}$ we have $|Tf(\phi)| \le \|\phi\|^*_{\mathrm{FM}}\|f\|_{\mathrm{FM}}$, so Tf is continuous with dual norm $\|Tf\|^* \le \|f\|_{\mathrm{FM}}$. So $Tf \in \left(\overline{\mathrm{Mol}}(S)_{\mathrm{FM}}\right)^*$ and T is well defined.

It is easy to prove that T is linear, using that any $\phi \in \overline{\mathrm{Mol}}(S)_{\mathrm{FM}}$ is a linear functional on $\mathrm{BL}(S)$. Also, from the inequality $\|Tf\|^* \le \|f\|_{\mathrm{FM}}$ we see that T is continuous with operator norm $\|T\| \le 1$.

Recall Definition 1.2.8 and the embedding ι from Lemma 1.2.7 $\iota(\mu)(f) = \int_S f\, d\mu$. Note that for $x \in S$ we have $\iota(\delta_x) \in \iota(\mathrm{Mol}(S)) \subset \overline{\mathrm{Mol}}(S)_{\mathrm{FM}}$. Let

$$L : \left(\overline{\mathrm{Mol}}(S)_{\mathrm{FM}}\right)^* \to \mathrm{BL}(S)_{\mathrm{FM}} : L\psi(x) = \psi(\iota(\delta_x)), \qquad \psi \in \left(\overline{\mathrm{Mol}}(S)_{\mathrm{FM}}\right)^*, x \in S.$$

We have

$$|L\psi(x) - L\psi(y)| = |\psi(\iota(\delta_x)) - \psi(\iota(\delta_y))| \le \|\psi\|^* \|\iota(\delta_x - \delta_y)\|^*_{\mathrm{FM}} \le \|\psi\|^* d(x, y). \tag{2.2}$$

The last inequality holds, since for $f \in \mathrm{B}_{\mathrm{FM}}$ we have $|\iota(\delta_x - \delta_y)(f)| = |f(x) - f(y)| \le |f|_L d(x, y) \le \|f\|_{\mathrm{FM}} d(x, y) \le d(x, y)$. By (2.2), $L\psi$ is Lipschitz continuous. Also, $L\psi$ is bounded, since

$$|L\psi(x)| = |\psi(\iota(\delta_x))| \le \|\psi\|^* \|\iota(\delta_x)\|^*_{\mathrm{FM}} = \|\psi\|^*, \qquad \text{for all } x \in S. \tag{2.3}$$

So L is well defined.

Linearity of L is immediate. For continuity, note that (2.3) yields $\|L\psi\|_\infty \leq \|\psi\|^*$. Furthermore, by (2.2) we have $|L\psi|_L \leq \|\psi\|^*$, hence $\|L\psi\|_{\mathrm{FM}} \leq \|\psi\|^*$. We conclude that L is continuous with $\|L\| \leq 1$.

It holds that $LT = \mathrm{Id}_{\mathrm{BL}(S)}$, since for any $f \in \mathrm{BL}(S)$ and $x \in S$, we have

$$LT(f)(x) = L(Tf)(x) = Tf(\iota(\delta_x)) = (\iota(\delta_x))(f) = \int_S f\, d\delta_x = f(x),$$

so $LT(f) = f$.

Now we show that $TL = \mathrm{Id}_{(\overline{\mathrm{Mol}}(S)_{\mathrm{FM}})^*}$. Let $\psi \in \big(\overline{\mathrm{Mol}}(S)_{\mathrm{FM}}\big)^*$ and $\phi \in \iota(\mathrm{Mol}(S))$. We can write $\phi = \iota(\sum_{i=1}^n \alpha_i \delta_{x_i}) = \sum_{i=1}^n \alpha_i \iota(\delta_{x_i})$, which yields

$$\begin{aligned} TL(\psi)(\phi) = T(L\psi)(\phi) = \phi(L\psi) &= \Big(\sum_{i=1}^n \alpha_i \iota(\delta_{x_i})\Big)(L\psi) \\ &= \sum_{i=1}^n \alpha_i \int_S L\psi\, d\delta_{x_i} \\ &= \sum_{i=1}^n \alpha_i L\psi(x_i) \\ &= \sum_{i=1}^n \alpha_i \psi(\iota(\delta_{x_i})) \\ &= \psi(\sum_{i=1}^n \alpha_i \iota(\delta_{x_i})) \\ &= \psi(\phi), \end{aligned} \tag{2.4}$$

where we used linearity of ψ in the second to last equality. Now let $\phi \in \overline{\mathrm{Mol}}(S)_{\mathrm{FM}}$. Pick a sequence $(\phi_n) \subset \mathrm{Mol}(S)$ converging to ϕ in $\|\cdot\|_{\mathrm{FM}}^*$. By (2.4), we have $TL(\psi)(\phi_n) = \psi(\phi_n)$ for all n, and since $TL(\psi), \psi \in \big(\overline{\mathrm{Mol}}(S)_{\mathrm{FM}}\big)^*$ are continuous, it follows that $TL(\psi)(\phi) = \psi(\phi)$. Therefore, we have shown that $TL(\psi) = \psi$.

Finally, we have for all $f \in \mathrm{BL}(S)$:

$$\|Tf\|^* \leq \|f\|_{\mathrm{FM}} = \|L(Tf)\|_{\mathrm{FM}} \leq \|Tf\|^*,$$

so $\|Tf\|^* = \|f\|_{\mathrm{FM}}$.

We conclude that T is a continuous linear isometric isomorphism with continuous inverse map L, and the proof is complete. ☐

Theorem 2.2.2. *It holds that* $\big(\overline{\mathrm{Mol}}(S)_{\mathrm{BL}}\big)^* \cong \mathrm{BL}(S)_{\mathrm{BL}}$ *as topological spaces and as normed linear spaces, via a linear isometric isomorphism.*

Proof. A proof similar to the proof of Theorem 2.2.1 can be given, the only difference is that the statement $\|L\| \leq 1$ requires a bit more effort for the BL-norm. The details can be found in [HW09, Theorem 3.6, Theorem 3.7]. ☐

Using the just obtained isomporphisms, we now define another topology on $\mathrm{BL}(S)$.

Definition 2.2.3. We define the $\sigma(\mathrm{BL}(S), \overline{\mathrm{Mol}}(S)_{\mathrm{FM}})$-topology on $\mathrm{BL}(S)$ via the identification $T : \mathrm{BL}(S)_{\mathrm{FM}} \cong \big(\overline{\mathrm{Mol}}(S)_{\mathrm{FM}}\big)^*$ from Theorem 2.2.1, i.e.,

$$\begin{aligned} f_a \to f \text{ wrt } \sigma(\mathrm{BL}(S), \overline{\mathrm{Mol}}(S)_{\mathrm{FM}}) &\iff Tf_a \to Tf \quad \text{ wrt } \sigma\big(\big(\overline{\mathrm{Mol}}(S)_{\mathrm{FM}}\big)^*, \overline{\mathrm{Mol}}(S)_{\mathrm{FM}}\big) = \mathrm{wk}^*, \\ &\iff Tf_a(\phi) \to Tf(\phi), \quad \text{for all } \phi \in \overline{\mathrm{Mol}}(S)_{\mathrm{FM}}, \\ &\iff \phi(f_a) \to \phi(f), \quad \text{for all } \phi \in \overline{\mathrm{Mol}}(S)_{\mathrm{FM}}. \end{aligned}$$

We define the $\sigma(\mathrm{BL}(S), \overline{\mathrm{Mol}}(S)_{\mathrm{BL}})$-topology on $\mathrm{BL}(S)$ likewise, via the identification $\mathrm{BL}(S)_{\mathrm{BL}} \cong \left(\overline{\mathrm{Mol}}(S)_{\mathrm{BL}}\right)^*$ from Theorem 2.2.2. This yields

$$f_a \to f \text{ wrt } \sigma(\mathrm{BL}(S), \overline{\mathrm{Mol}}(S)_{\mathrm{BL}}) \iff \phi(f_a) \to \phi(f), \qquad \text{for all } \phi \in \overline{\mathrm{Mol}}(S)_{\mathrm{BL}}.$$

We note that $\overline{\mathrm{Mol}}(S)_{\mathrm{FM}} = \overline{\mathrm{Mol}}(S)_{\mathrm{BL}}$ as sets by Corollary 1.2.20. So in fact, the topologies $\sigma(\mathrm{BL}(S), \overline{\mathrm{Mol}}(S)_{\mathrm{FM}})$ and $\sigma(\mathrm{BL}(S), \overline{\mathrm{Mol}}(S)_{\mathrm{BL}})$ are the same.

2.3 Extreme points and norm evaluation

We begin with the definition of an extreme point and an alternative characterization. Here, linear spaces are assumed to be defined over the field $\mathbb{R}$.

Definition 2.3.1. Let C be a convex subset of a linear space X. Then $z \in C$ is an *extreme point* if there is no open line segment that contains z and lies entirely in C.

This is equivalent to the statement that $z \in C$ is an extreme point if the following is satisfied (see [Day73, p. 101]):

$$z = \frac{x+y}{2}, \quad x, y \in C \iff x = y = z.$$

The set of extreme points of C is denoted by $\mathrm{ext}(C)$.

Lemma 2.3.2. *Let C be a convex subset of a linear space X. Then $z \in C$ is an extreme point if and only if it satisfies*

$$z \pm w \in C, \quad w \in X \iff w = 0. \tag{2.5}$$

Proof. If $z \in C$ is not an extreme point in the sense of Definition 2.3.1, then we can write $z = \frac{x+y}{2}$ for some $x, y \in C$ with $x \neq y$. Let $w := \frac{x-y}{2} \neq 0$. We have $z + w = x \in C$ and $z - w = y \in C$, so (2.5) is violated.

On the other hand, if (2.5) is not satisfied, then we have $z \pm w \in C$ for some $w \in X \setminus \{0\}$. Define $x := z + w \in C$ and $y := z - w \in C$. We have $x \neq y$ and $z = \frac{x+y}{2}$, violating the condition in Definition 2.3.1. ☐

The next proposition is the main motivation for our study of extreme points.

Proposition 2.3.3. *Let (S, d) be a Polish space and let $\mu \in \mathcal{M}(S)$. Then for $\bullet = \mathrm{FM}, \mathrm{BL}$, there exists $g^\bullet \in \mathrm{ext}(\mathrm{B}_\bullet)$ such that*

$$\|\mu\|_\bullet^* = \langle\, \mu, g^\bullet \,\rangle\,.$$

Proof. We use that any upper semi-continuous convex function on a non-empty, convex, compact subset of a locally convex Hausdorff space, attains its upper bound in at least one extreme point (see [Bou03, II.54, Proposition 1]).

Note that B_{FM} is convex. Therefore, to justify the use of this proposition, it suffices to show that B_{FM} is $\sigma(\mathrm{BL}(S), \overline{\mathrm{Mol}}(S)_{\mathrm{FM}})$-compact and $\langle\, \mu, \cdot \,\rangle$ is a continuous functional on B_{FM} with respect to the $\sigma(\mathrm{BL}(S), \overline{\mathrm{Mol}}(S)_{\mathrm{FM}})$-topology. The proof for the BL-norm can be given completely analogously.

Denote the closed unit ball of $\left(\overline{\mathrm{Mol}}(S)_{\mathrm{FM}}\right)^*$ by U^*. By Theorem 2.2.1, we have $\mathrm{B}_{\mathrm{FM}} \cong U^*$. The set U^* is weak*-compact by the Banach-Alaoglu Theorem. From Definition 2.2.3, it follows that $\mathrm{B}_{\mathrm{FM}} = T^{-1}(U^*)$ is $\sigma(\mathrm{BL}(S), \overline{\mathrm{Mol}}(S)_{\mathrm{FM}})$-compact.

Now we show that $\langle\, \mu, \cdot \,\rangle$ is continuous with respect to this topology. Suppose that (f_a) is a net in $\mathrm{BL}(S)$ such that $f_a \to f \in \mathrm{BL}(S)$ in the $\sigma(\mathrm{BL}(S), \overline{\mathrm{Mol}}(S)_{\mathrm{FM}})$-topology. Then $\phi(f_a) \to \phi(f)$ for all $\phi \in \overline{\mathrm{Mol}}(S)_{\mathrm{FM}}$ by Definition 2.2.3. Note that for $\phi := \langle\, \mu, \cdot \,\rangle$ it holds that $\phi = \iota(\mu) \in \iota(\mathcal{M}(S)) \subset \overline{\mathcal{M}}(S)_{\mathrm{FM}} = \overline{\mathrm{Mol}}(S)_{\mathrm{FM}}$ by Corollary 1.2.20. Therefore, $\langle\, \mu, f_a \,\rangle \to \langle\, \mu, f \,\rangle$, proving the desired continuity. ☐

Remark 2.3.4. *In view of Remark 1.2.19, one can similarly prove that Proposition 2.3.3 holds for non-Polish metric spaces, provided that μ is a tight or separable measure.*

2.4 Extreme points of the unit ball for the FM-norm

We have motivated the study of extreme points of B_{FM} and B_{BL} and now devote ourselves to determining the extreme points. In this section, we study the extreme points for the FM-norm. To be precise, we will determine a dense subset of $\mathrm{ext}(\mathrm{B}_{\mathrm{FM}})$ and describe some alternative dense subsets.

One of these dense subsets was already determined by Johnson ([Joh75, Proposition 1.1]) for the case in which (S,d) is a compact, connected metric space. For such S, density holds with respect to the supremum norm $\|\cdot\|_\infty$. We provide a detailed proof and show that the result can easily be extended for non-compact S, if we use a weaker, but still useful topology (in view of Corollary 2.6.1). The results and proofs are based on [Joh75] and [Hic20]. The difference with the results presented in this thesis, is the use of a slightly different dense subset E_{FM}. However, the reasoning remains virtually the same, with the exception of a few small details, as explained in Remarks 2.4.8 and 2.4.9.

After that, we consider some alternative dense subsets resembling E_{FM}, some a bit larger and some a bit smaller. Depending on the purpose, one can choose the subset that is most convenient to work with.

Definition 2.4.1. For $f \in \mathrm{BL}(S)$ we define $M_f^- := \{x \in S : f(x) = -\|f\|_\infty\}$ and

$$\begin{aligned}\mathrm{E}_{\mathrm{FM}} := \{f \in \mathrm{B}_{\mathrm{FM}} : \|f\|_\infty = 1, \exists \text{ finite } P_f \subset S \text{ s.t.}\\ \forall s \in S \setminus M_f^-, \exists p \in P_f \text{ with } f(s) = f(p) - d(s,p)\}.\end{aligned}$$

Lemma 2.4.2. *Let (S,d) be a connected metric space. Then,* $\mathrm{E}_{\mathrm{FM}} \subset \mathrm{ext}(\mathrm{B}_{\mathrm{FM}})$.

Proof. Let $f \in \mathrm{E}_{\mathrm{FM}}$ with corresponding set P_f. Suppose that $f \pm g \in \mathrm{B}_{\mathrm{FM}}$ for some $g \in \mathrm{BL}(S)$. We show that $g = 0$. From Lemma 2.3.2 it then follows that f is an extreme point.

For $s \in (M_f^-)^c \cap P_f^c$, there exists some $t_s \in P_f$ such that $\tilde{f}(s,t_s) := \frac{f(t_s)-f(s)}{d(s,t_s)} = 1$. Define $\tilde{g}$ analogously. Then

$$1 \geq \|f \pm g\|_{\mathrm{FM}} \geq |f \pm g|_L \geq |\tilde{f}(s,t_s) \pm \tilde{g}(s,t_s)| = |1 \pm \tilde{g}(s,t_s)|,$$

so $\tilde{g}(s,t_s)$ must be 0. This yields $g(s) = g(t_s)$, and therefore,

$$g((M_f^-)^c) \subset g((M_f^-)^c \cap P_f^c) \cup g(P_f) = g(P_f)$$

.

Define $M_f := \{x \in S : |f(x)| = \|f\|_\infty\}$. If $s \in M_f$, then $f(s) \in \{\pm 1\}$ and $1 \geq \|f \pm g\|_\infty \geq |f(s) \pm g(s)|$. Therefore, $g(s) = 0$ and we obtain

$$g(S) = g(M_f^-) \cup g((M_f^-)^c) \subset g(M_f) \cup g((M_f^-)^c) \subset \{0\} \cup g(P_f).$$

The set on the right-hand side is finite, so we conclude that $g(S)$ is finite.

If $M_f \neq \emptyset$, it holds that $\{0\} = g(M_f) \subset g(S)$. If $M_f = \emptyset$, in fact we also have $\{0\} \subset g(S)$. We prove this by contradiction. Suppose that $M_f = \emptyset$ and $0 \notin g(S)$. Pick a sequence $(x_n) \subset S$ with $\lim_{n\to\infty} |f(x_n)| = \|f\|_\infty = 1$. It holds that

$$|f| + |g| = \max(|f+g|, |f-g|) \leq \max(\|f+g\|_\infty, \|f-g\|_\infty) \leq 1. \tag{2.6}$$

Using that $0 \notin g(S)$, it follows from (2.6) that for all $n \in \mathbb{N}$:

$$0 < |g(x_n)| \leq 1 - |f(x_n)| \ \to\ 0 \quad \text{as } n \to \infty,$$

so $\lim_{n\to\infty} |g(x_n)| = 0$. In particular, for all $n \in \mathbb{N}$ we have for $m \in \mathbb{N}$ sufficiently large: $0 < |g(x_m)| < |g(x_n)|$, so $g(x_m) \neq g(x_n)$. But then $g(S)$ is not finite, a contradiction. We conclude that $0 \in g(S)$.

Furthermore, S is connected and g is continuous, so $g(S)$ is connected ([Rud76, Th 4.22]). Since $g(S)$ is also finite, $g(S)$ must be a singleton. We conclude that $g(S) = \{0\}$, i.e., $g = 0$. Thus $f \in \mathrm{ext}(\mathrm{B}_{\mathrm{FM}})$. ☐

We continue with some preparations for Theorem 2.4.7. The first is a rather technical proposition. After that, we give some results from functional analysis. These will all be used for proving that E_{FM} is dense in $\mathrm{ext}(\mathrm{B}_{\mathrm{FM}})$.

Proposition 2.4.3. *For all* $\phi \in \iota(\mathrm{Mol}(S)) \subset \mathrm{BL}(S)^*$ *it holds that* $\|\phi\|^*_{\mathrm{FM}} = \sup\{\phi(f) : f \in \mathrm{E}_{\mathrm{FM}}\}$. *Moreover, the supremum is attained: there exists* $f_\phi \in \mathrm{E}_{\mathrm{FM}}$ *such that* $\|\phi\|^*_{\mathrm{FM}} = \phi(f_\phi)$.

Proof. Let $\phi \in \iota(\mathrm{Mol}(S))$. By definition, it holds that $\mathrm{E}_{\mathrm{FM}} \subset \mathrm{B}_{\mathrm{FM}}$, so we have

$$\sup\{\phi(f) : f \in \mathrm{E}_{\mathrm{FM}}\} \leq \sup\{|\phi(f)| : f \in \mathrm{E}_{\mathrm{FM}}\} \leq \|\phi\|^*_{\mathrm{FM}}.$$

Therefore, it suffices to find $f \in \mathrm{E}_{\mathrm{FM}}$ with $\phi(f) = \|\phi\|^*_{\mathrm{FM}}$. This also shows that the supremum is attained.

Write $\phi = \iota(\sum_{j=1}^n a_j \delta_{s_j})$, with $a_j \in \mathbb{R}$, $s_j \in S$ distinct and $n \in \mathbb{N}$, and define $P := \{s_1, \ldots, s_n\}$. Let $(\mathrm{BL}(P), \|\cdot\|_{\mathrm{FM},P})$ be as in Definition 1.1.6, where P inherits the metric d from S.

Trivially, $f|_P \in \mathrm{BL}(P)$ for any $f \in \mathrm{BL}(S)$. Also, $\|f|_P\|_{\mathrm{FM},P} \leq \|f\|_{\mathrm{FM}}$, so $\{f|_P : f \in \mathrm{B}_{\mathrm{FM}}\} \subset \{h \in \mathrm{BL}(P) : \|h\|_{\mathrm{FM},P} \leq 1\} = \mathrm{B}^P_{\mathrm{FM}}$. Define

$$\phi|_P : \mathrm{BL}(P) \to \mathbb{R} : \phi|_P(h) = \sum_{j=1}^n a_j h(s_j).$$

Then $\phi|_P \in \mathrm{BL}(P)^*$ and it holds that $\phi|_P(f|_P) = \phi(f)$ for all $f \in \mathrm{BL}(S)$. This, together with the previous observation that $\{f|_P : f \in \mathrm{B}_{\mathrm{FM}}\} \subset \mathrm{B}^P_{\mathrm{FM}}$, yields

$$\|\phi\|^*_{\mathrm{FM}} \leq \|\phi|_P\|^*_{\mathrm{FM},P}. \tag{2.7}$$

The normed linear space $\mathrm{BL}(P)$ has dimension $n < \infty$, so it is complete and separable ([RY08, Corollary 2.19, Theorem 3.52]). In particular, it is a Polish space. So by Proposition 2.3.3 applied to $\mathrm{BL}(P)$ instead of $\mathrm{BL}(S)$, there exists $f^* \in \mathrm{ext}(\mathrm{B}^P_{\mathrm{FM}})$ such that $\|\phi|_P\|^*_{\mathrm{FM},P} = \sup_{h \in \mathrm{B}^P_{\mathrm{FM}}} \phi|_P(h) = \phi|_P(f^*)$.

We note that $\|f^*\|_\infty = 1$. Otherwise, we have $\varepsilon := 1 - \|f^*\|_\infty > 0$ and $f^* \pm \varepsilon \in \mathrm{B}^P_{\mathrm{FM}}$, contradicting the fact that f^* is an extreme point.

Now, let

$$f := (-1) \vee \bigvee_{i=1}^N (f^*(s_i) - d(s_i, \cdot)).$$

According to Lemma 2.1.5, we have $f \in \mathrm{B}_{\mathrm{FM}}$ and $f|_P = f^*$. Together with (2.7), this gives $\|\phi\|^*_{\mathrm{FM}} \geq \phi(f) = \phi|_P(f^*) = \|\phi|_P\|^*_{\mathrm{FM},P} \geq \|\phi\|^*_{\mathrm{FM}}$. Hence, $\|\phi\|^*_{\mathrm{FM}} = \phi(f)$. If we now prove that $f \in \mathrm{E}_{\mathrm{FM}}$, we are done. Note that $1 = \|f^*\|_\infty = |f^*(s_k)| = |f(s_k)|$ for some $k \in \{1, \ldots, n\}$, hence $\|f\|_\infty = 1$. It remains to show that for any $s \in S \setminus M^-_f$, there exists $p \in P$ with $f(p) - f(s) = d(s, p)$.

Let $s \in S \setminus M^-_f$. Since $s \notin M^-_f$, we have $f(s) > -1$, so $f(s) = f^*(s_j) - d(s_j, s)$ for some j. Using that $f^* = f$ on P, we obtain

$$f(s) = f(s_j) - d(s_j, s).$$

Thus, $f(s_j) - f(s) = d(s, s_j)$, as desired. As we already proved that $f \in \mathrm{B}_{\mathrm{FM}}$ and $\|f\|_\infty = 1$, we conclude that $f \in \mathrm{E}_{\mathrm{FM}}$. ☐

Definition 2.4.4. Let X be a topological vector space. The *convex hull* of a set $A \subset X$ is the intersection of all convex subsets of X that contain A. We denote it by $\mathrm{conv}(A)$. The *closed convex hull* of A is the intersection of all closed convex subsets of X that contain A.

Equivalently, $\mathrm{conv}(A)$ is the set of all convex combinations of points in A (by combining [Con90, Proposition IV.1.9, Definition IV.1.10]).

Lemma 2.4.5. *Let* X *be a Banach space,* F *a dense subset of* X *and* U^* *be the closed unit ball of* X^* *and* $A \subset U^*$. *Suppose that* $\|x\|_X = \sup\{\phi(x) : \phi \in A\}$ *for all* $x \in F$. *Then* U^* *is the weak*-closed convex hull of* A.

Proof. See [Joh75, Lemma 1.1]. ☐

The next theorem is known as the K^2-M^3-R *Theorem.*

Theorem 2.4.6. *Let K be a convex, compact set in a locally convex vector space L, let $E = \mathrm{ext}(K)$ and let $A \subset K$. Then the following are equivalent:*

- *(i) The closed convex hull of A is K.*
- *(ii) The closure of A contains E.*
- *(iii) The closure of A contains at least one point of each minimal facet of K.*
- *(iv) For each $f \in L^*$, $\sup f(A) = \sup f(K)$.*

Proof. See [Day73, p. 104]. ☐

We are now ready to prove that $\mathrm{E_{FM}}$ is dense in $\mathrm{ext}(\mathrm{B_{FM}})$. Our theorem is a slightly adapted version of [Joh75, Proposition 1.1], with Johnson's dense subset A replaced by $\mathrm{E_{FM}}$. In Remark 2.4.9, we demonstrate how density of Johnson's set A can be derived as well. In addition to the case where S is compact as assumed in [Joh75], we also prove density for non-compact S with respect to the $\sigma(\mathrm{BL}(S), \overline{\mathrm{Mol}}(S)_{\mathrm{FM}})$-topology.

Theorem 2.4.7. *Let (S, d) be a connected metric space. Then $\mathrm{E_{FM}}$ is a $\sigma(\mathrm{BL}(S), \overline{\mathrm{Mol}}(S)_{\mathrm{FM}})$-dense subset of $\mathrm{ext}(\mathrm{B_{FM}})$. If in addition, S is compact, then $\mathrm{E_{FM}}$ is a $\|\cdot\|_\infty$-dense subset of $\mathrm{ext}(\mathrm{B_{FM}})$.*

Proof. Recall that $\mathrm{E_{FM}} \subset \mathrm{B_{FM}}$ by Lemma 2.4.2. We now show that $\mathrm{ext}(\mathrm{B_{FM}}) \subset \overline{\mathrm{E_{FM}}}$. Denote the closed unit ball of $\big(\overline{\mathrm{Mol}}(S)_{\mathrm{FM}}\big)^*$ by U^*. By Theorem 2.2.1, we have $\big(\overline{\mathrm{Mol}}(S)_{\mathrm{FM}}\big)^* \cong \mathrm{BL}(S)_{\mathrm{FM}}$ isometrically via $T : \mathrm{BL}(S)_{\mathrm{FM}} \to \big(\overline{\mathrm{Mol}}(S)_{\mathrm{FM}}\big)^* : Tf(\mu) = \int f \, d\mu$, so

$$U^* = T(\mathrm{B_{FM}}) \cong \mathrm{B_{FM}}\,.$$

By Proposition 2.4.3 and the identification $\mathrm{E_{FM}} \cong T(\mathrm{E_{FM}})$, we have for all $\phi \in \mathrm{Mol}(S)$:

$$\sup\{\psi(\phi) : \psi \in T(\mathrm{E_{FM}})\} = \sup\{\phi(f) : f \in \mathrm{E_{FM}}\} = \|\phi\|^*_{\mathrm{FM}}.$$

From Lemma 2.4.5, it now follows that U^* is the weak*-closed convex hull of $T(\mathrm{E_{FM}})$ (apply it to $X = \overline{\mathrm{Mol}}(S)_{\mathrm{FM}}$, $F = \iota(\mathrm{Mol}(S))$ and $A = T(\mathrm{E_{FM}}) \subset T(\mathrm{B_{FM}}) = U^*$). We note that in this application, F is trivially dense in X, and $X = \overline{\mathrm{Mol}}(S)_{\mathrm{FM}}$ is a closed subspace of the Banach space $\mathrm{BL}(S)^*_{\mathrm{FM}}$, hence a Banach space itself ([Rud76, p. 54]). Now, from the K^2-M^3-R Theorem (Theorem 2.4.6, *(i)* $\Rightarrow$ *(iii)*), we conclude that $\mathrm{ext}(U^*) \subset \overline{T(\mathrm{E_{FM}})}^{\mathrm{wk}^*}$. Therefore,

$$\mathrm{ext}(\mathrm{B_{FM}}) = T^{-1}(\mathrm{ext}(U^*)) \subset T^{-1}\big(\overline{T(\mathrm{E_{FM}})}^{\mathrm{wk}^*}\big) = \overline{\mathrm{E_{FM}}}^{\sigma(\mathrm{BL}(S), \overline{\mathrm{Mol}}(S)_{\mathrm{FM}})}. \tag{2.8}$$

The first equality is true since extreme points are preserved under the isometric isomorphism T: we have $f \pm g \in \mathrm{B_{FM}} \iff T(f) \pm T(g) = T(f \pm g) \in T(\mathrm{B_{FM}}) = U^*$. The last equality in (2.8) follows almost immediately from Definition 2.2.3. Indeed, we have

$$\begin{aligned} f \in \overline{\mathrm{E_{FM}}}^{\sigma(\mathrm{BL}(S), \overline{\mathrm{Mol}}(S)_{\mathrm{FM}})} &\iff \exists \text{ net } (f_a) \subset \mathrm{E_{FM}}, f_a \to f \quad \text{wrt } \sigma(\mathrm{BL}(S), \overline{\mathrm{Mol}}(S)_{\mathrm{FM}}) \\ &\iff \exists \text{ net } (Tf_a) \subset T(\mathrm{E_{FM}}), Tf_a \overset{\mathrm{wk}^*}{\to} Tf \\ &\iff Tf \in \overline{T(\mathrm{E_{FM}})}^{\mathrm{wk}^*} \\ &\iff f \in T^{-1}\big(\overline{T(\mathrm{E_{FM}})}^{\mathrm{wk}^*}\big). \end{aligned}$$

Summarizing, we have proved that $\mathrm{E_{FM}} \subset \mathrm{ext}(\mathrm{B_{FM}}) \subset \overline{\mathrm{E_{FM}}}^{\sigma(\mathrm{BL}(S), \overline{\mathrm{Mol}}(S)_{\mathrm{FM}})}$. Therefore, $\mathrm{E_{FM}}$ is dense in $\mathrm{ext}(\mathrm{B_{FM}})$ with respect to the $\sigma(\mathrm{BL}(S), \overline{\mathrm{Mol}}(S)_{\mathrm{FM}})$-topology.

It remains to show that E_{FM} is also dense with respect to $\|\cdot\|_\infty$ when S is compact. Suppose that S is compact and let $f \in \operatorname{ext}(\mathrm{B}_{\mathrm{FM}})$. By the $\sigma(\mathrm{BL}(S), \overline{\mathrm{Mol}}(S)_{\mathrm{FM}})$ denseness, there exists a net $(f_a) \subset \mathrm{E}_{\mathrm{FM}}$ such that $f_a \to f$ with respect to $\sigma(\mathrm{BL}(S), \overline{\mathrm{Mol}}(S)_{\mathrm{FM}})$. Recall Definition 2.2.3. Since $\iota(\delta_x) \in \overline{\mathrm{Mol}}(S)_{\mathrm{FM}}$ for all $x \in S$, we have $f_a(x) = (\iota(\delta_x))(f_a) \to (\iota(\delta_x))(f) = f(x)$. So $f_a \to f$ pointwise.

Let $\varepsilon > 0$. S is compact and therefore totally bounded, so there exists $\{s_1, \ldots, s_n\} \subset S$ with $S = \cup_{i=1}^n B(s_i, \frac{\varepsilon}{3})$. Applying the convergence of each $f_a(s_i)$, we can find a_0 such that $|f_a(s_i) - f(s_i)| < \frac{\varepsilon}{3}$ for all $a \succeq a_0$ and for all $1 \leq i \leq n$.

Now, let $x \in S$ and pick s_i such that $d(x, s_i) < \frac{\varepsilon}{3}$. We then have, for all $a \succeq a_0$,

$$|f_a(x)-f(x)| \leq |f_a(x)-f_a(s_i)|+|f_a(s_i)-f(s_i)|+|f(s_i)-f(x)| < |f_a|_L d(x,s_i)+\frac{\varepsilon}{3}+|f|_L d(x,s_i) < \varepsilon\,.$$

We used that $f_a, f \in \mathrm{B}_{\mathrm{FM}}$, so $|f_a|_L, |f|_L \leq 1$. It follows that $\|f_a - f\|_\infty < \varepsilon$. We conclude that $\|f_a - f\|_\infty \to 0$ and that E_{FM} is dense in $\operatorname{ext}(\mathrm{B}_{\mathrm{FM}})$ with respect to $\|\cdot\|_\infty$. ☐

Remark 2.4.8. *Theorem 2.4.7 is also true when* E_{FM} *is replaced by*

$$\tilde{E}_{\mathrm{FM}} := \{f \in \mathrm{B}_{\mathrm{FM}} : \|f\|_\infty = 1, \exists \text{ finite } P_f \subset S \text{ s.t. } \forall s \in S \setminus M_f, \exists p \in P_f \text{ with } f(s) = f(p) - d(s,p)\},$$

where $M_f := \{x \in S : |f(x)| = \|f\|_\infty\}$.

To see this, note that $\mathrm{E}_{\mathrm{FM}} \subset \tilde{E}_{\mathrm{FM}}$, *since* $M_f^- \subset M_f$. *Moreover,* $\tilde{E}_{\mathrm{FM}} \subset \operatorname{ext}(\mathrm{B}_{\mathrm{FM}})$, *as we can copy the proof of Lemma 2.4.2. For* $s \in M_f^c \subset (M_f^-)^c$, *we conclude immediately from the proof that* $g(s) \in g(P_f)$. *Also, for* $s \in M_f$ *we already proved that* $g(s) = 0$, *so* $\{0\} \subset g(S) \subset \{0\} \cup g(P_f)$. *By the same reasoning as in the proof of Theorem 2.4.7 we obtain* $\mathrm{E}_{\mathrm{FM}} \subset \tilde{E}_{\mathrm{FM}} \subset \operatorname{ext}(\mathrm{B}_{\mathrm{FM}}) = \overline{\mathrm{E}_{\mathrm{FM}}}$, *proving density of* $\tilde{E}_{\mathrm{FM}}$ *in* $\operatorname{ext}(\mathrm{B}_{\mathrm{FM}})$.

Remark 2.4.9. *In [Joh75], a slightly different dense subset A is used, namely*

$$A = \{f \in \mathrm{B}_{\mathrm{FM}} : \|f\|_\infty = 1, \exists \text{ finite, nonempty } P_f \subset S \text{ s.t. } \forall s \in S \setminus M_f, \exists p \in P_f \text{ with } |f(s) - f(p)| = d(s,p)\}.$$

We note that the requirement that P_f *is non-empty precisely excludes the constant functions* $f = 1$ *and* $f = -1$. *It is then immediate that*

$$\mathrm{E}_{\mathrm{FM}} \subset \tilde{E}_{\mathrm{FM}} \subset A \cup \{-1\}. \tag{2.9}$$

Again, one can easily adapt the proof of Lemma 2.4.2 and Remark 2.4.8 to show that $A \subset \operatorname{ext}(\mathrm{B}_{\mathrm{FM}})$. *The only difference it that now we have to add the case* $\tilde{f}(s, t_s) = -1$ *next to the case where* $\tilde{f}(s, t_s) = 1$ *for* $s \in M_f^c \cap P_f^c$. *However, since* $1 \geq \|f \pm g\|_{\mathrm{FM}} \geq |\tilde{f}(s,t) \pm \tilde{g}(s,t_s)| = |-1 \pm \tilde{g}(s,t)|$ *we again conclude that* $\tilde{g}(s,t_s) = 0$ *and the proof still works.*

Also, $-1 \in \operatorname{ext}(\mathrm{B}_{\mathrm{FM}})$ *since* $-1 \pm g \in \mathrm{B}_{\mathrm{FM}}$ *implies* $\|-1 \pm g\|_\infty \leq 1$, *from which it follows that* $g = 0$. *So* $A \cup \{-1\} \subset \operatorname{ext}(\mathrm{B}_{\mathrm{FM}})$ *and from (2.9) and density of* E_{FM} *in* $\operatorname{ext}(\mathrm{B}_{\mathrm{FM}})$ *we conclude that* A *is* $\sigma(\mathrm{BL}(S), \overline{\mathrm{Mol}}(S)_{\mathrm{FM}})$*-dense as well and* $\|\cdot\|_\infty$*-dense in case* S *is compact. The latter (for compact* S*) is the result obtained in [Joh75, Proposition 1.1].*

2.5 Extreme points of the unit ball for the BL-norm

In this section, we state and prove a new characterization of a dense subset of $\operatorname{ext}(\mathrm{B}_{\mathrm{BL}})$, for any connected metric space (S, d). To our knowledge, such a dense subset of $\operatorname{ext}(\mathrm{B}_{\mathrm{BL}})$ has not been characterized for general metric spaces S up till now. Only in the very particular case $S = [0,1]$, $\operatorname{ext}(\mathrm{B}_{\mathrm{BL}})$ has been described in [RR70]. Some of the ideas in [RR70] have inspired the upcoming definitions and proofs, although they had to be generalized and substantially adapted to our general setting.

In [RR70, Theorem 2.4], Rao and Roy described the set $\operatorname{ext}(\mathrm{B}_{\mathrm{BL}})$ fully for the specific case where $S = [0,1]$. There, the bounded Lipschitz functions are complex-valued instead of real-valued (notation: $\mathrm{Lip}[0,1] = \mathrm{BL}_{\mathbb{C}}([0,1])$). We state the result here.

Theorem 2.5.1. *Let* $U := \{g \in \mathrm{BL}_{\mathbb{C}}([0,1]) : \|g\|_{\mathrm{BL}} \leq 1\}$*. If* $f \in U$ *is not of constant modulus, then* $f \in \mathrm{ext}(U)$ *if and only if*

(i) $|f'(x)| = 1 - \|f\|_\infty$ *a.e. off* $M_f := \{x \in [0,1] : |f(x)| = \|f\|_\infty\}$*, and*

(ii) $\inf_{n\in\mathbb{N}} \left[\alpha_n, \|f'\|_\infty - \|f'|_{M_f}\|_\infty\right] = 0$*.*

Here, one writes $M_f^c = \cup_{i=1}^\infty I_n$ *for intervals* I_n*, with one or both the endpoints of* I_n *in* M_f*, and* α_n *is defined by*

$$\alpha_n := \sup\{\alpha \geq 0 : \Big|1 + \frac{1+\alpha}{a_n} \int_{a_n}^{t} f'(\xi)\, d\xi\Big| \leq 1 \text{ for all } t \in I_n\}.$$

Proof. See [RR70, Theorem 2.4]. ☐

In [RR70, Lemma 2.7], a sufficient condition is given for the extreme points for the real-valued bounded Lipschitz functions as well, still for $S = [0,1]$.

Our ultimate goal is to prove an analogue of Proposition 2.4.3 for the BL-norm. We have used the same setup as for the FM-norm, and mimicked the reasoning from [Joh75]. However, the BL-norm turned out to be more complicated to work with, and some steps required considerably more effort. In these difficult steps, we gratefully used ideas from [RR70], and tried to generalize them from $S = [0,1]$ to a general metric space S.

In view of Theorem 2.5.1 and Theorem 2.4.7, a logical guess for a dense subset is given by

$$\begin{aligned} E = \{f \in \mathrm{B}_{\mathrm{BL}} : \|f\|_{\mathrm{BL}} = 1, \exists \text{ finite } P_f \subset S \text{ s.t. } \forall s \in S \setminus M_f,& \\ \exists p \in P_f \text{ with } |f(s) - f(p)| = (1 - \|f\|_\infty) d(s,p)\}.& \end{aligned}$$

However, we could not succeed in proving that $E \subset \mathrm{ext}(\mathrm{B}_{\mathrm{BL}})$. Therefore, we searched for additional conditions that could ensure the elements of E to be extreme points.

In the proof of Proposition 2.4.3, we worked with extreme points of $\mathrm{B}_{\mathrm{FM}}^P$, where P was a finite set. The extensions of these extreme points to B_{FM} turned out to be the essential elements of E_{FM}. Therefore, it is useful to study the extreme points of $\mathrm{B}_{\mathrm{BL}}^P$ first, before we adapt the definition of E.

The next lemma gives a property of $\mathrm{ext}(\mathrm{B}_{\mathrm{BL}}^P)$ that will be crucial for defining a suitable dense subset of $\mathrm{ext}(\mathrm{B}_{\mathrm{BL}})$. The main inspiration came from [RR70, Lemma 2.7].

Lemma 2.5.2. *Let* P *be a metric space with finitely many elements. Let* $f^* \in \mathrm{ext}(\mathrm{B}_{\mathrm{BL}}^P)$*, where* $\mathrm{B}_{\mathrm{BL}}^P := \{f \in \mathrm{BL}(P) : \|f\|_{\mathrm{BL},P} \leq 1\}$ *and* $\|\cdot\|_{\mathrm{BL},P}$ *is the* BL*-norm on* P*. Suppose that* f^* *is not constant. Then* f^* *attains both* $+\|f^*\|_\infty$ *and* $-\|f^*\|_\infty$*.*

Proof. By assumption, f^* is not constant, so P must contain at least two elements. Write $P = \{s_1, \dots, s_n\}$ for some $n \geq 2$ and let $\gamma := \|f^*\|_{\infty,P} \leq 1$. Since f^* is not constant, we have $0 < \gamma < 1$. Without loss of generality, we may assume that $f^*(s_j) = \gamma$ for some $j \in \{1, \dots, n\}$. Otherwise we must have $f^*(s_j) = -\gamma$ for some j, so $(-f^*)(s_j) = \gamma$ and $-f^* \in -\mathrm{ext}(\mathrm{B}_{\mathrm{BL}}^P) = \mathrm{ext}(\mathrm{B}_{\mathrm{BL}}^P)$. The last equality follows from Lemma 2.3.2 together with the observation that

$$f^* \pm g \in \mathrm{B}_{\mathrm{BL}}^P \iff -f^* \mp g \in -\mathrm{B}_{\mathrm{BL}}^P = \mathrm{B}_{\mathrm{BL}}^P \iff -f^* \pm g \in \mathrm{B}_{\mathrm{BL}}^P.$$

Note that $-f^*$ is not constant since f^* is not constant. The proof below only uses that $f^* \in \mathrm{ext}(\mathrm{B}_{\mathrm{BL}}^P)$ and $f^*(s_j) = \gamma$ for some j, and the fact that f^* is not constant. Therefore we can apply it to $-f^*$ and conclude that $-f^*$ attains both $+\|-f^*\|_{\infty,P} = +\|f^*\|_{\infty,P}$ and $-\|-f^*\|_{\infty,P} = -\|f^*\|_{\infty,P}$, but then $f^* = -(-f^*)$ attains these values too. So indeed, we may assume that $f^*(s_j) = \gamma$ for some $j \in \{1, \dots, n\}$.

Let

$$\alpha_i := \sup\{\alpha \geq 0 : |1 + \frac{1+\alpha}{\gamma}(f^*(s_i) - \gamma)| \leq 1\}, \qquad \alpha := \min_{i=1,\dots,n} \alpha_i.$$

We note that $\alpha_i = \infty \iff f^*(s_i) - \gamma = 0$, so

$$\alpha := \min_{i=1,\dots,n} \alpha_i = \infty \iff f^*(s_i) - \gamma = 0 \text{ for all } i \in \{1,\dots,n\} \iff f^* \equiv \gamma.$$

By assumption, f^* is not constant, so it follows that $0 \le \alpha < \infty$. Moreover, it holds that $\alpha = 0 \iff f^*(s_i) = -\gamma$ for some i, since

$$\begin{aligned}
\alpha = 0 &\iff \alpha_i = 0 \text{ for some } i \\
&\iff \exists i \text{ s.t. } \frac{1+\alpha}{\gamma}(f^*(s_i) - \gamma) \notin [-2, 0] \text{ for all } \alpha > 0 \\
&\overset{f^*(s_i) \le \gamma}{\iff} \exists i \text{ s.t. } \frac{1+\alpha}{\gamma}(f^*(s_i) - \gamma) < -2 \text{ for all } \alpha > 0 \\
&\iff \exists i \text{ s.t. } \alpha > \frac{-f^*(s_i) - \gamma}{f^*(s_i) - \gamma} \text{ for all } \alpha > 0 \\
&\iff \exists i \text{ s.t. } -f^*(s_i) - \gamma \ge 0 \\
&\iff \exists i \text{ s.t. } f^*(s_i) \le -\gamma \\
&\overset{\|f^*\|_{\infty,P} = \gamma}{\iff} \exists i \text{ s.t. } f^*(s_i) = -\gamma.
\end{aligned}$$

We shall now prove that $\alpha = 0$. Then, it follows that $f^*(s_i) = -\gamma$ for some i, so f^* attains both $+\gamma$ and $-\gamma$ as desired.

We argue by contradiction. Suppose that $\alpha > 0$. Pick

$$0 < c < \min_{i=1,\dots,n} [\frac{\alpha_i(1-\gamma)}{1+\alpha_i(1-\gamma)}, 1, \frac{1-\gamma}{\gamma}] \tag{2.10}$$

and define

$$g(x) := \begin{cases} c\gamma, & x \in M_{f^*}, \\ -\frac{c\gamma}{1-\gamma} f^*(x) + \frac{c\gamma}{1-\gamma}, & x \in P \setminus M_{f^*}. \end{cases}$$

Note that any real-valued function on P is automatically in $\mathrm{BL}(P)$, since P is a finite set of points. In particular, $g \in \mathrm{BL}(P)$. Note that $c > 0$, so $g \ne 0$. Now we show that $f^* \pm g \in \mathrm{B}^P_{\mathrm{BL}}$.

For $x \in M_{f^*}$, we have $|f^*(x) \pm g(x)| = (1 \pm c)\gamma$. Also, for $x \in P \setminus M_{f^*}$, we have

$$\begin{aligned}
|f^*(x) + g(x)| &= |(1 - \frac{c\gamma}{1-\gamma}) f^*(x) + \frac{c\gamma}{1-\gamma}| \\
&\le (1 - \frac{c\gamma}{1-\gamma}) |f^*(x)| + \frac{c\gamma}{1-\gamma} \\
&\le (1 - \frac{c\gamma}{1-\gamma}) \gamma + \frac{c\gamma}{1-\gamma} \\
&= \frac{\gamma}{1-\gamma}((1-\gamma) - c\gamma + c) \\
&= \gamma(1+c),
\end{aligned}$$

and

$$\begin{aligned}
|f^*(x) - g(x)| &= |(1 + \frac{c\gamma}{1-\gamma}) f^*(x) - \frac{c\gamma}{1-\gamma}| \\
&= |(1 + \frac{c\gamma}{1-\gamma})(f^*(x) - \gamma) + (1-c)\gamma| \\
&= (1-c)\gamma |1 + \frac{\frac{1+\frac{c\gamma}{1-\gamma}}{1-c}}{\gamma}(f^*(x) - \gamma)| \\
&\le (1-c)\gamma.
\end{aligned}$$

In the last line we used that $x = s_i$ for some $i \in \{1, \dots, n\}$ (f^* is a function on P), and that $\frac{1+\frac{c\gamma}{1-\gamma}}{1-c} < 1 + \alpha_i$ by (2.10), together with the definition of α_i. We conclude that $\|f^* \pm g\|_{\infty,P} \leq (1 \pm c)\gamma$.

Next, we determine an upper bound for $|f^* \pm g|_{L,P}$. We assumed that $\alpha > 0$, so $f^*(P) \subset (-\gamma, \gamma]$. Therefore, for $x, y \in M_{f^*}$, $x \neq y$, we have $f^*(x) = f^*(y) = \gamma$ and $g(x) = g(y) = c\gamma$, yielding

$$\frac{|f^*(x) \pm g(x) - f^*(y) \mp g(y)|}{d(x,y)} = \frac{0}{d(x,y)} = 0.$$

Now let $x \in M_{f^*}$ and $y \in P \setminus M_{f^*}$. We have $f^*(x) = \gamma$ and $\frac{|f^*(x) - f^*(y)|}{d(x,y)} \leq |f^*|_L = 1 - \gamma$, so

$$\begin{aligned}
\frac{|f^*(x) \pm g(x) - f^*(y) \mp g(y)|}{d(x,y)} &= \frac{|(1 \pm c)\gamma - f^*(y) \mp \frac{-c\gamma}{1-\gamma} f^*(y) \mp \frac{c\gamma}{1-\gamma}|}{d(x,y)} \\
&= \frac{|(1 \pm c \mp \frac{c}{1-\gamma}) f^*(x) - (1 \mp \frac{c\gamma}{1-\gamma}) f^*(y)|}{d(x,y)} \\
&= \frac{|(1 \mp \frac{c\gamma}{1-\gamma}) f^*(x) - (1 \mp \frac{c\gamma}{1-\gamma}) f^*(y)|}{d(x,y)} \\
&= (1 \mp \frac{c\gamma}{1-\gamma}) \frac{|f^*(x) - f^*(y)|}{d(x,y)} \\
&\leq (1 \mp \frac{c\gamma}{1-\gamma})(1-\gamma) \\
&= 1 - \gamma \mp c\gamma.
\end{aligned}$$

We used that $c < \frac{1-\gamma}{\gamma}$ so $\frac{c\gamma}{1-\gamma} < 1$. Finally, for $x, y \in P \setminus M_{f^*}$, $x \neq y$, we have

$$\begin{aligned}
\frac{|f^*(x) \pm g(x) - f^*(y) \mp g(y)|}{d(x,y)} &= \frac{|f^*(x) \mp \frac{c\gamma}{1-\gamma} f^*(x) \pm \frac{c\gamma}{1-\gamma} - f^*(y) \mp \frac{-c\gamma}{1-\gamma} f^*(y) \mp \frac{c\gamma}{1-\gamma}|}{d(x,y)} \\
&= \frac{|(1 \mp \frac{c\gamma}{1-\gamma}) f^*(x) - (1 \mp \frac{c\gamma}{1-\gamma}) f^*(y)|}{d(x,y)} \\
&= (1 \mp \frac{c\gamma}{1-\gamma}) \frac{|f^*(x) - f^*(y)|}{d(x,y)} \\
&\leq (1 \mp \frac{c\gamma}{1-\gamma})(1-\gamma) \\
&= 1 - \gamma \mp c\gamma.
\end{aligned}$$

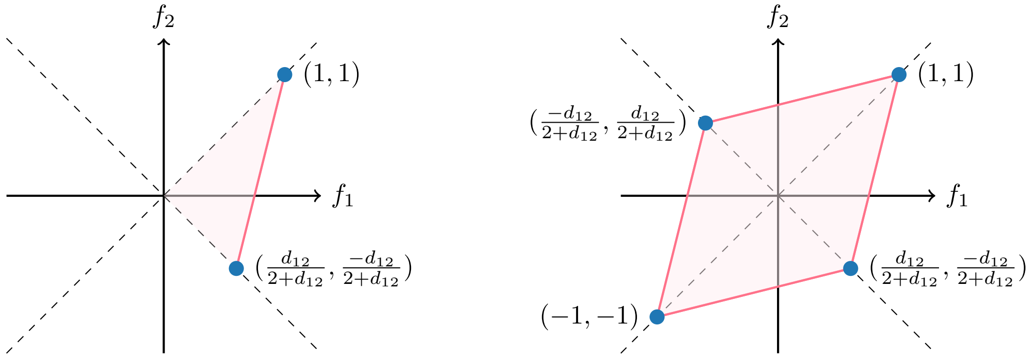
We conclude that $|f^* \pm g|_{L,P} \leq 1 - \gamma \mp c\gamma$. Together with our bound on $\|f^* \pm g\|_{\infty,P}$, this gives $\|f^* \pm g\|_{\mathrm{BL},P} \leq (1 \pm c)\gamma + 1 - \gamma \mp c\gamma = 1$, i.e., $f^* \pm g \in \mathrm{B}_{\mathrm{BL}}^P$. This contradicts the fact that $f^* \in \mathrm{ext}(\mathrm{B}_{\mathrm{BL}}^P)$. Therefore, our initial assumption that $\alpha > 0$ must false and this completes the proof. □

Example 2.5.3. *To illustrate the previous lemma, we consider the simple case where P exists of two points. Write $P = \{s_1, s_2\}$, $d_{12} = d(s_1, s_2)$ and identify $f \in \mathrm{BL}(P)$ with $(f_1, f_2) := (f(s_1), f(s_2)) \in \mathbb{R}^2$. Then, it holds that*

$$f \in \mathrm{B}_{\mathrm{BL}}^P \iff \|f\|_\infty + |f|_L = \max_{i=1,2} |f_i| + |f_1 - f_2| d_{12}^{-1} \leq 1. \tag{2.11}$$

The expression above is invariant under replacing f by $-f$ and under interchanging f_1 and f_2. Therefore, without loss of generality we can assume that $f_1 > 0$ and $|f_1| \geq |f_2|$. Then, from (2.11) we see that $f \in \mathrm{B}_{\mathrm{BL}}^P$ if and only if $f_1 + (f_1 - f_2) d_{12}^{-1} \leq 1$, i.e.,

$$f_2 \geq (1 + d_{12}) f_1 - d_{12}.$$



(a) $\mathrm{B}_{\mathrm{BL}}^{P} \cap \{f_1 \geq 0, |f_1| \geq |f_2|\}$ (b) $\mathrm{B}_{\mathrm{BL}}^{P}$

Figure 2.1: $\mathrm{B}_{\mathrm{BL}}^{P}$ for $d_{12} = 3$. The blue dots indicate $\mathrm{ext}(\mathrm{B}_{\mathrm{BL}}^{P})$.

At the boundary of $\mathrm{B}_{\mathrm{BL}}^{P}$ *it holds that* $f_2 = (1+d_{12})f_1 - d_{12}$ *and the two points at which this line intersects the boundary of the chosen quadrant* $f_1 \geq 0, |f_1| \geq |f_2|$, *satisfy* $f_1 = f_2$ *or* $f_1 = -f_2$, *respectively. Thus, we obtain equations for the intersection points:*

$$f_2 = (1+d_{12})f_2 - d_{12},\ f_1 = f_2 \qquad \textit{and} \qquad f_2 = -(1+d_{12})f_2 - d_{12},\ f_1 = -f_2,$$

which are solved by $(1,1)$ *and* $(\frac{d_{12}}{2+d_{12}}, \frac{-d_{12}}{2+d_{12}})$, *respectively.*

In the quadrant $f_1 \geq 0, |f_1| \geq |f_2|$, *we can now depict* $\mathrm{B}_{\mathrm{BL}}^{P}$ *as is done in Figure 2.1a. Using that* $\mathrm{B}_{\mathrm{BL}}^{P}$ *is invariant under* $f \mapsto -f$ *and* $(f_1, f_2) \mapsto (f_2, f_1)$, *we obtain the full picture, as shown in Figure 2.1b. The extreme points are drawn in blue and are given by*

$$\mathrm{ext}(\mathrm{B}_{\mathrm{BL}}^{P}) = \{(1,1), (-1,-1), (\frac{d_{12}}{2+d_{12}}, \frac{-d_{12}}{2+d_{12}}), (\frac{-d_{12}}{2+d_{12}}, \frac{d_{12}}{2+d_{12}}).$$

We see that all extreme points are either constant or satisfy $f_1 = -f_2$ *(thus attaining both* $+\|f\|_\infty$ *and* $-\|f\|_\infty$*). This illustrates the claim made in Lemma 2.5.2.*

Example 2.5.4. *Next, consider the case where* P *exists of three points. As in the previous example, write* $P = \{s_1, s_2, s_3\}$, $d_{ij} = d(s_i, s_j)$ *for* $i, j = 1, 2, 3$ *and identify* $f \in \mathrm{BL}(P)$ *with* $(f_1, f_2, f_3) := (f(s_1), f(s_2), f(s_3)) \in \mathbb{R}^3$. *We have*

$$f \in \mathrm{B}_{\mathrm{BL}}^{P} \iff \|f\|_\infty + |f|_L = \max_k |f_k| + \max_{i \neq j} |f_i - f_j| d_{ij}^{-1} \leq 1$$

A picture of $\mathrm{B}_{\mathrm{BL}}^{P}$, *created using* MATLAB® *([MAT19]), is given in Figure 2.2. The extreme points are indicated by a blue dot. Numerical inspection in* MATLAB® *yielded*

$$\mathrm{ext}(\mathrm{B}_{\mathrm{BL}}^{P}) = \{(\pm 1, \pm 1, \pm 1), (\pm\tfrac{1}{3}, \mp\tfrac{1}{3}, \mp\tfrac{1}{3}), (\pm\tfrac{1}{3}, \mp\tfrac{1}{3}, \pm\tfrac{1}{3}), (\pm\tfrac{1}{2}, 0, \mp\tfrac{1}{2}), (\pm\tfrac{1}{2}, \pm\tfrac{1}{2}, \mp\tfrac{1}{2}), (\pm\tfrac{1}{5}, \pm\tfrac{3}{5}, \mp\tfrac{3}{5})\}.$$

Again, all extreme points f *are either constant or attain both* $+\|f\|_\infty$ *and* $-\|f\|_\infty$, *illustrating Lemma 2.5.2.*

Unfortunately, it is extremely hard to find the extreme points of $\mathrm{B}_{\mathrm{BL}}^{P}$ *analytically when* P *consists of more than two points. It is in fact a special case of the problem of finding all vertices of a polytope defined by a finite number of constraints. We will elaborate on this later on, in Remark 4.5.5.*

We now present the contender E_{BL} for the dense subset of $\mathrm{ext}\,\mathrm{B}_{\mathrm{BL}}$.

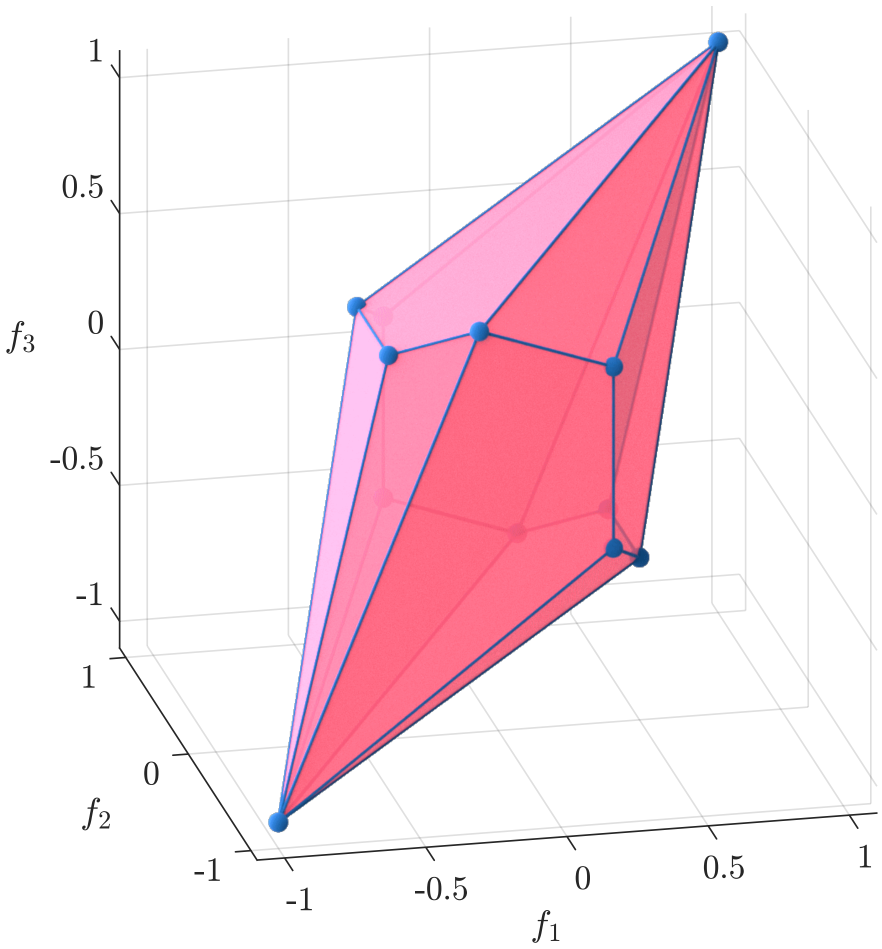


Figure 2.2: $\mathrm{B}^P_{\mathrm{BL}}$ for $d_{12} = 1, d_{13} = 2, d_{23} = 3$. The blue dots indicate $\mathrm{ext}(\mathrm{B}^P_{\mathrm{BL}})$.

Definition 2.5.5. For $f \in \mathrm{BL}(S)$, we define $M_f := \{x \in S : |f(x)| = \|f\|_\infty\}$ and

$$\begin{aligned}\tilde{E}_{\mathrm{BL}} := \{f \in \mathrm{B}_{\mathrm{BL}} : \|f\|_{\mathrm{BL}} = 1, \quad & f(M_f) = \{\|f\|_\infty, -\|f\|_\infty\}, \exists \text{ finite } P_f \subset S \text{ s.t.} \\ & \forall s \in S \setminus M_f, \exists p \in P_f \text{ with } |f(s) - f(p)| = (1 - \|f\|_\infty) d(s,p)\}, \\ \mathrm{E}_{\mathrm{BL}} := \tilde{E}_{\mathrm{BL}} \cup \{-1, 1\}. &\end{aligned}$$

Remark 2.5.6. *We make a few observations about $\tilde{E}_{\mathrm{BL}}$ and E_{BL}. These will be used directly and indirectly in the upcoming proof of Theorem 2.5.10.*

First of all, note that $\tilde{E}_{\mathrm{BL}}$ is non-empty, provided that S contains at least two distinct points x and y. Namely, one can define $f(s) := \max\{-\gamma, \gamma - (1-\gamma)d(x,s)\}$, with $\gamma := \frac{d(x,y)}{2+d(x,y)}$ and verify that $f \in \tilde{E}_{\mathrm{BL}}$.

Now let $f \in \tilde{E}_{\mathrm{BL}}$. Note that f is non-zero by the condition '$\|f\|_{\mathrm{BL}} = 1$'. Thus, $\|f\|_\infty > 0$. Moreover, the set M_f contains at least two points since $f \neq 0$ and $f(M_f) = \{\|f\|_\infty, -\|f\|_\infty\}$. In particular, M_f is non-empty. Moreover, $\|f\|_\infty < 1$, since otherwise we have $\|f\|_\infty = \|f\|_{\mathrm{BL}} = 1$, so $|f|_L = 0$, i.e., f is constant. The latter contradicts the condition $f(M_f) = \{\|f\|_\infty, -\|f\|_\infty\}$. We conclude that $\|f\|_\infty \in (0,1)$.

Finally, we note that $f \in \mathrm{E}_{\mathrm{BL}}$ implies that $-f \in \mathrm{E}_{\mathrm{BL}}$, so $\mathrm{E}_{\mathrm{BL}} = -\mathrm{E}_{\mathrm{BL}}$.

The next lemma is a reformulation of [RR70, Lemma 2.1] for real numbers. It will be used in the proof of Proposition 2.5.8.

Lemma 2.5.7. *Let $x, y \in \mathbb{R}$ and let $|x| + |y| = 1$. If $\alpha, \beta \in \mathbb{R}$ are such that $|x \pm \alpha| + |y \pm \beta| \leq 1$, then either $xy = \alpha = \beta = 0$, or*

$$xy \neq 0, \quad |\alpha| \leq \min\{|x|, |y|\} \quad \text{and} \quad \alpha\frac{|x|}{x} + \beta\frac{|y|}{y} = 0.$$

Proof. See [RR70, Lemma 2.1]. □

Although the next result applies to a much more general setting than $S = [0,1]$, several ideas were inspired by the proofs of [RR70, Theorem 2.4, Lemma 2.7] and adapted to the setup of [Joh75]. We once more stress that we consider *real-valued* bounded Lipschitz functions, while [RR70, Theorem 2.4] (Theorem 2.5.1) applies to $\mathrm{BL}_{\mathbb{C}}([0,1])$.

Proposition 2.5.8. *Let (S,d) be a connected metric space. Then, $\mathrm{E}_{\mathrm{BL}} \subset \mathrm{ext}(\mathrm{B}_{\mathrm{BL}})$.*

Proof. Suppose that $f \in \mathrm{E}_{\mathrm{BL}}$ and $f \pm g \in \mathrm{B}_{\mathrm{BL}}$, for some $g \in \mathrm{BL}(S)$. We will show that $g = 0$, so that we can conclude that $f \in \mathrm{ext}(\mathrm{B}_{\mathrm{BL}})$ by Lemma 2.3.2.

Recall that $\mathrm{E}_{\mathrm{BL}} = \{\pm 1\} \cup \tilde{E}_{\mathrm{BL}}$. If $f = \pm 1$, it is immediate that g must be zero. In the other case, we have $f \in \tilde{E}_{\mathrm{BL}}$. For $s, t \in S$, $s \neq t$, define $\tilde{f}(s,t) := \frac{f(s)-f(t)}{d(s,t)}$ and $\tilde{g}(s,t) := \frac{g(s)-g(t)}{d(s,t)}$. Let P_f be a finite subset as in the definition of $\tilde{E}_{\mathrm{BL}}$, and let $s \in M_f^c \cap P_f^c$. Set

$$\gamma := \|f\|_\infty,$$

and recall that $\gamma \in (0,1)$ by Remark 2.5.6. Now, let $p_s \in P_f$ be such that $|\tilde{f}(s,p_s)| = 1 - \gamma$. Such p_s exists according to the definition of E_{BL}. Then, for all $x \in M_f$ we have

$$\begin{cases} |f(x)| + |\tilde{f}(s,p_s)| = \gamma + 1 - \gamma = 1, \\ |f(x) \pm g(x)| + |\tilde{f}(s,p_s) \pm \tilde{g}(s,p_s)| \leq \|f \pm g\|_\infty + |f \pm g|_L = \|f \pm g\|_{\mathrm{BL}} \leq 1. \end{cases}$$

Note that $f(x) \neq 0 \neq \tilde{f}(s,p_s)$ since $\gamma \in (0,1)$, so Lemma 2.5.7 yields

$$g(x)\frac{|f(x)|}{f(x)} + \tilde{g}(s,p_s)\frac{|\tilde{f}(s,p_s)|}{\tilde{f}(s,p_s)} = 0, \qquad \text{for all } x \in M_f. \tag{2.12}$$

Keeping s (and p_s) fixed and varying x, this implies

$$g(x) = -\frac{\tilde{g}(s,p_s)|\tilde{f}(s,p_s)|}{\gamma\tilde{f}(s,p_s)}f(x) = cf(x), \qquad \text{for all } x \in M_f, \tag{2.13}$$

where $c := -\frac{\tilde{g}(s,p_s)|\tilde{f}(s,p_s)|}{\gamma\tilde{f}(s,p_s)} = \frac{g(x)}{f(x)}$ is constant. By Lemma 2.5.7, c satisfies

$$|c|\gamma = |cf(x)| = |g(x)| \leq \min\{|f(x)|, |\tilde{f}(s,p_s)|\} = \min\{\gamma, 1-\gamma\},$$

so $|c| \leq \min\{1, \frac{1-\gamma}{\gamma}\}$. Now, (2.12) becomes

$$c\gamma + \tilde{g}(s,p_s)\frac{|\tilde{f}(s,p_s)|}{\tilde{f}(s,p_s)} = 0,$$

so $\tilde{g}(s,p_s) = \frac{-c\gamma}{1-\gamma}\tilde{f}(s,p_s)$ (recall that $|\tilde{f}(s,p_s)| = 1-\gamma$). Therefore,

$$g(s) - g(p_s) = \frac{-c\gamma}{1-\gamma}(f(s) - f(p_s)). \tag{2.14}$$

Since $f \in \mathrm{E}_{\mathrm{BL}}$ there exist $x_\pm \in M_f$ with $f(x_\pm) = \pm\|f\|_\infty = \pm\gamma$. For the moment, assume the following:

$$\left\{\begin{array}{l} \text{There exist } n \in \mathbb{N} \text{ and } \{x_1,\dots,x_n\} \subset S, \text{ such that } x_1 = x_-, x_n = x_+ \\ \text{and } g(x_{i+1}) - g(x_i) = \frac{-c\gamma}{1-\gamma}(f(x_{i+1}) - f(x_i)) \text{ for } i = 1,\dots,n-1. \end{array}\right. \tag{2.15}$$

We will prove (2.15) below, but we finish the proof first, using this assumption. We have

$$\begin{aligned} 2c\gamma = cf(x_+) - cf(x_-) = g(x_+) - g(x_-) &= g(x_n) - g(x_1) \\ &= \sum_{i=1}^{n-1}\big(g(x_{i+1}) - g(x_i)\big) \\ &= \sum_{i=1}^{n-1}\frac{-c\gamma}{1-\gamma}\big(f(x_{i+1}) - f(x_i)\big) \\ &= \frac{-c\gamma}{1-\gamma}(f(x_n) - f(x_1)) \\ &= \frac{-c\gamma}{1-\gamma}(f(x_+) - f(x_-)) \\ &= \frac{-c\gamma}{1-\gamma}2\gamma. \end{aligned}$$

So either $c = 0$ or $\gamma = 0$ or $1 = \frac{-\gamma}{1-\gamma}$. The last two options cannot hold since $\gamma \in (0,1)$. We conclude that $c = 0$.

Now, (2.13) implies that $g = cf = 0$ on $M_f \supset \{x_+, x_-\}$ and from (2.14), we derive that $g(s) \in g(P_f)$ for all $s \in S \setminus P_f$. Thus, $\{0\} \subset g(S) \subset \{0\} \cup g(P_f)$, so $g(S)$ is finite and contains zero. Since S is connected and g is continuous, $g(S)$ is connected. Also, it is finite, so it must be a singleton. As $0 \in g(S)$, it follows that $g(S) = \{0\}$, i.e., $g = 0$. We conclude that $f \in \mathrm{ext}(\mathrm{B}_{\mathrm{BL}})$.

It remains to prove (2.15). To this end, define for $x \in S$:

$$\begin{aligned} M_x := \{s \in S : &\exists n \in \mathbb{N}, \exists x_1,\dots,x_n \in S \text{ such that } x_1 = x, x_n = s, \\ &g(x_{i+1}) - g(x_i) = \frac{-c\gamma}{1-\gamma}(f(x_{i+1}) - f(x_i)) \text{ for } 1 \leq i \leq n-1\}. \end{aligned} \tag{2.16}$$

We write $x \sim y$ if and only if $y \in M_x$. Clearly, if $x_+ \in M_{x_-}$, we have proved (2.15).

We first show that $\sim$ is an equivalence relation. By taking $n = 1$ in the definition of M_x we see that trivially $x \in M_x$, proving reflexivity. For symmetry, suppose that $y \in M_x$, with corresponding $\{x_1, \ldots, x_n\}$ as in the definition of M_x. Define $\bar{x}_i := x_{n-i+1}$ for $i = 1, \ldots, n$. Then $\bar{x}_1 = x_n = y$, $\bar{x}_n = x_1 = x$, and

$$\begin{aligned} g(\bar{x}_{i+1}) - g(\bar{x}_i) = -\Big(g(x_{n-i+1}) - g(x_{n-i})\Big) &= -\Big(\frac{-c\gamma}{1-\gamma}(f(x_{n-i+1}) - f(x_{n-i}))\Big) \\ &= \frac{-c\gamma}{1-\gamma}(f(\bar{x}_{i+1}) - f(\bar{x}_i)), \end{aligned}$$

so $x \in M_y$. For transitivity, suppose that $x \in M_y$ with corresponding $\{x_1, \ldots, x_n\}$ and $y \in M_z$ with corresponding $y_1, \ldots, y_m$. Define $N := n + m$ and $\bar{x}_i := x_i$ for $1 \leq i \leq n$, $\bar{x}_i := y_{i-n}$ for $n+1 \leq i \leq N$. Note that $\bar{x}_n = \bar{x}_{n+1} = y$ and note that all the properties are satisfied to conclude that $x \in M_z$. We conclude that $\sim$ is an equivalence relation. Consequently, any two equivalence classes M_x, M_y are either equal or disjoint.

Next, we show that the equivalence classes M_x are closed subsets of S. Suppose that $(s_n) \subset M_x$ and $s_n \to s \in S$. By continuity of f, we have $f(s_n) \to f(s)$. Since $f \in \mathrm{E}_{\mathrm{BL}}$, we have for each $n \in \mathbb{N}$ either $s_n \in M_f$, so $|f(s_n)| = \gamma$, or $|f(s_n) - f(p)| = (1-\gamma)d(s,p)$ for some $p \in P_f$. Write $P_f = \{p^1, \ldots, p^k\}$ with $p^i \in S$ and $k \in \mathbb{N}$. Define

$$\begin{aligned} I_i &:= \{n \in \mathbb{N} : |f(s_n) - f(p^i)| = (1-\gamma)d(s_n, p^i)\}, \\ I^{\gamma} &:= \{n \in \mathbb{N} : f(s_n) = \gamma\}, \\ I^{-\gamma} &:= \{n \in \mathbb{N} : f(s_n) = -\gamma\}. \end{aligned}$$

It holds that $\mathbb{N} = \cup_{i=1}^k I_i \cup I^{\gamma} \cup I^{-\gamma}$, so at least one of the sets in the finite union on the right-hand side must be infinite. Let I be such an infinite set on the right-hand side and write $I = \{n_1, n_2, \ldots\}$ with $n_j < n_{j+1}$ for all $j \in \mathbb{N}$, so that (s_{n_j}) is a subsequence of (s_n).

If $I = I_i$ for some $i \in \{1, \ldots, k\}$, then

$$|f(s) - f(p^i)| = \lim_{j\to\infty} |f(s_{n_j}) - f(p^i)| = \lim_{j\to\infty} (1-\gamma)d(s_{n_j}, p^i) = (1-\gamma)d(s, p^i),$$

using that $f(s_{n_j}) \to f(s)$ and $d(s_{n_j}, s) \to 0$. By (2.14), it now follows that $s \in M_{p^i}$ (take $n = 2, x_1 = p^i, x_2 = s$ in the definition (2.16), note that $s \in M_{p^i}$ trivially holds when $s = p^i$). Moreover, $s_{n_j} \in M_{p^i}$ by (2.14), so $p^i \sim s$ and $p^i \sim s_{n_j}$ for all $j \in \mathbb{N}$. Using symmetry and transitivity, this yields $s_{n_j} \sim s$. Also, $s_{n_j} \in M_x$ for all $j \in \mathbb{N}$, so $x \sim s_{n_j}$ and again by transitivity: $x \sim s$, i.e., $s \in M_x$.

The other cases are $I = I^{\pm\gamma}$. In these cases, we have $f(s_{n_j}) = \pm\gamma$ for all $j \in \mathbb{N}$, so $f(s) = \lim_{j\to\infty} f(s_{n_j}) = \pm\gamma = f(s_{n_j})$. Therefore, $s, s_{n_j} \in M_f$, and (2.13) yields $g(s_{n_j}) = g(s) = \pm c\gamma$. Now, trivially we have $g(s_{n_j}) - g(s) = \frac{-c\gamma}{1-\gamma}(f(s_{n_j}) - f(s))$ as both sides are zero, and it follows that $s_{n_j} \in M_s$. Thus, $s \sim s_{n_j}$ and $x \sim s_{n_j}$ for all $j \in \mathbb{N}$, and by symmetry and transitivity: $x \sim s$, i.e., $s \in M_x$. We conclude that M_x is closed.

Finally, observe that

$$S = \cup_{i=1}^k M_{p^i} \cup M_{x_+} \cup M_{x_-}. \tag{2.17}$$

For any $s \in S \setminus M_f$, (2.14) holds for some $p_s \in \{p^1, \ldots, p^k\} = P_f$, hence $s \in M_{p_s}$. For $s \in M_f$ we have $f(s) = \pm\gamma = f(x_\pm)$ and $g(s) = \pm c\gamma = g(x_\pm)$, so taking $n = 2, x_1 = x_\pm, x_2 = s$ in the definition of $M_{x_\pm}$, we see that $s \in M_{x_\pm}$. So indeed, (2.17) holds.

Our goal was to show that $x_+ \in M_{x_-}$. Suppose that the latter is not true. Then $M_{x_+} \cap M_{x_-} = \emptyset$. Let $J \subset \{1, \ldots, k\}$ be the collection of precisely all indices i such that $p^i \notin M_{x_+}$ and define $M := \cup_{i\in J} M_{p^i} \cup M_{x_-}$. Then M is a finite union of closed sets, hence closed. Moreover, $M \cap M_{x_+} = \emptyset$ and $x_- \in M_{x_-} \subset M$, so $M \neq \emptyset$. Also, M_{x_+} is closed and contains x_+, and we have

$$S = M_{x_+} \dot{\cup} M. \tag{2.18}$$

Note that $M_{x_+} = M^c$ and $M = M_{x_+}^c$, so both sets are also open. Therefore, (2.18) contradicts the connectedness of S. We conclude that $x_+ \in M_{x_-}$, justifying our assumption (2.15). ☐

The following proposition is similar to Proposition 2.4.3.

Proposition 2.5.9. *For all* $\phi \in \iota(\mathrm{Mol}(S)) \subset \mathrm{BL}(S)^*$, *it holds that* $\|\phi\|_{\mathrm{BL}}^* = \sup\{\phi(f) : f \in \mathrm{E}_{\mathrm{BL}}\}$. *Moreover, there exists* $f_\phi \in \mathrm{E}_{\mathrm{BL}}$ *at which the the supremum is attained:* $\|\phi\|_{\mathrm{BL}}^* = \phi(f_\phi)$.

Proof. A similar argument as in the proof of Proposition 2.4.3 shows that there exists $f^* \in \mathrm{ext}(\mathrm{B}_{\mathrm{BL}}^P)$ with $\phi|_P(f^*) = \|\phi|_P\|_{\mathrm{BL},P}^* \geq \|\phi\|_{\mathrm{BL}}^*$.

Now, it suffices to construct $f \in \mathrm{E}_{\mathrm{BL}}$ such that $f|_P = f^*$. Indeed, once we have done that, we have $\phi(f) = \phi|_P(f^*) = \|\phi|_P\|_{\mathrm{BL},P}^* \geq \|\phi\|_{\mathrm{BL}}^*$. Since $f \in \mathrm{E}_{\mathrm{BL}}$, we obtain $\|\phi\|_{\mathrm{BL}}^* \leq \sup\{\phi(f) : f \in \mathrm{E}_{\mathrm{BL}}\}$. The other inequality also holds, since for any $f \in \mathrm{E}_{\mathrm{BL}}$, we have $\phi(f) \leq \|\phi\|_{\mathrm{BL}}^* \|f\|_{\mathrm{BL}} \leq \|\phi\|_{\mathrm{BL}}^*$, as $\mathrm{E}_{\mathrm{BL}} \subset \mathrm{B}_{\mathrm{BL}}$. The inequalities together yield $\|\phi\|_{\mathrm{BL}}^* = \sup\{\phi(f) : f \in \mathrm{E}_{\mathrm{BL}}\}$.

To construct $f \in \mathrm{E}_{\mathrm{BL}}$ with $f|_P = f^*$, let $\gamma = \max_{1 \leq j \leq n} |f^*(s_j)| = \|f^*\|_\infty$ and distinguish between two cases:

1. Suppose that f^* is not constant. Note that $\|f^*\|_{\mathrm{BL},P} = 1$. Otherwise, we would have $f^* \pm \varepsilon \in \mathrm{B}_{\mathrm{BL}}^P$ for some small ε, contradicting Lemma 2.3.2. Therefore, $|f^*|_L = \|f^*\|_{\mathrm{BL},P} - \|f^*\|_\infty = 1 - \gamma$.

Now, define

$$f_0(s) := \max_{1 \leq j \leq n} \Big(f^*(s_j) - (1-\gamma) d(s_j, s) \Big), \qquad f(s) := \max(f_0(s), -\gamma).$$

By Proposition 1.1.5, we have $f = f^*$ on P, $\|f\|_\infty = \|f^*\|_\infty = \gamma$ and $|f|_L = |f^*|_L$. If we now prove that $f \in \mathrm{E}_{\mathrm{BL}}$, we are done. From Lemma 2.5.2, we know that f^* attains both $+\gamma$ and $-\gamma$. Since $f^* = f|_P$, this proves that f attains both $+\gamma$ and $-\gamma$. Thus, it only remains to show:

$$\forall s \in S \setminus M_f,\ \exists p \in P \text{ with } |f(s) - f(p)| = (1-\gamma) d(s,p).$$

Let $s \in S \setminus M_f$. Then $|f(s)| < \gamma$, hence $|f_0(s)| < \gamma$. Pick j with $f_0(s) = f^*(s_j) - (1-\gamma)d(s_j, s)$. Since $f^* = f$ on P, we have

$$f(s) = f_0(s) = f^*(s_j) - (1-\gamma)d(s_j,s) = f(s_j) - (1-\gamma) d(s_j, s),$$

so $\frac{f(s_j) - f(s)}{d(s, s_j)} = 1 - \gamma$.

2. Now suppose that f^* is constant, i.e., $f^* \equiv \pm\gamma$. Then it follows that $|f^*|_L = 0$, so $\gamma = \|f^*\|_\infty = \|f^*\|_{\mathrm{BL}} = 1$. Hence, $f^* \equiv \pm 1$. Now, for the trivial extension $f := \pm 1$, it holds that $f|_P = f^*$ and $f \in \mathrm{E}_{\mathrm{BL}}$, as follows immediately from the definition of E_{BL}. ☐

We are now ready to state and prove an analogue of [Joh75, Proposition 1.1] and Theorem 2.4.7 for the bounded Lipschitz norm on $\mathrm{BL}(S)$, instead of the Fortet-Mourier norm as appeared in Johnson's result. The hard work has already been done, especially by establishing $\mathrm{E}_{\mathrm{BL}} \subset \mathrm{ext}(\mathrm{B}_{\mathrm{BL}})$ in Proposition 2.5.8. As we mentioned, a characterization of the extreme points of B_{BL} for a general connected metric space was not known until now.

Theorem 2.5.10. *Let* (S, d) *be a connected metric space. Then* E_{BL} *is a* $\sigma(\mathrm{BL}(S), \overline{\mathrm{Mol}}(S)_{\mathrm{BL}})$-*dense subset of* $\mathrm{ext}(\mathrm{B}_{\mathrm{BL}})$. *If in addition, S is compact, then* E_{BL} *is a* $\|\cdot\|_\infty$-*dense subset of* $\mathrm{ext}(\mathrm{B}_{\mathrm{BL}})$.

Proof. We can copy all arguments in the proof of Theorem 2.4.7, replacing Theorem 2.2.1 by Theorem 2.2.2, Lemma 2.4.2 by Proposition 2.5.8 and Proposition 2.4.3 by Proposition 2.5.9. Then, only the functional analytic part remains. But this part can be proved similarly, by literally replacing every FM-norm by the BL-norm.

☐

2.6 Concluding observations

Using the dense subsets of the extreme points derived in the previous sections, we can now adjust Proposition 2.3.3 for connected Polish spaces. For such spaces, the supremum can be taken over the smaller sets E_{FM} and E_{BL}.

Corollary 2.6.1. *Let (S, d) be a connected Polish space and let $\mu \in \mathcal{M}(S)$ be a finite signed measure. Then, for $\bullet = \mathrm{FM}, \mathrm{BL}$, it holds that*

$$\|\mu\|_{\bullet}^{*} = \sup_{g \in \mathrm{E}_{\bullet}} \langle\, \mu, g \,\rangle,$$

where E_{BL} is the set from Theorem 2.5.10 and E_{FM} is as in Definition 2.4.1.

Proof. The proof is completely analogous for both cases. We provide the proof for the FM-norm here. By Proposition 2.3.3, there exists some $g \in \mathrm{ext}(\mathrm{B}_{\mathrm{FM}})$ such that $\|\mu\|_{\mathrm{FM}}^{*} = \langle\, \mu, g \,\rangle$.

We note that sets of the form

$$V_{\mu,g,\varepsilon} := \{h \in \mathrm{BL}(S) : |\langle\, \mu, h - g \,\rangle| < \varepsilon\}$$

are $\sigma(\mathrm{BL}(S), \overline{\mathrm{Mol}}(S)_{\mathrm{FM}})$-open neighbourhoods of g (see Definition 2.2.3 and [Con90, p. 100, Definition V.1.1] and note that $\langle\, \mu, \cdot \,\rangle \in \iota(\mathcal{M}(S)) \subset \overline{\mathcal{M}}(S)_{\mathrm{FM}} = \overline{\mathrm{Mol}}(S)_{\mathrm{FM}}$ by Corollary 1.2.20). Since E_{FM} is $\sigma(\mathrm{BL}(S), \overline{\mathrm{Mol}}(S)_{\mathrm{FM}})$-dense in $\mathrm{ext}(\mathrm{B}_{\mathrm{FM}})$ we can pick a sequence $(g_n) \subset \mathrm{E}_{\mathrm{FM}}$ with $g_n \in V_{\mu,g,\frac{1}{n}}$ for all $n \in \mathbb{N}$, so $|\langle\, \mu, g_n - g \,\rangle| < \frac{1}{n}$. It follows that

$$|\langle\, \mu, g_n \,\rangle - \langle\, \mu, g \,\rangle| = |\langle\, \mu, g_n - g \,\rangle| < \frac{1}{n},$$

so $\|\mu\|_{\mathrm{FM}}^{*} \leq \sup_{g \in \mathrm{E}_{\mathrm{FM}}} \langle\, \mu, g \,\rangle$. Also, we have $\|\mu\|_{\mathrm{FM}}^{*} := \sup_{g \in \mathrm{B}_{\mathrm{FM}}} \langle\, \mu, g \,\rangle \geq \sup_{g \in \mathrm{E}_{\mathrm{FM}}} \langle\, \mu, g \,\rangle$, since $\mathrm{E}_{\mathrm{FM}} \subset \mathrm{B}_{\mathrm{FM}}$. Thus, the corollary is proved. ☐

We conclude by giving thought to some side results that follow from the proofs of Proposition 2.4.3 and Proposition 2.5.9. Although the results are not used in the remainder of this thesis, they are interesting by themselves and deserve some attention.

Remark 2.6.2. *Let (S, d) be a connected metric space and let $P = \{s_1, \ldots, s_n\} \subset S$. If we combine the proof of Proposition 2.4.3 with that of Theorem 2.4.7, we can derive a rather remarkable side result. Namely, we have in fact shown that*

$$\mathcal{E}_{P,S}^{\mathrm{FM}} : \mathrm{BL}(P) \to \mathrm{BL}(S) : f^{*} \mapsto (-1) \vee \bigvee_{i=1}^{n} (f^{*}(s_j) - d(s_j, \cdot))$$

maps $\mathrm{ext}(\mathrm{B}_{\mathrm{FM}}^{P})$ into $\mathrm{ext}(\mathrm{B}_{\mathrm{FM}}^{S})$. Indeed, in the proof of Proposition 2.4.3 it was established that $\mathcal{E}_{P,S}^{\mathrm{FM}}(f^{*}) \in \mathrm{E}_{\mathrm{FM}}$ for $f^{*} \in \mathrm{ext}(\mathrm{B}_{\mathrm{FM}}^{P})$, and in Theorem 2.4.7 we proved that $\mathrm{E}_{\mathrm{FM}} \subset \mathrm{ext}(\mathrm{B}_{\mathrm{FM}}^{S})$.

Likewise, the proof of Proposition 2.5.9 and that of Theorem 2.5.10, together imply that

$$\mathcal{E}_{P,S}^{\mathrm{BL}} : \mathrm{BL}(P) \to \mathrm{BL}(S) : \begin{cases} f^{*} \mapsto (-1) \vee \bigvee_{i=1}^{n} (f^{*}(s_j) - d(s_j, \cdot)), & f^{*} \text{ not constant}, \\ f^{*} \mapsto f^{*}(s_1), & f^{*} \text{ constant}. \end{cases}$$

maps $\mathrm{ext}(B_{\mathrm{BL}}^{P})$ into $\mathrm{ext}(B_{\mathrm{BL}}^{S})$.

One could consider the smallest subset $\mathrm{E}^{\bullet}$ of $\mathrm{ext}(\mathrm{B}_{\bullet}^{S})$ ($\bullet = \mathrm{FM}, \mathrm{BL}$), for which the proofs of Proposition 2.4.3 and Proposition 2.5.9 would still work. It can be verified that this set will given by

$$\mathrm{E}^{\bullet} := \bigcup_{P \subset S \text{ finite}} \mathcal{E}_{P,S}^{\bullet}(\mathrm{ext}(\mathrm{B}_{\bullet}^{P})).$$

By the earlier observations we have $\mathcal{E}_{P,S}^{\bullet}(\mathrm{ext}(\mathrm{B}_{\bullet}^{P})) \subset \mathrm{ext}(\mathrm{B}_{\bullet}^{S})$, so Theorem 2.4.7 and Theorem 2.5.10 are also true when $\mathrm{E}_{\bullet}$ is replaced by $\mathrm{E}^{\bullet}$. This gives an even smaller dense subset, which *could be useful when trying to compute* $\|\mu\|_{\bullet}^{*}$ *for* $\mu \in \mathcal{M}(S)$. *Similarly as was proved in Corollary 2.6.1, one has*

$$\|\mu\|_{\bullet}^{*} = \sup_{g \in \mathrm{E}^{\bullet}} \langle\, \mu, g \,\rangle,$$

and the supremum on the right-hand side now only has to be taken over $\mathrm{E}^{\bullet}$.

Chapter 3

Fortet-Mourier distance between probability measures

In this chapter, we derive expressions for Fortet-Mourier distances between Borel probability measures ν and μ on a metric space S, where ν has finite support.

In particular, we establish an explicit expression for $\|\delta_x - \mu\|_{\mathrm{FM}}^*$, with $x \in S$ and $\mu \in \mathcal{P}(S)$. This expression is presented in Proposition 3.1.2. Until now, only an expression for $\|\delta_x - \delta_y\|_{\mathrm{FM}}^*$ has appeared in the literature. Our general expression for $\mu \in \mathcal{P}(S)$ is, as far as we are aware, a novel result! In Section 4.1, we will generalize further and derive an expression for $\|\delta_x - \mu\|_{\mathrm{FM}}^*$ that applies to all $\mu \in \mathcal{M}^+(S)$.

We found the expressions in this chapter originally via Corollary 2.6.1, using the dense subset E_{FM} of $\mathrm{ext}(\mathrm{B}_{\mathrm{FM}})$. Eventually, we discovered that the proofs for these expressions remained valid when working only with the definition of the Fortet-Mourier distance. Consequently, the results became valid for all metric spaces, S did no longer need to be connected and Polish.

However, without our journey in Chapter 2, we might not have considered the crucial functions in B_{FM} that enable us to compute the distances in this chapter. Indeed, all the functions that play a key role here, are elements of $\mathrm{E}_{\mathrm{FM}} \subset \mathrm{ext}(\mathrm{B}_{\mathrm{FM}})$.

Throughout this chapter we assume that (S, d) is a metric space.

3.1 Distance between a Dirac measure and a probability measure

The next lemma will help to find an expression for the distance between a Dirac measure and a probability measure.

Lemma 3.1.1. *Let $x \in S$ and $\mu \in \mathcal{P}(S)$. Then*

$$\|\delta_x - \mu\|_{\mathrm{FM}}^* = \sup_{\substack{g \in \mathrm{B}_{\mathrm{FM}}, \\ g(x)=1}} \langle\, \delta_x - \mu, g \,\rangle .$$

Proof. By definition, we have

$$\|\delta_x - \mu\|_{\mathrm{FM}}^* = \sup_{g \in \mathrm{B}_{\mathrm{FM}}} \langle\, \delta_x - \mu, g \,\rangle .$$

Let $g \in \mathrm{B}_{\mathrm{FM}}$ and define $h := g(\cdot) \vee (1 - d(x, \cdot))$. By Lemma 2.1.2, it holds that $h \in \mathrm{B}_{\mathrm{FM}}$, $h(x) = 1$

and $|g-h| \leq 1-g(x)$. We obtain

$$\begin{aligned}\langle\, \delta_x-\mu, h\,\rangle = h(x)-\int h\, d\mu = 1-\int h\, d\mu& \\ &= g(x)+1-g(x)-\int (g(s)+h(s)-g(s))\, d\mu(s) \\ &\geq g(x)+1-g(x)-\int g\, d\mu-\int |g-h|\, d\mu \\ &\geq g(x)+1-g(x)-\int g\, d\mu-(1-g(x))\mu(S) \\ &= g(x)-\int g\, d\mu \\ &= \langle\, \delta_x-\mu, g\,\rangle\,.\end{aligned}$$

Therefore,

$$\sup_{\substack{g\in \mathrm{B}_{\mathrm{FM}},\\ g(x)=1}} \langle\, \delta_x-\mu, g\,\rangle \geq \sup_{g\in \mathrm{B}_{\mathrm{FM}}} \langle\, \delta_x-\mu, g\,\rangle\,.$$

The other inequality holds trivially, so we have proved the result. □

Proposition 3.1.2. *Let (S,d) be a metric space and let $x\in S$, $\mu\in\mathcal{P}(S)$. Then*

$$\begin{aligned}\|\delta_x-\mu\|_{\mathrm{FM}}^{*} = 1-\int_S \big((1-d(x,s))\vee(-1)\big)\, d\mu(s) &= \langle\, \delta_x-\mu, (1-d(x,\cdot))\vee(-1)\,\rangle \qquad (3.1)\\ &= \langle\, \mu, 2\wedge d(x,\cdot)\,\rangle\,. \qquad (3.2)\end{aligned}$$

Proof. By Lemma 3.1.1, we have

$$\|\delta_x-\mu\|_{\mathrm{FM}}^{*} = \sup_{\substack{g\in \mathrm{B}_{\mathrm{FM}},\\ g(x)=1}} \langle\, \delta_x-\mu, g\,\rangle = \sup_{\substack{g\in \mathrm{B}_{\mathrm{FM}},\\ g(x)=1}} 1-\langle\, \mu, g\,\rangle = 1-\inf_{\substack{g\in \mathrm{B}_{\mathrm{FM}},\\ g(x)=1}} \int g\, d\mu. \qquad (3.3)$$

Let $\tilde{g} := (1-d(x,\cdot))\vee(-1)$. By Lemma 2.1.3, we have $\tilde{g}\in \mathrm{B}_{\mathrm{FM}}$, $\tilde{g}(x)=1$ and $\tilde{g}\leq g$ for any $g\in \mathrm{B}_{\mathrm{FM}}$ with $g(x)=1$.

These properties immediately yield

$$\inf_{\substack{g\in \mathrm{B}_{\mathrm{FM}},\\ g(x)=1}} \int g\, d\mu = \int_S \tilde{g}\, d\mu.$$

Together with (3.3), this gives (3.1).

Finally, (3.2) follows from the fact that for all $s\in S$:

$$(1-d(x,s))\vee(-1) = -((d(x,s)-1)\wedge 1) = -\big((d(x,s)\wedge 2)-1\big) = -(2\wedge d(x,s))+1.$$

□

It is worth to note that $(1-d(x,\cdot))\vee(-1)$ is an element of E_{FM} (see Definition 2.4.1). So we have found an extreme point of B_{FM} that yields the Fortet-Mourier norm as in Proposition 2.3.3.

Example 3.1.3. *Applying (3.2) to $\mu=\delta_y$, we obtain*

$$\|\delta_x-\delta_y\|_{\mathrm{FM}}^{*} = \langle\, \delta_y, 2\wedge d(x,\cdot)\,\rangle = \min(2, d(x,y)),$$

which is precisely the expression of [HW09, p. 8, Remark] that was already known.

Proposition 3.1.2 allows us to compute norms for which explicit expressions have not been known until now. For example, for any $y, x_1, x_2\in S$ and $\alpha\in(0,1)$, we have by (3.2):

$$\begin{aligned}\|\delta_y-\alpha\delta_{x_1}-(1-\alpha)\delta_{x_2}\|_{\mathrm{FM}}^{*} &= \langle\, \alpha\delta_{x_1}+(1-\alpha)\delta_{x_2}, 2\wedge d(y,\cdot)\,\rangle \\ &= \alpha\big(2\wedge d(y,x_1)\big)+(1-\alpha)\big(2\wedge d(y,x_2)\big). \qquad (3.4)\end{aligned}$$

This is a new result. It will be generalized in the proof of Proposition 5.2.2, see (5.3).

Example 3.1.4. *Let $S = [0,1]$ and let λ be the Borel-Lebesgue measure on S. Then*

$$\|\delta_x - \lambda\|^*_{\mathrm{FM}} = 1 - \int_0^x (1 - x + s)\, ds - \int_x^1 (1 + x - s)\, ds = \frac{1}{2} - x + x^2.$$

The function $x \mapsto \frac{1}{2} - x + x^2$ is minimal at $x = \frac{1}{2}$ with value $\frac{1}{4}$. Therefore,

$$\inf_{x \in S} \|\delta_x - \lambda\|^*_{\mathrm{FM}} = \|\delta_{\frac{1}{2}} - \lambda\|^*_{\mathrm{FM}} = \frac{1}{4}.$$

We note that $x = 1/2$ is the median of the uniform distribution on $[0,1]$, which is given by λ.

In Chapter 5, we will discuss in depth the problem of approximating a probability measure by a convex combination of at most N Dirac measures. Example 3.1.4 shows that for $N = 1$, $S = [0,1]$ and $\mu = \lambda$, a best approximation exists and is given by $\delta_{\frac{1}{2}}$. The next proposition provides a generalization.

Proposition 3.1.5. *Let $S = [0,1]$ and let f be a continuous probability density function, i.e., $f \in C[0,1]$, $f \geq 0$ and $\int f\, d\lambda = 1$. Then*

$$\inf_{x \in S} \|\delta_x - f d\lambda\|^*_{\mathrm{FM}} = \|\delta_{\tilde{x}} - f d\lambda\|^*_{\mathrm{FM}} = \int_{\tilde{x}}^1 s f(s)\, ds - \int_0^{\tilde{x}} s f(s)\, ds,$$

where $\tilde{x}$ is a median of $f d\lambda$, i.e., $\tilde{x}$ satisfies $\int_0^{\tilde{x}} f(s)\, ds = \int_{\tilde{x}}^1 f(s)\, ds$.

Proof. Using the expression from Proposition 3.1.2, we have

$$\begin{aligned}
\|\delta_x - f d\lambda\|^*_{\mathrm{FM}} &= 1 - \int_0^x (1 - x + s) f(s)\, ds - \int_x^1 (1 + x - s) f(s)\, ds \\
&= 1 - \int_0^1 f(s)\, ds + \int_0^x (x - s) f(s)\, ds + \int_x^1 (s - x) f(s)\, ds \\
&= \int_0^x (x - s) f(s)\, ds + \int_x^1 (s - x) f(s)\, ds \\
&= x \int_0^x f(s)\, ds + x \int_1^x f(s)\, ds - \int_0^x s f(s)\, ds - \int_1^x s f(s)\, ds.
\end{aligned}$$

By the Fundamental Theorem of Calculus, it follows that $\psi : S \to \mathbb{R} : x \mapsto \|\delta_x - f d\lambda\|^*_{\mathrm{FM}}$ is differentiable, with

$$\frac{d\psi}{dx} = (\int_0^x f(s)\, ds + x f(x)) + (\int_1^x f(s)\, ds + x f(x)) - x f(x) - x f(x) = \int_0^x f(s)\, ds + \int_1^x f(s)\, ds.$$

We see that $\frac{d\psi}{dx}(x) = 0 \iff x = \tilde{x}$, where $\tilde{x}$ is a median (note that the median is not necessarily unique).

For any median $\tilde{x}$, we have

$$\psi(\tilde{x}) = -\int_0^{\tilde{x}} s f(s)\, ds + \int_{\tilde{x}}^1 s f(s)\, ds = \int_0^{\tilde{x}} (1 - s) f(s)\, ds - \int_{\tilde{x}}^1 (1 - s) f(s)\, ds, \tag{3.5}$$

where we use that $\int_0^{\tilde{x}} f(s)\, ds = \int_{\tilde{x}}^1 f(s)\, ds$ for the second equality. Let $\tilde{x} > \tilde{y}$, and suppose that $\tilde{x}$ and $\tilde{y}$ are both medians. By the definition of a median and since $f \geq 0$, we have $f|_{(\tilde{x},\tilde{y})} = 0$. Thus,

$$\psi(\tilde{x}) - \psi(\tilde{y}) = -2 \int_{\tilde{y}}^{\tilde{x}} s f(s) ds = 0,$$

i.e., ψ is constant on the set of all medians. Now, we fix one median $\tilde{x}$.

S is compact, and ψ is continuous (even differentiable), so ψ attains a global minimum on S. It is attained either at the boundary or at $\tilde{x}$.

We show that the global minimum is attained at $\tilde{x}$. It holds that $\psi(0) = \int_0^1 sf(s)\,ds \geq \psi(\tilde{x})$, as we see from the first expression in (3.5). Furthermore, $\psi(1) = \int_0^1 f(s)\,ds - \int_0^1 sf(s)\,ds = \int_0^1 (1-s)f(s)\,ds \geq \psi(\tilde{x})$, by the second expression in (3.5). We conclude that ψ attains a global minimum at $\tilde{x}$, with $\psi(\tilde{x}) = \int_{\tilde{x}}^1 sf(s)\,ds - \int_0^{\tilde{x}} sf(s)\,ds$. □

Remark 3.1.6. *An obvious question, is whether an analogue of Lemma 3.1.1 and Proposition 3.1.2 can be derived for the norm* $\|\delta_x - \mu\|_{\mathrm{BL}}^*$*, for* $x \in S$ *and* $\mu \in \mathcal{P}(S)$*. The idea for these results was to pick the extreme point* $g \in \mathrm{E}_{\mathrm{FM}} \subset \mathrm{B}_{\mathrm{FM}}$ *that has the largest possible value at* x *(i.e.,* $g(x) = 1$*), and such that* g *is as small as possible outside* $\{x\}$*.*

Unfortunately, this strategy does not work for the bounded Lipschitz norm. The underlying reason is that g *does not remain in* B_{BL} *when it is 'shifted upward'. Indeed, when* $\|g\|_\infty$ *increases,* g *can only remain in* B_{BL} *if* $|g|_L$ *decreases, since* $\|g\|_{\mathrm{BL}}$ *has to stay below 1. But then,* g *must decrease less 'steeply' outside* $\{x\}$*. In contrast, for the Fortet-Mourier norm,* $\|g\|_\infty$ *and* $|g|_L$ *could be changed independently, as long as both values remained below 1.*

We will illustrate this with an example. Let $x \in S, \mu \in \mathcal{P}(S)$ *and suppose that* S *is compact, so that* $d(x, y_0) = \sup_{y \in S} d(x,y) < \infty$ *for some* $y_0 \in S$*. For non-constant* $g \in \mathrm{E}_{\mathrm{BL}}$*, the greatest possible value for* $\gamma := g(x)$ *is then* $\frac{d(x,y_0)}{2 + d(x,y_0)}$*. To see this, note that* g *has to attain both* $\gamma = \|g\|_\infty$ *and* $-\gamma = -\|g\|_\infty$ *by the definition of* E_{BL} *and note that* $|g|_L$ *is at most* $1 - \gamma$*. The range of* g *is the largest when* g *attains* $-\gamma$ *at the point at the greatest distance of* x*, i.e.,* $g(y_0) = -\gamma$ *and when* g *decreases as fast as possible outside* $\{x\}$*, meaning that*

$$g = \gamma - (1-\gamma)d(x,\cdot). \tag{3.6}$$

We then have $-\gamma = \gamma - (1-\gamma)d(x,y_0)$*, yielding* $\gamma = \frac{d(x,y_0)}{2+d(x,y_0)}$ *as claimed. We note that*

$$\langle\, \delta_x - \mu, g \,\rangle = \gamma - \int g d\mu \geq \gamma - \|g\|_\infty \mu(S) = 0 = \langle\, \delta_x - \mu, \pm 1 \,\rangle,$$

so it would not have been useful to look at the constant elements $\pm 1 \in \mathrm{E}_{\mathrm{BL}}$*, justifying our assumption that* g *is non-constant.*

However, g *does not maximize* $\langle\, \delta_x - \mu, \cdot \,\rangle$*. For a counterexample, let* $S = [0,2], x = 0, \mu = \delta_1$*. Then,* $y_0 = 2$*,* $\gamma = \frac{1}{2}$ *and*

$$\langle\, \delta_x - \mu, g \,\rangle = \langle\, \delta_x - \mu, \frac{1}{2} - \frac{1}{2} d(x,\cdot) \;= \frac{1}{2} - \frac{1}{2} + \frac{1}{2} d(x,1) = \frac{1}{2},$$

while

$$\langle\, \delta_x - \mu, \frac{1}{3} - \frac{2}{3} d(x,\cdot) \,\rangle = \frac{2}{3} > \frac{1}{2}.$$

Note that $\frac{1}{3} - \frac{2}{3} d(x,\cdot) \in \mathrm{E}_{\mathrm{BL}}$*. Apparently, if we define* g *by* (3.6)*, using the strategy from the Fortet-Mourier norm results,* g *does not give the bounded Lipschitz norm.*

In fact, one can show that $\|\delta_x - \delta_y\|_{\mathrm{BL}}^* = \langle\, \delta_x - \delta_y, \frac{d(y,\cdot) - d(x,\cdot)}{2 + d(x,y)} \,\rangle$ *([HW09, Lemma 3.5]). Here, we see that the element of* E_{BL} *that maximizes* $\langle\, \delta_x - \delta_y, \cdot \,\rangle$ *depends on* y*, i.e., on the support of* $\mu = \delta_y$*. This is opposed to the* μ*-independent function* $g = 1 - d(x,\cdot)$ *that led to* $\|\delta_x - \mu\|_{\mathrm{FM}}^*$ *for any* $\mu \in \mathcal{P}(S)$*. This indicates that the bounded Lipschitz norm will be 'trickier' to work with than the Fortet-Mourier norm, from an analytical-computational perspective.*

3.2 Distance between a convex combination of Dirac measures and a probability measure

In this section, we study distances $\|\nu - \mu\|_{\mathrm{FM}}^*$, where ν is a convex combination of N Dirac measures and μ is a probability measure. By definition, $\|\nu - \mu\|_{\mathrm{FM}}^* = \sup_{g \in \mathrm{B}_{\mathrm{FM}}} \langle\, \nu - \mu, g \,\rangle$. The next lemma shows that we can take the supremum over a smaller subset of test functions, in the setting of this section. Loosely said, it suffices to only consider the B_{FM}-functions that are the maximum of at most N hat-shaped functions, with hats located at the points in $\operatorname{supp}(\nu)$ and with at least one hat of height 1. This is already a considerable reduction of the original problem of computing $\|\nu-\mu\|^*_{\mathrm{FM}}$.

Lemma 3.2.1. *Let* $\nu=\sum_{i=1}^N \alpha_i\delta_{x_i}$, *with* $\alpha_i\in[0,1]$, $\sum_{i=1}^N\alpha_i=1$, $x_i\in S$ *and* $\mu\in\mathcal{P}(S)$. *Then*

$$\|\nu-\mu\|^*_{\mathrm{FM}}=\sup_{\substack{\theta_1,\dots,\theta_N\in[-1,1],\\ \exists k:\,\theta_k=1}}\left\langle\,\nu-\mu,(-1)\vee\bigvee_{i=1}^N(\theta_i-d(x_i,\cdot))\,\right\rangle \tag{3.7}$$

Proof. By definition, $\|\nu-\mu\|^*_{\mathrm{FM}}=\sup_{g\in\mathrm{B}_{\mathrm{FM}}}\langle\,\nu-\mu,g\,\rangle$. For any $\theta_1,\dots,\theta_N\in[-1,1]$, define

$$h_{\theta_1,\dots,\theta_N}(s):=(-1)\vee\bigvee_{i=1}^N(\theta_i-d(x_i,s)).$$

By Lemma 2.1.1, $h_{\theta_1,\dots,\theta_N}\in\mathrm{B}_{\mathrm{FM}}$, implying the inequality '$\geq$' in (3.7) immediately.

For the other inequality, let $g\in\mathrm{B}_{\mathrm{FM}}$. Define $\varepsilon:=\min_{1\leq i\leq N}(1-g(x_i))\geq 0$ and $\theta_i:=g(x_i)+\varepsilon$ for $i=1,\dots,N$. Define

$$h:=h_{\theta_1,\dots,\theta_N}.$$

By Lemma 2.1.6, h satisfies $h\in\mathrm{B}_{\mathrm{FM}}$, $h\leq g+\varepsilon$ on S, $h|_P=g|_P+\varepsilon$ and $\max h|_P=1$. Therefore, $\max_{1\leq i\leq N}\theta_i=\max(g|_P+\varepsilon)=\max h|_P=1$, so h is precisely of the form of the test functions on the right-hand side of (3.7).

The properties of h imply

$$\begin{aligned}\langle\,\nu-\mu,h\,\rangle&=\sum_{i=1}^N\alpha_i h(x_i)-\int h d\mu\\ &\geq\sum_{i=1}^N\alpha_i(g(x_i)+\varepsilon)-\int(g+\varepsilon)d\mu\\ &=\sum_{i=1}^N\alpha_i g(x_i)+\varepsilon\sum_{i=1}^N\alpha_i-\int gd\mu-\varepsilon\,\mu(S)\\ &=\sum_{i=1}^N\alpha_i g(x_i)-\int gd\mu\\ &=\langle\,\nu-\mu,g\,\rangle,\end{aligned}$$

proving the inequality '$\leq$'. □

Remark 3.2.2. *In the last lines of the proof above, we have used that the total mass of* μ *and* ν *are equal. If we want to generalize the lemma to measures with different mass, the condition '*$\exists k:\theta_k=1$*' has to be removed from the supremum. The details will be given in Lemma 4.0.1 and Remark 4.0.2.*

When both μ and ν are are convex combinations of Dirac measures, Lemma 3.2.1 provides two different sufficient subsets of test functions. Indeed, $\|\nu-\mu\|^*_{\mathrm{FM}}=\|\mu-\nu\|^*_{\mathrm{FM}}$, so one can either choose to locate the 'hats' at the support points of ν, or locate them at the support points of μ.

In the next example, we work out both ways for a simple example, and obtain two different functions for which $\langle\,\mu-\nu,\cdot\,\rangle$ is maximal.

Example 3.2.3. *Let* $\mu=\delta_y$, $\nu=\alpha\delta_{x_1}+(1-\alpha)\delta_{x_2}$, *with* $y,x_1,x_2\in S$ *and* $\alpha\in(0,1)$. *Using* (3.1.3) *derived from Proposition 3.1.2, we have*

$$\|\nu-\mu\|^*_{\mathrm{FM}}=\|\mu-\nu\|^*_{\mathrm{FM}}=\alpha\big(2\wedge d(y,x_1)\big)+(1-\alpha)\big(2\wedge d(y,x_2)\big).$$

If we further assume that Diam(S) $:= \sup\{d(x,y) : x, y \in S\} \leq 2$*, this reduces to*

$$\|\nu - \mu\|^*_{\mathrm{FM}} = \alpha d(y, x_1) + (1-\alpha) d(y, x_2). \tag{3.8}$$

On the other hand, we can call on Lemma 3.2.1, to obtain

$$\|\nu - \mu\|^*_{\mathrm{FM}} = \max\left(\sup_{\theta \in [-1,1]} \langle\, \nu - \mu, \psi_{1,\theta} \,\rangle, \sup_{\theta \in [-1,1]} \langle\, \nu - \mu, \psi_{2,\theta} \,\rangle \right), \tag{3.9}$$

where $\psi_{1,\theta}(s) := -1 \vee (1 - d(x_1, s)) \vee (\theta - d(x_2, s)$ *and* $\psi_{2,\theta}(s) := -1 \vee (\theta - d(x_1, s)) \vee (1 - d(x_2, s)$*. With our additional assumption Diam(S)* ≤ 2*, we have for all* $\theta \in [-1, 1]$*:*

$$\begin{aligned}
\langle\, \nu - \mu, \psi_{1,\theta} \,\rangle &= \alpha + (1-\alpha)\max(1 - d(x_1, x_2), \theta) - \max(1 - d(x_1, y), \theta - d(x_2, y)) \\
&= \begin{cases} -(1-\alpha) d(x_1, x_2) + d(x_1, y), & \theta \leq 1 - d(x_1, x_2), \\ (1-\alpha)(\theta - 1) + d(x_1, y), & 1 - d(x_1, x_2) < \theta < 1 - d(x_1, y) + d(x_2, y), \\ \alpha(1 - \theta) + d(x_2, y), & \theta \geq 1 - d(x_1, y) + d(x_2, y). \end{cases}
\end{aligned}$$

The supremum of $\langle\, \nu - \mu, \psi_{1,\theta} \,\rangle$ *is attained at* $\theta = \min(1 - d(x_1, y) + d(x_2, y), 1)$*, so*

$$\begin{aligned}
\sup_{\theta \in [-1,1]} \langle\, \nu - \mu, \psi_{1,\theta} \,\rangle &= \begin{cases} \langle\, \nu - \mu, \psi_{1,1-d(x_1,y)+d(x_2,y)} \,\rangle, & 1 - d(x_1, y) + d(x_2, y) \leq 1, \\ \langle\, \nu - \mu, \psi_{1,1} \,\rangle, & 1 - d(x_1, y) + d(x_2, y) > 1, \end{cases} \\
&= \begin{cases} \langle\, \nu - \mu, \psi_{1,1-d(x_1,y)+d(x_2,y)} \,\rangle, & d(x_1, y) \geq d(x_2, y), \\ \langle\, \nu - \mu, \psi_{1,1} \,\rangle, & d(x_1, y) < d(x_2, y), \end{cases} \\
&= \begin{cases} \alpha d(x_1, y) + (1-\alpha) d(x_2, y), & d(x_1, y) \geq d(x_2, y), \\ d(x_1, y), & d(x_1, y) < d(x_2, y). \end{cases}
\end{aligned}$$

By interchanging (x_1, α) *and* $(x_2, 1-\alpha)$*, we immediately also obtain*

$$\begin{aligned}
\sup_{\theta \in [-1,1]} \langle\, \nu - \mu, \psi_{2,\theta} \,\rangle &= \begin{cases} \langle\, \nu - \mu, \psi_{2,1-d(x_2,y)+d(x_1,y)} \,\rangle, & d(x_2, y) \geq d(x_1, y), \\ \langle\, \nu - \mu, \psi_{2,1} \,\rangle, & d(x_2, y) < d(x_1, y), \end{cases} \\
&= \begin{cases} \alpha d(x_1, y) + (1-\alpha) d(x_2, y), & d(x_2, y) \geq d(x_1, y), \\ d(x_2, y), & d(x_2, y) < d(x_1, y). \end{cases}
\end{aligned}$$

Combining these expressions with (3.9), it follows that

$$\|\nu - \mu\|^*_{\mathrm{FM}} = \begin{cases} \langle\, \nu - \mu, \psi_{1,1-d(x_1,y)+d(x_2,y)} \,\rangle, & d(x_1, y) \geq d(x_2, y), \\ \langle\, \nu - \mu, \psi_{2,1-d(x_2,y)+d(x_1,y)} \,\rangle, & d(x_2, y) \geq d(x_1, y), \end{cases} = \alpha d(x_1, y) + (1-\alpha) d(x_2, y).$$

This corresponds precisely with the expression in (3.8) that was obtained via Proposition 3.1.2. However, the test function that maximizes $\langle\, \nu - \mu, \cdot \,\rangle$ *now consists of two 'hats' instead of one.*

For general $\mu \in \mathcal{P}(S)$ and $N > 1$, it seems impossible to derive an explicit formula for $\|\nu - \mu\|^*_{\mathrm{FM}}$ from Lemma 3.2.1. However, in Section 4.2, we do describe a method to compute $\|\nu - \mu\|^*_{\mathrm{FM}}$ numerically in some cases.

Chapter 4

Distances between measures with different mass

In the previous chapter, we found expressions for Fortet-Mourier distances between probability measures μ and ν, with ν a convex combination of N Dirac measures. We continue by extending these results for measures with different mass. More precisely, we assume that $\mu \in \mathcal{M}^+(S)$ and $\nu = \sum_{i=1}^N \alpha_i \delta_{x_i}$ with $\alpha_i \geq 0$ and $x_i \in S$.

In Section 4.2, we show that computing the Fortet-Mourier distance between such measures can be reduced to minimizing a convex functional over a compact and convex subset of $\mathbb{R}^N$. We demonstrate how convex minimization of this functional can be done numerically when $S = \mathbb{R}^n$ and when μ is absolutely continuous with respect to the Borel-Lebesgue measure.

But we start with a simpler setting. Namely, when $N = 1$, i.e., $\nu = \alpha\delta_x$ for some $\alpha \geq 0$ and $x \in S$. In Section 4.1, we express the Fortet-Mourier distance explicitly for that case. In particular, we derive an explicit expression for $\|\delta_x - \mu\|^*_{\mathrm{FM}}$, for any $\mu \in \mathcal{M}^+(S)$.

The last three sections are devoted to the computation of $\|\nu - \mu\|^*_\bullet$, for μ and ν both positive linear combinations of Dirac measures. We do this for both $\bullet = \mathrm{FM}$ and $\bullet = \mathrm{BL}$. Put differently, we compute $\|\tau\|^*_\bullet$ for $\tau \in \mathrm{Mol}(S)$.

The just described problem has been considered before, in [JMC13] and [SFG$^+$12]. However, the problem was studied only for much more specific settings. In [SFG$^+$12], an algorithm is offered for the case in which ν and μ are both empirical probability measures and $\bullet = \mathrm{BL}$. On the other hand, the algorithm presented in [JMC13] only applies to $S \subset \mathbb{R}$ an interval or $S = \mathbb{R}$, and only for $\bullet = \mathrm{FM}$. In Section 4.4, we develop a novel exact algorithm for general metric spaces S, using functional analytic insights and linear programming, that works for both $\bullet = \mathrm{FM}$ and $\bullet = \mathrm{BL}$. Thus, it generalizes the previous result from [JMC13] in two directions: different norms and general space.

In this chapter, we assume that (S, d) is a metric space. We start with a reformulation and generalization of Lemma 3.2.1. This will be the main ingredient for the first two sections.

Lemma 4.0.1. *Let* $\nu = \sum_{i=1}^N \alpha_i \delta_{x_i}$, $\alpha_i \geq 0$, $x_i \in S$ *and let* $\mu \in \mathcal{M}^+(S)$. *Define* $P := \{x_1, \ldots, x_N\}$. *Then*

$$\|\nu - \mu\|^*_{\mathrm{FM}} = \sup_{g \in \mathrm{B}_{\mathrm{FM}}} \langle\, \nu - \mu, g \,\rangle = \sup_{f \in \mathrm{B}^P_{\mathrm{FM}}} \langle\, \nu - \mu, (-1) \vee \bigvee_{i=1}^N (f(x_i) - d(x_i, \cdot)) \,\rangle$$

Proof. Let $g \in \mathrm{B}_{\mathrm{FM}}$. We define

$$h := (-1) \vee \bigvee_{i=1}^N (g(x_i) - d(x_i, \cdot)).$$

By Lemma 2.1.4, we have $h \in \mathrm{B}_{\mathrm{FM}}$, $h|_P = g|_P$ and $h \leq g$. Therefore,

$$\langle\, \nu - \mu, h \,\rangle = \sum_{i=1}^N \alpha_i h(x_i) - \langle\, h, \mu \,\rangle = \sum_{i=1}^N \alpha_i g(x_i) - \langle\, h, \mu \,\rangle \geq \sum_{i=1}^N \alpha_i g(x_i) - \langle\, g, \mu \,\rangle = \langle\, \nu - \mu, g \,\rangle\,.$$

Note that $g|_P \in \mathrm{B}_{\mathrm{FM}}^P$ and $g(x_i) = g|_P(x_i)$ for all $i \in \{1, \dots, N\}$. This proves the inequality '$\leq$' of the statement in this lemma.

The other inequality is an immediate consequence of the fact that for any $f \in \mathrm{B}_{\mathrm{FM}}^P$, the function $(-1) \vee \bigvee_{i=1}^N (f(x_i) - d(x_i, \cdot))$ is an element of B_{FM}, see Lemma 2.1.5. ☐

Remark 4.0.2. *Alternatively, one can use the expression*

$$\|\nu - \mu\|_{\mathrm{FM}}^* = \sup_{\theta_1,\dots,\theta_N \in [-1,1]} \langle\, \nu - \mu, (-1) \vee \bigvee_{i=1}^N (\theta_i - d(x_i, \cdot)) \,\rangle\,. \tag{4.1}$$

This expression has the advantage that the supremum can be taken over the simpler set $[-1,1]^N$*. On the other hand, the downside is that for* $h = (-1) \vee \bigvee_{i=1}^N (\theta_i - d(x_i, \cdot))$*, it does not need to hold that* $h(x_i) = \theta_i$*, while we do have* $h(x_i) = f(x_i)$ *for* $h = (-1) \vee \bigvee_{i=1}^N (f(x_i) - d(x_i, \cdot))$ *with* $f \in \mathrm{B}_{\mathrm{FM}}^P$.

Let us explain why (4.1) *holds. Actually, it is an immediate consequence of Lemma 4.0.1 and the fact that*

$$\{(-1) \vee \bigvee_{i=1}^N (f(x_i) - d(x_i, \cdot)) : f \in \mathrm{B}_{\mathrm{FM}}^P\} = \{(-1) \vee \bigvee_{i=1}^N (\theta_i - d(x_i, \cdot)) : \theta \in [-1,1]^N\}. \tag{4.2}$$

We prove (4.2)*.*

Proof. For '$\subseteq$', let $f \in \mathrm{B}_{\mathrm{FM}}^P$ and $h := (-1) \vee \bigvee_{i=1}^N (f(x_i) - d(x_i, \cdot))$. Define $\theta_i := f(x_i)$. Then $\theta := (\theta_1, \dots, \theta_N) \in [-1,1]^N$ (since $f \in \mathrm{B}_{\mathrm{FM}}^P$) and $h = (-1) \vee \bigvee_{i=1}^N (\theta_i - d(x_i, \cdot))$.

For '$\supseteq$', let $\theta \in [-1,1]^N$ and $h := (-1) \vee \bigvee_{i=1}^N (\theta_i - d(x_i, \cdot))$. We have $h \in \mathrm{B}_{\mathrm{FM}}$ by Lemma 2.1.1, so $h|_P \in \mathrm{B}_{\mathrm{FM}}^P$. Let

$$\tilde{h} := (-1) \vee \bigvee_{i=1}^N (h(x_i) - d(x_i, \cdot)) = (-1) \vee \bigvee_{i=1}^N (h|_P(x_i) - d(x_i, \cdot)).$$

We show that $\tilde{h} = h$. By Lemma 2.1.4, we have $\tilde{h} \in \mathrm{B}_{\mathrm{FM}}$ and $\tilde{h} \leq h$. So it suffices to prove that $\tilde{h} \geq h$. For all $i \in \{1, \dots, N\}$, we have $h(x_i) \geq \theta_i - d(x_i, x_i) = \theta_i$, so $h(x_i) - d(x_i, \cdot) \geq \theta_i - d(x_i, \cdot)$. From the definitions of $\tilde{h}$ and h, it now immediately follows that $\tilde{h} \geq h$. We conclude that $\tilde{h} = h$ and hence, h contained in the set on the left-hand side of (4.2). ☐

4.1 FM-distance between a Dirac measure and a positive measure

In this section we derive a generalization of Proposition 3.1.2. The additional difficulty is that we no longer assume that μ has mass 1, an assumption that was explicitly used in the proof of Lemma 3.1.1.

First of all, the following corollary is an immediate consequence of Lemma 4.0.1 and Remark 4.0.2 (taking $N = 1$).

Corollary 4.1.1. *Let* $x \in S$ *and* $\mu \in \mathcal{M}^+(S)$*. Then*

$$\|\delta_x - \mu\|_{\mathrm{FM}}^* = \sup_{\theta \in [-1,1]} \langle\, \delta_x - \mu, (-1) \vee (\theta - d(x, \cdot)) \,\rangle\,.$$

We now present a novel expression for the distance between a Dirac measure and any finite positive measure.

Proposition 4.1.2. *Let* $x \in S$*,* $\mu \in \mathcal{M}^+(S)$*. It holds that*

$$\|\delta_x - \mu\|^*_{\mathrm{FM}} = \langle\, \delta_x - \mu, (-1) \vee (\theta_0 - d(x,\cdot))\, \rangle,$$

where

$$\theta_0 := \begin{cases} \inf\{\theta \in [-1,1] : \mu\big(B(x,\theta+1)\big) \geq 1\}, & \text{if } \mu\big(B(x,\theta+1)\big) \geq 1 \text{ for some } \theta \in [-1,1], \\ 1, & \text{otherwise,} \end{cases}$$

and $B(x,\theta+1) := \{s \in S : d(x,s) < \theta + 1\}$*.*

Proof. Define $\phi(\theta) := \langle\, \delta_x - \mu, (-1) \vee (\theta - d(x,\cdot))\, \rangle$. In view of Corollary 4.1.1, we need to maximize ϕ over $[-1,1]$. Let $\theta > \tilde\theta$. It holds that

$$\begin{aligned}
\phi(\theta) - \phi(\tilde\theta) &= \theta - \int_{B(x,\theta+1)} \theta - d(x,s)\, d\mu(s) - \int_{B(x,\theta+1)^c} -1\, d\mu(s) \\
&\qquad - \tilde\theta + \int_{B(x,\tilde\theta+1)} \tilde\theta - d(x,s)\, d\mu(s) + \int_{B(x,\tilde\theta+1)^c} -1\, d\mu(s) \\
&= \theta(1 - \mu(B(x,\theta+1)) + \int_{B(x,\theta+1)} d(x,s)\, d\mu(s) + \mu(S) - \mu(B(x,\theta+1)) \\
&\qquad - \tilde\theta(1 - \mu(B(x,\tilde\theta+1)) - \int_{B(x,\tilde\theta+1)} d(x,s)\, d\mu(s) - \mu(S) + \mu(B(x,\tilde\theta+1)) \\
&= (\theta - \tilde\theta)\Big(1 - \mu\big(B(x,\tilde\theta+1)\big)\Big) - \theta\mu(B(x,\theta+1) \setminus B(x,\tilde\theta+1)) \\
&\qquad + \int_{B(x,\theta+1)\setminus B(x,\tilde\theta+1)} d(x,s)\, d\mu(s) - \mu(B(x,\theta+1) \setminus B(x,\tilde\theta+1)) \\
&= (\theta - \tilde\theta)\Big(1 - \mu\big(B(x,\tilde\theta+1)\big)\Big) - \int_{B(x,\theta+1)\setminus B(x,\tilde\theta+1)} \theta - d(x,s) + 1\, d\mu(s).
\end{aligned}$$

Hence, for $-1 \leq \tilde\theta < \theta \leq 1$, we have $\phi(\theta) > \phi(\tilde\theta)$ if and only if

$$(\theta - \tilde\theta)\Big(1 - \mu\big(B(x,\tilde\theta+1)\big)\Big) > \int_{B(x,\theta+1)\setminus B(x,\tilde\theta+1)} \theta - d(x,s) + 1\, d\mu(s). \tag{4.3}$$

The right-hand side of (4.3) is always nonnegative, since $d(x,s) \leq \theta + 1$ for all $s \in B(x,\theta+1) \setminus B(x,\tilde\theta+1)$. Note that $\mu\big(B(x,\theta+1)\big)$ is non-decreasing in θ since μ is a positive measure. Using the definition of θ_0, it follows that $\mu\big(B(x,\tilde\theta+1)\big) \geq 1$ for all $\tilde\theta > \theta_0$. Now, if $\mu\big(B(x,\tilde\theta+1)\big) \geq 1$, then (4.3) cannot hold, as the right-hand side is nonnegative. Therefore, we have $\phi(\theta) \leq \phi(\tilde\theta)$ for all $\theta > \tilde\theta > \theta_0$. We conclude that ϕ is non-increasing on $(\theta_0, 1]$. Note that when $\theta_0 = 1$, it holds that $(\theta_0, 1] = \emptyset$. So in that case, the same statement is trivially true.

On the other hand, for all $s \in B(x,\theta+1) \setminus B(x,\tilde\theta+1)$ it holds that $d(x,s) \geq \tilde\theta + 1$, hence $\theta - \tilde\theta \geq \theta - d(x,s) + 1$. So if the condition

$$(\theta - \tilde\theta)\Big(1 - \mu\big(B(x,\tilde\theta+1)\big)\Big) > \int_{B(x,\theta+1)\setminus B(x,\tilde\theta+1)} \theta - \tilde\theta\, d\mu(s) \tag{4.4}$$

holds, then (4.3) is also satisfied. Now, (4.4) can be simplified. We have

$$\begin{aligned}
&(\theta - \tilde\theta)\Big(1 - \mu\big(B(x,\tilde\theta+1)\big)\Big) > \int_{B(x,\theta+1)\setminus B(x,\tilde\theta+1)} \theta - \tilde\theta\, d\mu(s) \\
&\iff 1 - \mu\big(B(x,\tilde\theta+1)\big) > \mu\big(B(x,\theta+1) \setminus B(x,\tilde\theta+1)\big) \\
&\iff 1 - \mu\big(B(x,\tilde\theta+1)\big) > \mu\big(B(x,\theta+1)\big) - \mu\big(B(x,\tilde\theta+1)\big) \\
&\iff 1 > \mu\big(B(x,\theta+1)\big).
\end{aligned}$$

So if $\mu\big(B(x,\theta+1)\big) < 1$, then (4.3) is satisfied and $\phi(\theta) > \phi(\tilde{\theta})$. Note that $\mu\big(B(x,\theta+1)\big) < 1$ for all $\theta < \theta_0$. Thus, ϕ is strictly increasing on $[-1,\theta_0)$. Note that the reasoning also applies when $\mu\big(B(x,\theta+1) < 1$ for all $\theta \in [-1,1]$ (i.e., $\theta_0 = 1$).

Finally, ϕ is continuous. To see this, note that $\theta \mapsto (-1) \vee (\theta - d(x,s))$ is continuous for all $s \in S$ and apply the Dominated Convergence Theorem. Together with the fact that ϕ is strictly increasing on $[-1,\theta_0)$ and non-increasing on $(\theta_0, 1]$, this proves that ϕ attains its supremum at θ_0. Using Corollary 4.1.1, we thus obtain

$$\|\delta_x - \mu\|^*_{\mathrm{FM}} = \sup_{\theta\in[-1,1]} \phi(\theta) = \phi(\theta_0) = \langle\, \delta_x - \mu, (-1) \vee (\theta_0 - d(x,\cdot))\,\rangle\,.$$

□

Remark 4.1.3. *For $\mu \in \mathcal{P}(S)$, Proposition 4.1.2 in some cases provides a different function $g \in \mathrm{B}_{\mathrm{FM}}$ with $\|\delta_x - \mu\|_{\mathrm{FM}} = \langle\, \delta_x - \mu, g\,\rangle$ than the function $(-1) \vee (1 - d(x,\cdot))$ that we found in Proposition 3.1.2. This may happen when $\theta_0 < 1$ for some μ and x.*

For example, suppose that $x, y \in S$, $d(x,y) = 1$, $\mu = \delta_y$. Then, $\theta_0 = \inf\{\theta \in [-1,1] : \mu(B(x,\theta+1)) \geq 1\} = 0$. The values $\langle\, \delta - \mu, (-1) \vee (\theta_0 - d(x,\cdot))\,\rangle$ and $\langle\, \delta - \mu, (-1) \vee (1 - d(x,\cdot))\,\rangle$ are the same:

$$\langle\, \delta_x - \delta_y, (-1) \vee (0 - d(x,\cdot))\,\rangle = 0 - (-1) = 1 = 1 - 0 = \langle\, \delta_x - \delta_y, (-1) \vee (1 - d(x,\cdot))\,\rangle\,.$$

This is consistent with the proof of Proposition 4.1.2: θ_0 is the smallest point at which ϕ attains its supremum. Since ϕ is only known to be non-increasing on $(\theta_0, 1]$, it may be that ϕ attains its supremum at larger points than θ_0 as well.

We consider some applications of Proposition 4.1.2.

Corollary 4.1.4. *Let $x \in S$, $\mu \in \mathcal{M}^+(S)$ and $\mu(S) < 1$. Then $\mu\big(B(x,\theta+1)\big) < 1$ for all $\theta \in [-1,1]$. Therefore, $\theta_0 = 1$ and $\|\delta_x - \mu\|^*_{\mathrm{FM}} = \langle\, \delta_x - \mu, (-1) \vee (1 - d(x,\cdot))\,\rangle = 1 - \mu(S) + \langle\, \mu, 2 \wedge d(x,\cdot)\,\rangle$.*

Corollary 4.1.5. *Let $\mu \in \mathcal{M}^+(S)$, $x \in S$ and $\alpha > 0$. Then,*

$$\|\alpha\delta_x - \mu\|^*_{\mathrm{FM}} = \alpha\theta_0 - \langle\, \mu, (-1) \vee (\theta_0 - d(x,\cdot))\,\rangle,$$

where

$$\theta_0 = \begin{cases} \inf\{\theta \in [-1,1] : \mu\big(B(x,\theta+1)\big) \geq \alpha\}, & \textit{if } \mu\big(B(x,\theta+1)\big) \geq \alpha \textit{ for some } \theta \in [-1,1], \\ 1, & \textit{otherwise.} \end{cases}$$

Proof. Applying Proposition 4.1.2 to $\alpha^{-1}\mu$ instead of μ, we obtain

$$\begin{aligned} \|\alpha\delta_x - \mu\|^*_{\mathrm{FM}} &= \alpha\|\delta_x - \alpha^{-1}\mu\|^*_{\mathrm{FM}} \\ &= \alpha\,\langle\, \delta_x - \alpha^{-1}\mu, (-1) \vee (\theta_0 - d(x,\cdot))\,\rangle \\ &= \alpha\theta_0 - \langle\, \mu, (-1) \vee (\theta_0 - d(x,\cdot))\,\rangle, \end{aligned}$$

with

$$\begin{aligned} \theta_0 &= \begin{cases} \inf\{\theta \in [-1,1] : \alpha^{-1}\mu\big(B(x,\theta+1)\big) \geq 1\}, & \text{if } \alpha^{-1}\mu\big(B(x,\theta+1)\big) \geq 1 \text{ for some } \theta \in [-1,1], \\ 1, & \text{otherwise.} \end{cases} \\ &= \begin{cases} \inf\{\theta \in [-1,1] : \mu\big(B(x,\theta+1)\big) \geq \alpha\}, & \text{if } \mu\big(B(x,\theta+1)\big) \geq \alpha \text{ for some } \theta \in [-1,1], \\ 1, & \text{otherwise.} \end{cases} \end{aligned}$$

This proves the statement. □

Corollary 4.1.6. *Let $\alpha, \beta \geq 0$ and $x, y \in S$. Then*

$$\|\alpha\delta_x - \beta\delta_y\|^*_{\mathrm{FM}} = |\alpha - \beta| + (\alpha \wedge \beta)(2 \wedge d(x,y)).$$

Proof. By Proposition 3.1.2, we have

$$\|\delta_x - \delta_y\|_{\mathrm{FM}}^* = \langle\, \delta_y, 2 \wedge d(x,\cdot)\,\rangle = 2 \wedge d(x,y).$$

Now, if we let $z = x$ when $\alpha \geq \beta$ and $z = y$ when $\alpha < \beta$, we have by the triangle inequality:

$$\begin{aligned}\|\alpha\delta_x - \beta\delta_y\|_{\mathrm{FM}}^* &= \|(\alpha \wedge \beta)(\delta_x - \delta_y) + |\alpha - \beta|\|\delta_z\|_{\mathrm{FM}}^* \\ &\leq (\alpha \wedge \beta)\|\delta_x - \delta_y\|_{\mathrm{FM}}^* + |\alpha - \beta|\|\delta_z\|_{\mathrm{FM}}^* \\ &= (\alpha \wedge \beta)(2 \wedge d(x,y)) + |\alpha - \beta|.\end{aligned}$$

Using Corollary 4.1.5, we can even obtain equality!

If $\alpha = 0$, then $\alpha \wedge \beta = 0$, so we have

$$\|\alpha\delta_x - \beta\delta_y\|_{\mathrm{FM}}^* = \|\beta\delta_y\|_{\mathrm{FM}}^* = \beta = |\alpha - \beta| + (\alpha \wedge \beta)(2 \wedge d(x,y)).$$

On the other hand, for $\alpha > 0$, we have

$$\|\alpha\delta_x - \beta\delta_y\|_{\mathrm{FM}}^* = \alpha\theta_0 - \beta((-1) \vee (\theta_0 - d(x,y)), \tag{4.5}$$

where

$$\begin{aligned}\theta_0 &= \begin{cases} \inf\{\theta \in [-1,1] : \beta\delta_y\big(B(x,\theta+1)\big) \geq \alpha\}, & \text{if } \exists\theta \in [-1,1] :\ \beta\delta_y\big(B(x,\theta+1)\big) \geq \alpha, \\ 1, & \text{otherwise,} \end{cases} \\ &= \begin{cases} d(x,y) - 1, & \text{if } \alpha \leq \beta, d(x,y) < 2, \\ 1, & \text{otherwise.} \end{cases}\end{aligned} \tag{4.6}$$

Combining (4.5) and (4.6), we obtain

$$\begin{aligned}\|\alpha\delta_x - \beta\delta_y\|_{\mathrm{FM}}^* &= \begin{cases} \alpha(d(x,y) - 1) - \beta(((-1) \vee ((d(x,y) - 1) - d(x,y)), & \text{if } \alpha \leq \beta, d(x,y) < 2, \\ \alpha - \beta((-1) \vee (1 - d(x,y)), & \text{otherwise.} \end{cases} \\ &= \begin{cases} \alpha(d(x,y) - 1) + \beta, & \text{if } \alpha \leq \beta, d(x,y) < 2, \\ \alpha - \beta((-1) \vee (1 - d(x,y)), & \text{otherwise.} \end{cases} \\ &= \begin{cases} \alpha(d(x,y) - 1) + \beta, & \text{if } \alpha \leq \beta, d(x,y) < 2, \\ \alpha - \beta(1 - d(x,y)), & \text{if } \alpha > \beta, d(x,y) < 2, \\ \alpha + \beta, & \text{if } d(x,y) \geq 2, \end{cases} \\ &= |\alpha - \beta| + (\alpha \wedge \beta)(2 \wedge d(x,y)),\end{aligned}$$

where we have used that $2(\alpha \wedge \beta) = \alpha + \beta - |\alpha - \beta|$ for the case $d(x,y) \geq 2$. Thus, we have obtained the desired expression for $\|\alpha\delta_x - \beta\delta_y\|_{\mathrm{FM}}^*$.

□

4.2 FM-distance between a positive linear combination of Dirac measures and a positive measure

In this section, we let $\nu = \sum_{i=1}^N \alpha_i\delta_{x_i}$, $\alpha_i \geq 0$, $x_i \in S$ and $\mu \in \mathcal{M}^+(S)$. We will derive expressions for $\|\nu - \mu\|_{\mathrm{FM}}^*$ that allow to compute or approximate the distance numerically for some classes of measures. We define $P := \{x_1, \ldots, x_N\}$ and

$$\psi : \mathrm{B}_{\mathrm{FM}}^P \to \mathbb{R} : f \mapsto \langle\, \nu - \mu, (-1) \vee \bigvee_{i=1}^N (f_i - d(x_i,\cdot))\,\rangle, \tag{4.7}$$

where $f_i := f(x_i)$. Due to Lemma 4.0.1, we have

$$\|\nu - \mu\|^*_{\mathrm{FM}} = \sup_{f \in \mathrm{B}^P_{\mathrm{FM}}} \psi(f). \tag{4.8}$$

Therefore, we can compute the norm $\|\nu - \mu\|^*_{\mathrm{FM}}$ by maximizing ψ over $\mathrm{B}^P_{\mathrm{FM}}$.

Some useful properties of the functional ψ are given in Proposition 4.2.2. In its proof we will make use of some elementary properties of maxima of real numbers. These are collected in the next lemma.

Lemma 4.2.1. *Let $n \in \mathbb{N}$ and $a_i, b_i \in \mathbb{R}$ for $i = 1, \dots, n$. It holds that*

(i) $\max_{i=1,\dots,n} (a_i + b_i) \leq \max_{i=1,\dots,n} a_i + \max_{i=1,\dots,n} b_i$,

(ii) $|\max_{i=1,\dots,n} a_i - \max_{i=1,\dots,n} b_i| \leq \max_{i=1,\dots,n} |a_i - b_i|$.

Proof. Part *(i)* is obvious. For *(ii)*, without loss of generality, assume that $\max_{i=1,\dots,n} a_i \geq \max_{i=1,\dots,n} b_i$ and let $j \in \{1, \dots, n\}$ be such that $a_j = \max_{i=1,\dots,n} a_i$. Then

$$|\max_{i=1,\dots,n} a_i - \max_{i=1,\dots,n} b_i| = a_j - \max_{i=1,\dots,n} b_i \leq a_j - b_j \leq |a_j - b_j| \leq \max_{i=1,\dots,n} |a_i - b_i|.$$

□

Proposition 4.2.2. *Let ψ be as defined in (4.7). Then ψ is concave and Lipschitz continuous with $|\psi|_L \leq \nu(S) + \mu(S)$.*

Proof. We first prove concavity. Write $\psi = \psi_1 - \psi_2$, with

$$\psi_1(f) := \langle \nu, (-1) \vee \bigvee_{i=1}^N (f_i - d(x_i, \cdot)) \rangle, \qquad \psi_2(f) := \langle \mu, (-1) \vee \bigvee_{i=1}^N (f_i - d(x_i, \cdot)) \rangle$$

for $f \in \mathrm{B}^P_{\mathrm{FM}}$. Lemma 2.1.5 shows that $(-1) \vee \bigvee_{i=1}^N (f_i - d(x_i, \cdot)) \in \mathrm{BL}(S)$ is an extension of $f \in \mathrm{B}^P_{\mathrm{FM}}$. Hence, $f_k = f(x_k) = (-1) \vee \bigvee_{i=1}^N (f_i - d(x_i, x_k))$ for all $k \in \{1, \dots, N\}$ and

$$\psi_1(f) = \langle \sum_{i=1}^N \alpha_i \delta_{x_i}, (-1) \vee \bigvee_{i=1}^N (f_i - d(x_i, \cdot)) \rangle = \sum_{k=1}^N \alpha_k f_k.$$

Therefore, ψ_1 is linear on $\mathrm{B}^P_{\mathrm{FM}}$ and in particular concave.

Next, we show that ψ_2 is convex. Let $f, g \in \mathrm{B}^P_{\mathrm{FM}}$ and $\gamma \in [0, 1]$. We have

$$\begin{aligned}
\psi_2\big(\gamma f + (1-\gamma) g\big) &= \int (-1) \vee \bigvee_{i=1}^N (\gamma f_i + (1-\gamma) g_i - d(x_i, s))\, d\mu(s) \\
&= \int (-1) \vee \bigvee_{i=1}^N \Big(\gamma\big(f_i - d(x_i, s)\big) + (1-\gamma)\big(g_i - d(x_i, s)\big)\Big)\, d\mu(s) \\
&\leq \int (-1) \vee \Big(\gamma \bigvee_{i=1}^N \big(f_i - d(x_i, s)\big) + (1-\gamma) \bigvee_{i=1}^N \big(g_i - d(x_i, s)\big)\Big)\, d\mu(s) \\
&= \int (-\gamma + (\gamma - 1)) \vee \Big(\gamma \bigvee_{i=1}^N \big(f_i - d(x_i, s)\big) + (1-\gamma) \bigvee_{i=1}^N \big(g_i - d(x_i, s)\big)\Big)\, d\mu(s) \\
&\leq \int \Big((-\gamma) \vee \gamma \bigvee_{i=1}^N \big(f_i - d(x_i, s)\big)\Big) + \Big((\gamma - 1) \vee (1-\gamma) \bigvee_{i=1}^N \big(g_i - d(x_i, s)\big)\Big)\, d\mu(s) \\
&= \gamma \int (-1) \vee \bigvee_{i=1}^N \big(f_i - d(x_i, s)\big) d\mu(s) + (1-\gamma) \int (-1) \vee \bigvee_{i=1}^N \big(g_i - d(x_i, s)\big)\, d\mu(s) \\
&= \gamma \psi_2(f) + (1-\gamma) \psi_2(g).
\end{aligned}$$

The inequalities in the lines above follow from the fact that $\gamma, 1-\gamma \geq 0$, positivity of μ and Lemma 4.2.1*(i)*. We conclude that ψ_2 in convex, and hence, $-\psi_2$ is concave. Since ψ_1 is also concave, it follows that the sum $\psi = \psi_1 + (-\psi_2)$ is concave.

Now we show that ψ is Lipschitz continuous. We have for all $f, g \in \mathrm{B}^P_{\mathrm{FM}}$:

$$|\psi_1(f) - \psi_1(g)| = |\sum_{i=1}^N \alpha_i (f_i - g_i)| \leq \sum_{i=1}^N \alpha_i |f_i - g_i| \leq \sum_{i=1}^N \alpha_i \|f-g\|_\infty \leq \sum_{i=1}^N \alpha_i \|f-g\|_{\mathrm{FM}}.$$

So ψ_1 is Lipschitz with $|\psi_1|_L \leq \sum_{i=1}^N \alpha_i = \nu(S)$. Also, using Lemma 4.2.1*(ii)*, we have

$$\big|(-1) \vee \bigvee_{i=1}^N (f_i - d(x_i, s)) - (-1) \vee \bigvee_{i=1}^N (g_i - d(x_i, s))\big| \leq \bigvee_{i=1}^N |f_i - g_i| = \|f-g\|_\infty \leq \|f-g\|_{\mathrm{FM}}.$$

This yields

$$\begin{aligned} |\psi_2(f) - \psi_2(g)| &= \big|\,\langle\, \mu, (-1) \vee \bigvee_{i=1}^N (f_i - d(x_i, \cdot)) - (-1) \vee \bigvee_{i=1}^N (g_i - d(x_i, \cdot))\,\rangle\,\big| \\ &\leq \langle\, \mu, \|f-g\|_{\mathrm{FM}}\, \mathbb{1}_S \,\rangle \\ &= \mu(S)\|f-g\|_{\mathrm{FM}}. \end{aligned}$$

So ψ_2 is Lipschitz as well, with $|\psi_2|_L \leq \mu(S)$. Finally, using that

$$|\psi_1(f) - \psi_2(f) - (\psi_1(g) - \psi_2(g))| \leq |\psi_1(f) - \psi_1(g)| + |\psi_2(f) - \psi_2(g)|,$$

we see that the difference $\psi = \psi_1 - \psi_2$ is Lipschitz continuous with $|\psi|_L \leq \nu(S) + \mu(S)$. ☐

The problem of maximizing the concave and Lipschitz continuous function ψ over the convex set $\mathrm{B}^P_{\mathrm{FM}}$ as posed in (4.8) is equivalent to minimizing the convex and Lipschitz continuous function $-\psi$ over $\mathrm{B}^P_{\mathrm{FM}}$. Note that $-\psi$ is continuous and $\mathrm{B}^P_{\mathrm{FM}}$ is compact, so at least we know that the minimum is attained at some point in $\mathrm{B}^P_{\mathrm{FM}}$.

Minimization problems for convex functions are widely studied, since they arise naturally in many disciplines. To mention a few, they appear in engineering, automatic control systems, network design and operation, finance, supply chain management, scheduling, among many other areas ([BV04, p. 3]). The theory of minimization of a convex function on a convex set is totally different from the theory of maximization ([Roc72, p. 342]). The minimum is generally attained in the interior of the set and not in an extreme point. Conditions for a minimizer can be derived, as can be found in [Roc72, §28, Corollary 28.3.1], but these conditions do not give a practical recipe for computing the minimizer or minimum.

The great thing is that a whole variety of algorithms have been developed for convex minimization. The mathematical subfield that studies the minimization of convex functions is called *convex optimization.* Due to all the activity in this subfield, convex optimization problems can be solved very efficiently, or as Boyd and VandenBerghe state in [BV04, p. 8]:

> "With only a bit of exaggeration, we can say that, if you formulate a practical problem as a convex optimization problem, then you have solved the original problem."

In our context, one could use subgradient methods (see [Ber15, Chapter 3]). These methods are very popular when the function that is minimized is not differentiable in the classical sense.

There are many packages available for convex optimization. In MATLAB®, one could use the 'CVX' package or the more generally applicable built-in 'fmincon' function. Alternatively, one could also use an optimization method for Lipschitz functions. For example, an applicable algorithm is presented in [MV17].

In order to use one of the algorithms, the expression for ψ given in (4.7) needs to be computable. Integration with respect to ν is easy since ν is a linear combination of Dirac measures. In contrast, integration with respect to a positive measure μ can generally not be done in programs such as MATLAB®.

However, if S is a hyperrectangle in $\mathbb{R}^n$, and μ is absolutely continuous with respect to the n-dimensional Borel-Lebesgue measure λ^n, then ψ can be evaluated. For such μ we have $\mu = hd\lambda^n$, where h is the Radon-Nikodym derivative. Therefore, $\langle \mu, f \rangle = \int_S f(s)h(s)d\lambda^n(s)$ for all $f \in \mathrm{B}^P_{\mathrm{FM}}$, so indeed, programs such as MATLAB® can compute $\psi(s)$ for $s \in S$. In the Introduction, we explained that this rather specific setting is particularly interesting for applications. We work out an example of a norm computation.

Example 4.2.3. *We consider the special case that $S = (S_{\min}, S_{\max}) \subset \mathbb{R}$. Here, $S_{\min}$ and $S_{\max}$ are allowed to be $-\infty$ and $+\infty$, respectively. Using the 'fmincon' function in* MATLAB®*, we implemented an algorithm that computes the norm $\|\nu - \mu\|^*_{\mathrm{FM}}$ for $\nu \in \mathrm{Mol}^+(S)$ and $\mu \in \mathcal{M}^+(S)$, where we assumed that $\mu = hd\lambda^n$. The code can be found in Appendix A.3.*

Letting $S = (0, \infty)$, $\mu = \exp(-s^2)d\lambda$ and $\nu = \frac{1}{2}\delta_0 + 2\delta_{\frac{1}{3}} + \frac{1}{5}\delta_{\frac{1}{2}} + \frac{1}{3}\delta_3$, we obtain the function $f \in \mathrm{B}^P_{\mathrm{FM}}$ that minimizes $-\psi$, and we find the norm $\|\nu - \mu\|^*_{\mathrm{FM}} = -\psi(f)$:

$$\textit{norm} = 2.392..., \qquad f = [1\ 1\ \tfrac{5}{6}\ 1].$$

4.3 Algorithm by Jabłoński and Marciniak-Czochra

As we have seen, computing $\|\nu - \mu\|^*_{\mathrm{FM}}$ for $\mu \in \mathcal{M}^+(S)$ and ν a positive linear combination of N Dirac measures is complicated when $N \geq 2$. We have described a numerical method, but this method only applies if the functional ψ in (4.7) can be evaluated by the chosen software. The computation of norms turns out to be more pleasant when both ν and μ are linear combinations of Dirac measures. In Section 4.4, we present an exact algorithm that computes $\|\nu - \mu\|^*_\bullet$ for such μ and ν and for $\bullet = \mathrm{FM}, \mathrm{BL}$. But before that, we shortly describe the algorithm by Jabłoński and Marciniak-Czochra that was already known.

The algorithm in [JMC13, §3.3] applies to the setting $\bullet = \mathrm{FM}$ and $S \subset \mathbb{R}$, where S is either an interval or $S = \mathbb{R}$. For such S, it computes the distance $\|\nu - \mu\|^*_{\mathrm{FM}}$ for μ and ν positive linear combinations of Dirac measures. Note that in [JMC13], the Fortet-Mourier distance is called the *flat metric*.

We write $\nu - \mu = \sum_{i=1}^n \alpha_i \delta_{x_i}$ with $\alpha_i \in \mathbb{R}$, $x_i \in S$ and, without loss of generality, $x_1 \leq x_2 \leq \ldots \leq x_n$. We define $\Delta_k := x_k - x_{k-1}$ for $2 \leq k \leq n$. Let us explain the algorithm. Detailed mathematical proofs can be found in [Eve15, Appendix D, Appendix E]. Define for $m \leq n$ and $\theta \in [-1, 1]$:

$$F^m(\theta) := \sup\{\sum_{k=1}^m \alpha_k f_k : f_m = \theta, |f_k - f_{k-1}| \leq |x_k - x_{k-1}|, |f_k| \leq 1 \ \text{ for all } k \leq m\}.$$

It is easy to verify that

$$\|\nu - \mu\|^*_{\mathrm{FM}} = \sup_{\theta \in [-1,1]} F^n(\theta), \tag{4.9}$$

see [Eve15, Lemma D.1]. Also, the following recursive relation holds:

$$\begin{cases} F^1(\theta) = \alpha_1 \theta, & \\ F^m(\theta) = \alpha_m \theta + \sup\limits_{f_{m-1} \in [\theta - \Delta_m, \theta + \Delta_m] \cap [-1,1]} F^{m-1}(f_{m-1}), & m \geq 2. \end{cases} \tag{4.10}$$

The functions F^m are concave, continuous, piecewise linear, and satisfy

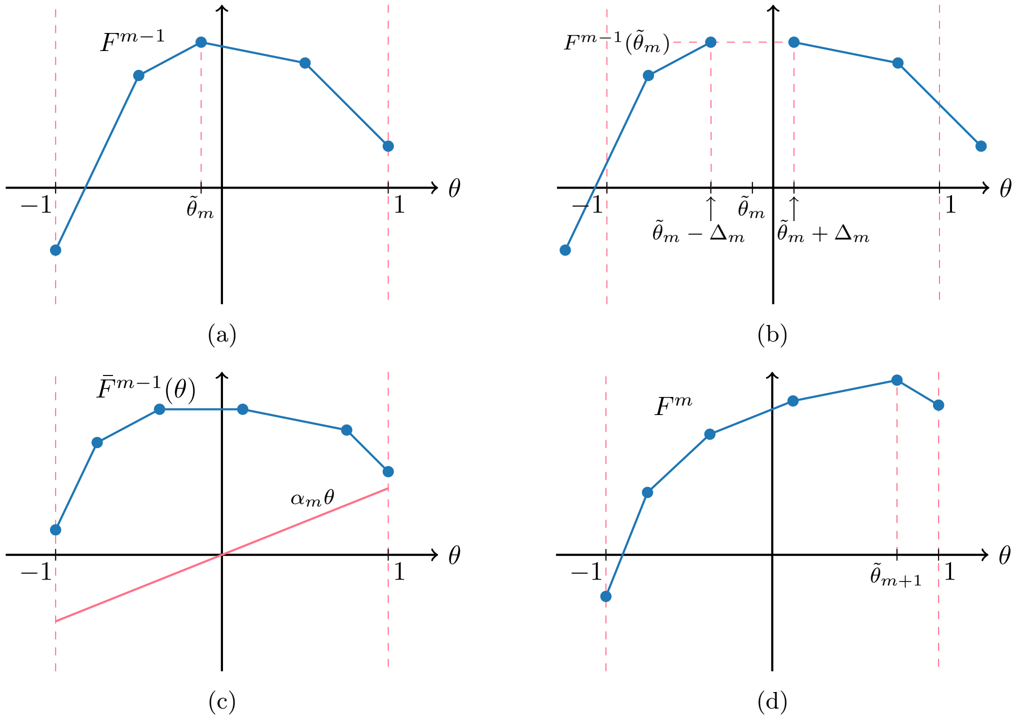
$$\sup_{\tilde{\theta} \in [\theta - \Delta_m, \theta + \Delta_m] \cap [-1,1]} F^{m-1}(\tilde{\theta}) = \begin{cases} F^{m-1}(\theta + \Delta_m), & \theta \in [-1, \tilde{\theta}_m - \Delta_m] \cap [-1, 1] \\ F^{m-1}(\tilde{\theta}_m), & \theta \in [\tilde{\theta}_m - \Delta_m, \tilde{\theta}_m + \Delta_m] \cap [-1, 1] \\ F^{m-1}(\theta - \Delta_m), & \theta \in [\tilde{\theta}_m + \Delta_m, 1] \cap [-1, 1], \end{cases} \tag{4.11}$$

where $\tilde{\theta}_m := \max\{\tilde{\theta} \in [-1,1] : F^{m-1}(\theta) \leq F^{m-1}(\tilde{\theta}) \text{ for all } \theta \in [-1,1]\}$. For detailed inductive proofs, see [Eve15, Lemma E. 1, Lemma E. 2]). Combining (4.10) and (4.11), we see that the supremum of F^n can now be computed easily. Hence, by (4.9), we can compute $\|\nu - \mu\|^*_{\mathrm{FM}}$. An illustration of the process can be found in Figure 4.1.

We conclude with a remark.

Remark 4.3.1. *Note that any $\tau \in \mathrm{Mol}(\mathbb{R})$ can be written as $\tau = \nu - \mu$ with μ and ν positive linear combinations of Dirac measures, so we can use the algorithm to compute the norm of any molecular measure on $\mathbb{R}$.*

Furthermore, we want to stress that the method uses the natural total order '$\leq$' on $\mathbb{R}$ in an essential way. Indeed, (4.10) *exploits the fact that $x_1 \leq x_2 \leq \ldots \leq x_n$. A similar recursive relation cannot be naturally derived for general metric spaces S. Even for $S = \mathbb{R}^d$ ($d \in \mathbb{N}_{>1}$), there exists no meaningful total order in this context, as was the case for $S = \mathbb{R}$. Therefore, we take another approach in the next sections, in which a total order on S is not needed.*



(a) (b) (c) (d)

Figure 4.1: The Jabłoński-Marciniak-Czochra-algorithm in operation. In (a), the piecewise linear and concave function F^{m-1} is shown. In (b), F^{m-1} is split at the argmax $\tilde{\theta}_m$ and translated over Δ_m to the left and right. In (c), we see the function $\bar{F}^{m-1}$, which we define by either side of (4.11). It is obtained by constant interpolation of the function in (b) on the interval $[\tilde{\theta}_m - \Delta_m, \tilde{\theta}_m + \Delta_m]$, and by restricting the resulting function to $[-1,1]$. Also, the linear function $\theta \mapsto \alpha_m\theta$ is shown. In (d), the next function F^m is revealed, which equals the sum of the two functions in (c). Moreover, the argmax $\tilde{\theta}_{m+1}$ is indicated, so that we are back in the situation of (a), and all steps can be repeated until $m = n$. Once $m = n$, the distance $\|\nu - \mu\|^*_{\mathrm{FM}}$ is equal to the supremum of F^m by (4.11). This figure has been adapted from [Eve15].

4.4 Exact algorithms for FM- and BL-distances between linear combinations of Dirac measures

Let (S,d) be a any metric space. In this section, we present exact algorithms that compute the norms $\|\tau\|_\bullet^*$ for $\bullet = \mathrm{FM}, \mathrm{BL}$ and for any molecular measure τ. In particular, the algorithms can be used to compute distances between measures μ and ν, when both are a linear combination of Dirac measures.

Let $\tau \in \mathrm{Mol}(S)$. Write $\tau = \sum_{i=1}^n \alpha_i \delta_{x_i}$ with $\alpha_i \in \mathbb{R}, x_i \in S$ and define $P := \{x_1, \ldots, x_n\}$. It holds that

$$\|\tau\|_\bullet^* = \sup_{g \in \mathrm{B}_\bullet^S} \langle\, \tau, g \,\rangle = \sup_{f \in \mathrm{B}_\bullet^P} \langle\, \tau|_P, f \,\rangle, \qquad \bullet = \mathrm{FM},\ \mathrm{BL}\ .$$

The last equality follows from the fact that $\langle\, \tau, g \,\rangle = \langle\, \tau|_P, g|_P \,\rangle$ for any $g \in \mathrm{B}_\bullet^S$, together with the fact that $R_P : \mathrm{BL}(S)_\bullet \to \mathrm{BL}(P)_\bullet : g \mapsto g|_P$ maps $\mathrm{B}_\bullet^S$ onto $\mathrm{B}_\bullet^P$, as was proved in Corollary 1.1.7.

Moreover, by Proposition 2.3.3 (applied to $\mathrm{BL}(P)$ instead of $\mathrm{BL}(S)$), there exists $f^* \in \mathrm{ext}(\mathrm{B}_\bullet^P)$ such that $\sup_{f \in \mathrm{B}_\bullet^P} \langle\, \tau|_P, f \,\rangle = \langle\, \tau|_P, f^* \,\rangle$, so

$$\|\tau\|_\bullet^* = \langle\, \tau|_P, f^* \,\rangle\,. \tag{4.12}$$

For $\bullet = \mathrm{BL}$ we have already seen pictures of $\mathrm{B}_\bullet^P$ and its extreme points, see Figures 2.1b and 2.2. Two examples of $\mathrm{B}_{\mathrm{FM}}^P$ and its extreme points are shown in Figures 4.2 and 4.3, for P consisting of three points. It turns out that $\mathrm{B}_\bullet^P$ is a *polytope* (we define this later) and can be defined via linear inequalities. The extreme point $f^* \in \mathrm{ext}(\mathrm{B}_\bullet^P)$ that satisfies (4.12) can be found using linear programming. Once we have found such f^*, (4.12) immediately yields the desired norm of τ.

We now put our problem of finding $\sup_{f \in \mathrm{B}_\bullet^P} \langle\, \tau|_P, f \,\rangle$ in a linear programming framework. After we have done that, any linear programming algorithm can produce the desired extreme point f^* and the corresponding value of $\|\tau\|_\bullet^*$.

In what follows, we will be using some shorthand notations. We define

$$f_i := f(x_i), \quad d_{ij} := d(x_i, x_j), \qquad f \in \mathrm{BL}(P), 1 \le i, j \le n. \tag{4.13}$$

Also, for any map $\phi : \mathrm{BL}(P) \to \mathbb{R}$, we define

$$\{\phi(f) \le 1\} := \{f \in \mathrm{BL}(P) : \phi(f) \le 1\}. \tag{4.14}$$

For example, $\{|f_k| \le 1\}$ denotes the set $\{f \in \mathrm{BL}(P) : |f_k| \le 1\}$.

Consider the FM-norm first. It holds that

$$\mathrm{B}_{\mathrm{FM}}^P = \bigcap_{1 \le k \le n} \{|f_k| \le 1\} \cap \bigcap_{1 \le i < j \le n} \{|f_i - f_j| d_{ij}^{-1} \le 1\}$$

and

$$\langle\, \tau|_P, f \,\rangle = \sum_{i=1}^n \alpha_i f_i.$$

Note that maximizing $\sum_{i=1}^n \alpha_i f_i$ is equivalent to minimizing $-\sum_{i=1}^n \alpha_i f_i$. Therefore, the problem of finding f^* that satisfies (4.12) can be rephrased as:

$$\text{Minimize } -\sum_{i=1}^n \alpha_i f_i \text{ subject to } \begin{cases} f_k \le 1, & 1 \le k \le n, \\ -f_k \le 1, & 1 \le k \le n, \\ (f_i - f_j) d_{ij}^{-1} \le 1, & 1 \le i < j \le n, \\ (f_j - f_i) d_{ij}^{-1} \le 1, & 1 \le i < j \le n. \end{cases} \tag{$\mathrm{LP}_{\mathrm{FM}}$}$$

This already is a standard linear programming formulation.

For the BL-norm, a linear programming formulation is slightly more complicated. We first need a small lemma.

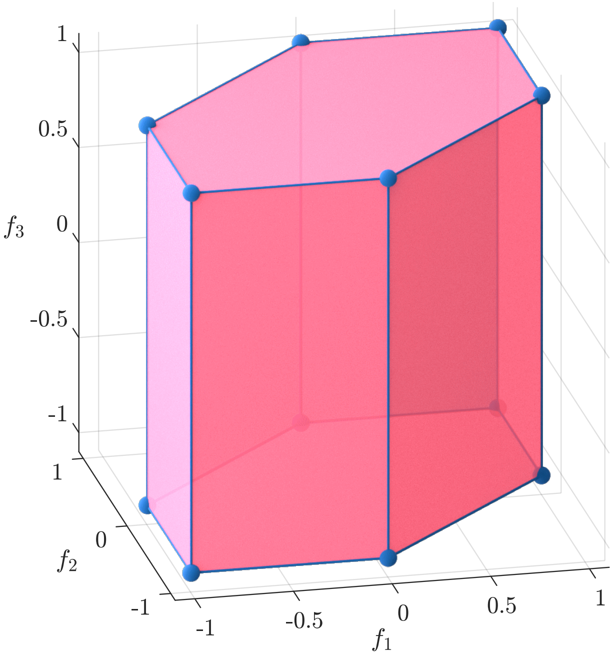


Figure 4.2: $\mathrm{B}^{P}_{\mathrm{FM}}$ for $d_{12} = 1, d_{13} = 2, d_{23} = 3$

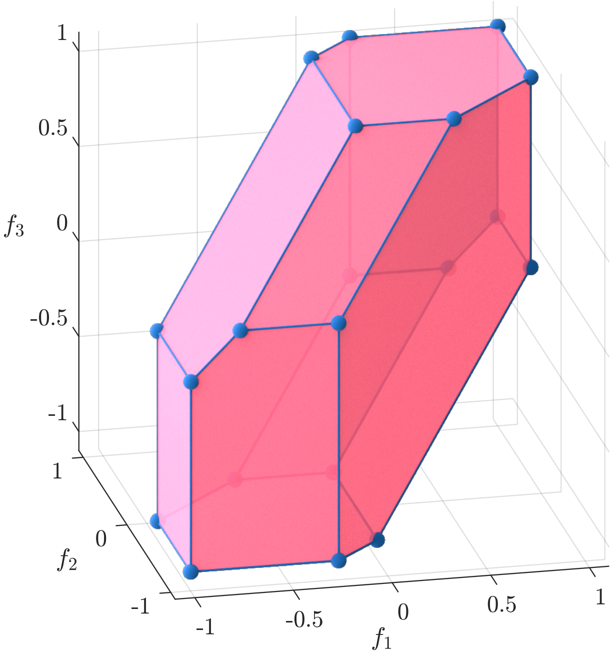


Figure 4.3: $\mathrm{B}^{P}_{\mathrm{FM}}$ for $d_{12} = 0.75, d_{13} = 1, d_{23} = 1.25$

Lemma 4.4.1. *Let $P = \{x_1, \dots, x_n\}$ with $n \geq 2$. We use the notation defined in* (4.13) *and* (4.14)*. It holds that*

$$\mathrm{B}_{\mathrm{BL}}^P = \bigcap_{1\leq i,j,k\leq n, k\neq i\neq j\neq k} \{f_k + (f_i - f_j)d_{ij}^{-1} \leq 1\} \cap \{-f_k - (f_i - f_j)d_{ij}^{-1} \leq 1\} \quad \cap \bigcap_{1\leq i,k\leq n, i\neq k} \{f_k + (f_k - f_i)d_{ik}^{-1} \leq 1\} \cap \{-f_k - (f_k - f_i)d_{ik}^{-1} \leq 1\}.$$

Furthermore,

$$\mathrm{B}_{\mathrm{BL}}^P = \bigcap_{1\leq i,j,k\leq n, i\neq j} \{|f_k| + |f_i - f_j|d_{ij}^{-1} \leq 1\}.$$

Proof. The second expression was added because of its more elegant appearance. However, only the first expression for $\mathrm{B}_{\mathrm{BL}}^P$ will be used in the derivation of the algorithm below. We provide a full proof for this first expression. The second expression can be proved in a similar fashion (even in less steps, as one does not need to distinguish between all the cases).

We start by proving "$\supset$". Let $f \in \mathrm{BL}(P)$ be contained in the right-hand side. Let $i, j, k \in \{1, \dots, n\}$, $i \neq j$ be such that $|f_k| = \|f\|_\infty$, $f_i - f_j = |f_i - f_j|$ and $(f_i - f_j)d_{ij}^{-1} = |f|_L$.

If $|f|_L = 0$, then f is constant and $f \in \{\pm f_k \pm (f_k - f_i)d_{ik}^{-1} \leq 1\} = \{\pm f_k \pm 0 \leq 1\}$ for all $i \neq k$, giving $\|f\|_\infty \leq 1$. Together with $|f|_L = 0$, this implies that $f \in \mathrm{B}_{\mathrm{BL}}^P$.

Now consider the other case: $|f|_L > 0$. We split the proof for this case in three parts. First, suppose that $k \notin \{i, j\}$. If $f_k = |f_k|$, then we use that $f \in \{f_k + (f_i - f_j)d_{ij}^{-1} \leq 1\}$ by assumption. This yields $\|f\|_{\mathrm{BL}} = \|f\|_\infty + |f|_L = f_k + (f_i - f_j)d_{ij}^{-1} \leq 1$, so $f \in \mathrm{B}_{\mathrm{BL}}^P$. If $-f_k = |f_k|$, we use that $f \in \{-f_k - (f_j - f_i)d_{ji}^{-1} \leq 1\}$, similarly giving $\|f\|_{\mathrm{BL}} = \|f\|_\infty + |f|_L = -f_k + (f_i - f_j)d_{ij}^{-1} = -f_k - (f_j - f_i)d_{ji}^{-1} \leq 1$, so $f \in \mathrm{B}_{\mathrm{BL}}^P$.

Secondly, suppose that $k = i$. Then it holds that $f_k - f_j = d_{kj}|f|_L > 0$, so $f_k > f_j$. If $f_k < 0$, then $|f_k| < |f_j|$, contradicting the fact that $|f_k| = \|f\|_\infty$. We conclude that $f_k = |f_k| = \|f\|_\infty$. Since f is an element of the right-hand side and $k = i \neq j$, we have $f \in \{f_k + (f_k - f_j)d_{jk}^{-1} \leq 1\}$. Hence, $\|f\|_{\mathrm{BL}} = \|f\|_\infty + |f|_L = f_k + (f_k - f_j)d_{jk}^{-1} \leq 1$. In other words, $f \in \mathrm{B}_{\mathrm{BL}}^P$.

Finally, suppose that $k = j$. Then, $f_i - f_k = d_{ik}|f|_L > 0$, so $f_i > f_k$. If $f_k > 0$, then $|f_i| > |f_k| = \|f\|_\infty$, a contradiction. Therefore, $-f_k = |f_k| = \|f\|_\infty$. By assumption, $f \in \{-f_k - (f_k - f_i)d_{ik}^{-1} \leq 1\}$. Hence, $\|f\|_{\mathrm{BL}} = \|f\|_\infty + |f|_L = -f_k - (f_k - f_i)d_{ik}^{-1} \leq 1$. Thus, $f \in \mathrm{B}_{\mathrm{BL}}^P$.

For the inclusion "$\subset$", suppose that $f \in \mathrm{B}_{\mathrm{BL}}^P$ and let $i, j, k \in \{1, \dots, n\}, k \neq i \neq j$ be arbitrary. Then, $\pm f_k \leq |f_k| \leq \|f\|_\infty$ and $\pm(f_i - f_j)d_{ij}^{-1} \leq |f_i - f_j|d_{ij}^{-1} \leq |f|_L \leq 1 - \|f\|_\infty$, so $\pm f_k \pm (f_i - f_j)d_{ij}^{-1} \leq \|f\|_\infty + 1 - \|f\|_\infty = 1$. Likewise, $\pm f_k \mp (f_i - f_j)d_{ij}^{-1} \leq 1$. Now, distinguishing between $k = j$ and $k \neq j$, we see that f is contained in the intersection on the right-hand side.

□

By the first expression in Lemma 4.4.1, the problem of finding f^* such that (4.12) holds can be rephrased as:

$$\text{Minimize } -\sum_{i=1}^n \alpha_i f_i \text{ subject to}$$
$$\begin{cases} f_k + (f_k - f_i)d_{ik}^{-1} \leq 1, & 1 \leq i, k \leq n, i \neq k \\ -f_k - (f_k - f_i)d_{ik}^{-1} \leq 1, & 1 \leq i, k \leq n, i \neq k \\ f_k + (f_i - f_j)d_{ij}^{-1} \leq 1, & 1 \leq i, j, k \leq n, k \neq i \neq j \neq k \\ -f_k - (f_i - f_j)d_{ij}^{-1} \leq 1, & 1 \leq i, j, k \leq n, k \neq i \neq j \neq k. \end{cases} \tag{LP$_{\mathrm{BL}}$}$$

The problems (LP$_{\mathrm{FM}}$) and (LP$_{\mathrm{BL}}$) are now formulated as a standard linear programming problem of the form: 'Minimize $c^T f$ subject to $A^\bullet f \leq b$' ($\bullet = \mathrm{FM}, \mathrm{BL}$), where $A^\bullet$ is an $m \times n$-matrix and b is a vector containing only ones, representing the linear constraints, $f = (f_1, \dots, f_n) \in \mathbb{R}^n$

and $c = -\alpha = -(\alpha_1, \dots, \alpha_n) \in \mathbb{R}^n$. For example, for $n = 2$ we can write

$$A^{\mathrm{FM}} = \begin{bmatrix} 1 & 0 \\ 0 & 1 \\ -1 & 0 \\ 0 & -1 \\ d_{12}^{-1} & -d_{12}^{-1} \\ -d_{12}^{-1} & d_{12}^{-1} \end{bmatrix}, \qquad A^{\mathrm{BL}} = \begin{bmatrix} 1 + d_{12}^{-1} & -d_{12}^{-1} \\ -d_{12}^{-1} & 1 + d_{12}^{-1} \\ -1 - d_{12}^{-1} & d_{12}^{-1} \\ d_{12}^{-1} & -1 - d_{12}^{-1} \end{bmatrix}. \tag{4.15}$$

Counting the number of inequalities in (LP$_{\mathrm{FM}}$), we find for the FM-norm: $m = 2n + 2\binom{n}{2} = n^2 + n$. For the BL-norm, we obtain from (LP$_{\mathrm{BL}}$): $m = 2n(n-1) + 2n(n-1)(n-2) = 2n(n-1)^2$. In our setting, the function $f \mapsto -\sum_{i=1}^n \alpha_i f_i = -\alpha^T f$ is called the *objective function.*

Linear programming problems can be solved exactly. The simplex algorithm is the most used algorithm that achieves this. The algorithm starts at one vertex of the polytope defined by the finite set of constraints. If this vertex does not minimize the objective function, then there exists an edge on which the objective function is strictly decreasing, and the algorithm turns to the vertex on the other side of this edge. Repeating this step, it finds a locally minimizing vertex in finitely many steps. Indeed, the number of vertices is finite and in each step one cannot come back to one of the vertices of the previous steps, since the objective function has strictly decreased in each step. Using the convexity of the object function and the convexity of the polytope, one can show that local minimizers are in fact global minimizers, thus one has found a globally minimizing vertex ([Ber97, Chapter 3, Exercise 3.1]).

There exist plenty of very fast optimization solvers that use linear programming, such as Gurobi and CPLEX. We chose to use the built-in 'linprog' function in MATLAB® and used it to compute FM-norms and BL-norms of molecular measures. The codes can be found in Appendix A.1 and Appendix A.2.

Theoretically, the simplex algorithm may need exponentially many steps to find the minimizing vertex. For example, if $d_{ij} \geq 2$ for all $i \neq j$, then $\mathrm{B}_{\mathrm{FM}}^P$ is equal to the n-cube $\{f : |f_i| \leq 1, i = 1, \dots, n\}$, and this cube has already 2^n vertices.

However, in practice, the number of steps is a low degree polynomial in m and n, and for real-life problems even typically linear ([Sha87, p. 302]). The rather mysterious reason is extensively studied. For a survey, see [Sha87]. Regardless of the reason, the low degree polynomial practical efficiency of the simplex algorithm is of course great news! Especially since our purpose is to compute norms of linear combinations of a possibly very large, finite number of Dirac measures, in which case n and m are large.

Example 4.4.2. *To test our algorithms, let τ be of the form $\sum_{i=1}^3 \alpha_i \delta_{x_i}, \alpha_i \in \mathbb{R}$ with $d_{12} = 1, d_{13} = 2, d_{23} = 3$ and $P := \{x_1, x_2, x_3\}$. In Figures 2.2 and 4.2 we have already included a picture of $\mathrm{B}_{\mathrm{BL}}^P$ and $\mathrm{B}_{\mathrm{FM}}^P$, respectively.*

Let $\alpha_1 = 1, \alpha_2 = -\frac{1}{3}$ and $\alpha_3 = -\frac{2}{3}$. Using Proposition 3.1.2, we can compute $\|\tau\|_{\mathrm{FM}}^*$ explicitly:

$$\|\tau\|_{\mathrm{FM}}^* = \langle\, \tau, (1 - d(x_1, \cdot)) \vee (-1)\,\rangle = \sum_{i=1}^3 \alpha_i((1 - d(x_1, x_i)) \vee -1) = 1 - \frac{1}{3}(1-1) - \frac{2}{3} \cdot -1 = \frac{5}{3}.$$

On the other hand, when we use

$$a = [1\ -\frac{1}{3}\ -\frac{2}{3}], \qquad dist = \begin{bmatrix} 0 & 1 & 2 \\ 1 & 0 & 3 \\ 2 & 3 & 0 \end{bmatrix}$$

as input for our MATLAB® *algorithm 'FMdualnorm' from Appendix A.1, we obtain as output*

$$norm = \frac{5}{3}, \qquad f = (1, 0, -1).$$

This not only shows that the norm is indeed $\frac{5}{3}$*, it also gives an extreme point* $f = (1, 0, -1)$ *that satisfies* (4.12). *In Figure 4.2 we see that* $f = (1, 0, -1)$ *is indeed one of the extreme points. It corresponds to the function* $(-1) \vee (1 - d(x_1, \cdot))$ *(recall that* $d_{12} = 1$, $d_{13} = 2$*), which is precisely the same function as appears in the expression for the* FM*-norm in Proposition 3.1.2!*

Unfortunately, we do not have an explicit expression for $\|\tau\|^*_{\mathrm{BL}}$*. However, the* MATLAB® *algorithm 'BLdualnorm' from Appeldix A.2 yields*

$$norm = \frac{5}{6}, \qquad f = (\frac{1}{2}, 0, -\frac{1}{2}),$$

and at least from Figure 2.2 we see that $f = (\frac{1}{2}, 0, -\frac{1}{2})$ *is one of the extreme points.*

Lastly, it is worth noting that in general, we have $\|\tau\|^*_{\mathrm{BL}} \leq \|\tau\|^*_{\mathrm{FM}} \leq 2\|\tau\|^*_{\mathrm{BL}}$ *by Lemma 1.2.2. In the above setting, we see that* $\|\tau\|^*_{\mathrm{FM}} = 2\|\tau\|^*_{\mathrm{BL}}$*, making the second bound sharp.*

Remark 4.4.3. *For the specific linear programming problems* ($\mathrm{LP}_{\mathrm{FM}}$) *and* ($\mathrm{LP}_{\mathrm{BL}}$)*, the number of steps executed by the simplex algorithm can be reduced in a few ways. For example, the points* $(1, \ldots, 1)$ *and* $(-1, \ldots, -1)$ *are always vertices of* $\mathrm{B}^P_\bullet$*, both for* $\bullet = \mathrm{FM}$ *and* $\bullet = \mathrm{BL}$*. Therefore, the first step of finding an initial vertex can be skipped, as one can let the algorithm start at* $(1, \ldots, 1)$ *or* $(-1, \ldots, -1)$*.*

We can reduce the steps further by exploiting the point symmetry of $\mathrm{B}^P_\bullet$ *about the origin. Let* $vert(\mathrm{B}^P_\bullet)$ *be the set of all extreme points (vertices) of* $\mathrm{B}^P_\bullet$*. We have* $\mathrm{B}^P_\bullet = -\mathrm{B}^P_\bullet$*, so* $vert(\mathrm{B}^P_\bullet) = -vert(\mathrm{B}^P_\bullet)$*. Also, the objective function satisfies* $-\alpha^T(-f) = -(-\alpha^T)f$*, so it holds that*

$$\#\{f \in vert(\mathrm{B}^P_\bullet) : -\alpha^T f < 0\} \leq \frac{1}{2}\#vert(\mathrm{B}^P_\bullet). \tag{4.16}$$

Now, if we take $(1, ..., 1)$ *as initial vertex* f_0 *when* $\sum_{i=1}^n \alpha_i \geq 0$*, and* $f_0 = (-1, ..., -1)$ *when* $\sum_{i=1}^n \alpha_i < 0$*, then we have already eliminated half of the vertices! Indeed, for these choices, we have* $-\alpha^T f_0 \leq 0$*. In each step the objective function decreases strictly, so all next vertices* f *satisfy* $-\alpha^T f < 0$*. From* (4.16)*, we see that the maximal number of steps is now at least halved.*

4.5 Alternative approach via polars of polytopes

In this section, we describe an alternative method for the computation of $\|\tau\|^*_\bullet$, making use of the polar of $\mathrm{B}^P_\bullet$. Although this method will turn out to be complicated and less efficient than the method from Section 4.4, we still found it useful to include the idea, since it provides a geometric picture to the optimization problems ($\mathrm{LP}_{\mathrm{FM}}$) and ($\mathrm{LP}_{\mathrm{BL}}$). We start with some definitions.

Definition 4.5.1. For $D \subset \mathbb{R}^n$, the *polar set* D^Δ is defined by

$$D^\Delta := \{y \in \mathbb{R}^n : y^T x \leq 1 \text{ for all } x \in D\}.$$

Definition 4.5.2. A *polytope* in a vector space is the convex hull (see Definition 2.4.4) of a finite set, that is, a subset of the form $T = \mathrm{conv}(P) \subset \mathbb{R}^n$ for some finite set $P \subset \mathbb{R}^n$.

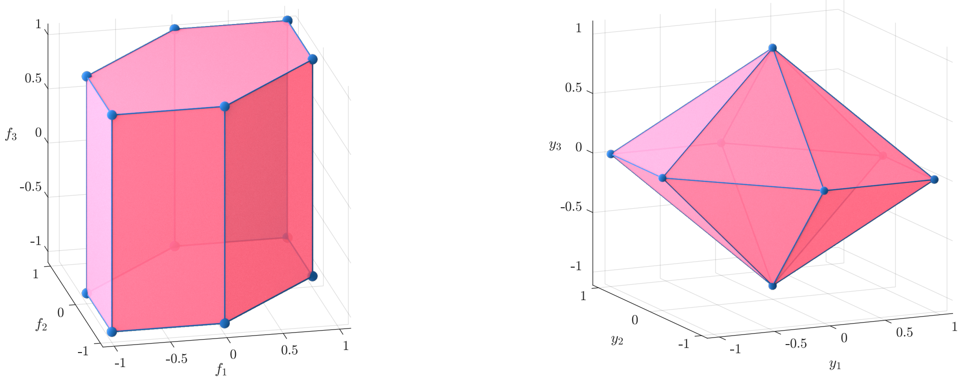
A *face* of a convex polytope T is any subset of the form $F = \{x \in T : a^T x = c\}$, where the linear inequality $a^T x \leq c$ holds for all $x \in T$. The *dimension* of a face F is the dimension of its *affine hull*, which is defined as the intersection of all affine subspaces of $\mathbb{R}^n$ containing F.

A *facet* of a polytope is a face of one dimension lower than the dimension of the polytope itself.

Remark 4.5.3. *We will not dive too deeply into polytope theory. However, there are two useful properties of polytopes that we need for the upcoming discussion.*

Firstly, a polytope is equivalently an intersection of finitely many closed halfspaces $\{x \in \mathbb{R}^n : a^T x \leq c\}$ *(see [Zie95, Definition 0.1, Theorem 1.1]).*

Secondly, if T *is a polytope, then every facet in* T^Δ *corresponds with a vertex in* T *and vice versa. Details can be found in [Zie95, §2.3, Corollary 2.4, p. 64].*



(a) $\mathrm{B}_{\mathrm{FM}}^{P}$ (b) $(\mathrm{B}_{\mathrm{FM}}^{P})^{\Delta}$

Figure 4.4: Closed unit ball and its polar for $P = \{x_1, x_2, x_3\}$, $d_{12} = 1, d_{13} = 2, d_{23} = 3$.

As mentioned before, using the formulations ($\mathrm{LP}_{\mathrm{FM}}$) and ($\mathrm{LP}_{\mathrm{BL}}$), we can write the closed unit balls $\mathrm{B}_{\bullet}^{P}$ in the form $\{f \in \mathbb{R}^n : A^{\bullet} f \leq 1\}$, where $A^{\bullet} \in \mathbb{R}^{m \times n}$ represents all constraints (see (4.15) for the example $n = 2$). Let $row(A^{\bullet})^T \subset \mathbb{R}^n$ denote the set of the m rows of $A^{\bullet}$, where each row is transposed so that $row(A^{\bullet})^T$ consists of column vectors. Note that

$$\mathrm{B}_{\bullet}^{P} = \{f \in \mathbb{R}^n : A^{\bullet} f \leq 1\} = \cap_{a \in row(A^{\bullet})^T} \{f \in \mathbb{R}^n : a^T f \leq 1\}.$$

It now follows immediately from Remark 4.5.3 that $\mathrm{B}_{\bullet}^{P}$ is a polytope. Moreover, by [Zie95, Theorem 2.11(vii)], we have

$$(\mathrm{B}_{\bullet}^{P})^{\Delta} = \{f \in \mathbb{R}^n : A^{\bullet} f \leq 1\}^{\Delta} = \operatorname{conv}(row(A^{\bullet})^T).$$

Note that $(\mathrm{B}_{\bullet}^{P})^{\Delta}$ is the convex hull of m vectors and hence a polytope itself by Definition 4.5.2. An example of a polar is shown in Figure 4.4, where we have plotted the ball $\mathrm{B}_{\mathrm{FM}}^{P}$ from Figure 4.2 and its polar.

As before, write $\tau = \sum_{i=1}^{n} \alpha_i \delta_{x_i}$ and $\alpha = (\alpha_1, \ldots, \alpha_n)$. Now consider the ray $\mathbb{R}_+ \alpha := \{\lambda \alpha : \lambda \geq 0\}$. Note that it will intersect at least one facet of $(\mathrm{B}_{\bullet}^{P})^{\Delta}$ (and possibly more than one if the intersection occurs at the boundary of a facet). Let F_α be such a facet. Then we have $\lambda \alpha \in F_\alpha$ for a unique $\lambda > 0$. Note that the facet F_α is a polytope itself. Hence, it is the convex hull of finitely many vertices, and these vertices are also vertices of $(\mathrm{B}_{\bullet}^{P})^{\Delta}$ by [Sim11, Proposition 8.6]. So F_α is the convex hull of finitely many elements of $row(A^{\bullet})^T$, and we denote these elements by $A_1^{\alpha}, \ldots, A_N^{\alpha}$. Then, we have $\lambda \alpha \in F_\alpha = \operatorname{conv}(\{A_1^{\alpha}, \ldots, A_N^{\alpha}\})$, so $\lambda \alpha = \sum_{i=1}^{N} \lambda_i A_i^{\alpha}$ for some $\lambda_i \in [0, 1]$ with $\sum_{i=1}^{N} \lambda_i = 1$.

We note that the upcoming reasoning and the estimation given in (4.18) apply independently of the choice of the coefficients λ_i in the convex combination representation $\lambda \alpha = \sum_{i=1}^{N} \lambda_i A_i^{\alpha}$. Also, if $\mathbb{R}_+ \alpha$ intersects multiple facets, we can choose any of these facets and apply the argument below.

By Remark 4.5.3, F_α corresponds precisely with one vertex f_α of $\mathrm{B}_{\bullet}^{P}$. This vertex can be found solving

$$\begin{bmatrix} (A_1^{\alpha})^T \\ \vdots \\ (A_N^{\alpha})^T \end{bmatrix} f_\alpha = \begin{bmatrix} 1 \\ \vdots \\ 1 \end{bmatrix}. \tag{4.17}$$

We show that $\langle\, \tau|_P, f_\alpha \,\rangle = \sup_{f\in \mathrm{B}_\bullet^P} \langle\, \tau|_P, f \,\rangle$. For any $f \in \mathrm{B}_\bullet^P$, we have

$$\langle\, \tau|_P, f \,\rangle = \alpha^T f = \lambda^{-1} \sum_{i=1}^{N} \lambda_i (A_i^\alpha)^T f \leq \lambda^{-1} \sum_{i=1}^{N} \lambda_i \cdot 1 = \lambda^{-1}, \tag{4.18}$$

where the second last inequality follows from the fact that $\mathrm{B}_\bullet^P = \{f \in \mathbb{R}^n : A^\bullet f \leq 1\}$. Moreover, we have equality when $f = f_\alpha$, as follows from (4.17). We conclude that $\|\tau\|_\bullet^* = \langle\, \tau|_P, f_\alpha \,\rangle = \lambda^{-1}$.

To compute the norm $\|\tau\|_\bullet^*$, one can now either compute

$$\lambda^{-1} = \sup\{l \geq 0 : l\alpha \in (\mathrm{B}_\bullet^P)^\Delta\}^{-1} = \inf\{t \geq 0 : \alpha \in t(\mathrm{B}_\bullet^P)^\Delta\}, \tag{4.19}$$

or compute f_α via (4.17). One can omit computing the extreme point f_α by using (4.19). Note that the expression for λ^{-1} in (4.19) is precisely the Minkowski functional of $(\mathrm{B}_\bullet^P)^\Delta$ at α. Summarizing, we have proved the following:

Proposition 4.5.4. *Let $\tau = \sum_{i=1}^n \alpha_i \delta_{x_i}$ with $\alpha_i \in \mathbb{R}$, $x_i \in S$. Put $P := \{x_1, \ldots, x_n\}$. For any $K \subset \mathbb{R}^n$, let p_K denote the Minkowski functional of the set K in $\mathbb{R}^n$. Then $\|\tau\|_\bullet^* = p_{(B_\bullet^P)^\Delta}(\alpha)$ for* $\bullet = \mathrm{FM}, \mathrm{BL}$.

We now reflect on the feasibility of a method that uses the principles above to compute $\|\tau\|_\bullet^*$. Unfortunately, although the principles described above are appealing, a practical application cannot be done elegantly nor efficiently.

First of all, finding the intersection of a ray and a polytope is hard. If $(\mathrm{B}_\bullet^P)^\Delta$ is a 2- or 3-dimensional polytope, the problem of intersecting a ray $\mathbb{R}_+\,\alpha$ with $(\mathrm{B}_\bullet^P)^\Delta$ is a version of the line clipping problem, where one determines the intersection of a line with a *polygon* (a 2D polytope) or *polyhedron* (a 3D polytope). The problem has been widely studied. It is of vital importance for computer graphics, where one needs to remove the parts of lines that are outside a viewing area. The Cyrus-Beck-algorithm [CB78] is a well-known algorithm that applies to our setting. It has an efficiency of $\mathcal{O}(\tilde{n})$, where $\tilde{n}$ denotes the number of facets of $(\mathrm{B}_\bullet^P)^\Delta$, which is equal to the number of vertices of $\mathrm{B}_\bullet^P$ by [Zie95, §2.3]. Improved algorithms can be found in [Ska94] (for 2D, efficiency $\mathcal{O}(\log \tilde{n})$) and in [Ska97] (for 3D, expected efficiency $\mathcal{O}(\sqrt{\tilde{n}})$, efficiency $\mathcal{O}(\tilde{n})$ for the worst case).

We note that $\tilde{n}$, the number of vertices of $\mathrm{B}_\bullet^P$, is also the maximal number of steps in the simplex algorithm. Therefore, if we would use the Cyrus-Beck algorithm, with efficiency $\mathcal{O}(\tilde{n})$, this would not structurally improve the approach via the simplex algorithm as described in Section 4.4. The Skala algorithms could improve the efficiency in theory. However, $\sqrt{\tilde{n}}$ is still exponential in n and $\log \tilde{n}$ is polynomial in n. As mentioned before, the practical efficiency of the simplex algorithm is also polynomial in n. So the approach via the polar, using an algorithm by Skala, will not be a major improvement. Also, we want to compute norms of linear combinations of many Dirac measures, and not just two or three, so we would need higher dimensional line clipping algorithms first! We have not been able to find line clipping algorithms for higher dimensional polytopes, but the problem is unlikely to get easier in higher dimensions.

Next, we have to be aware that there is another obstacle, that we have not even taken into account yet. The line-clipping algorithms assumes that we already have a list of the vertices of $(\mathrm{B}_\bullet^P)^\Delta$ ([Ska05, p. 907]). In our case, we do know that $(\mathrm{B}_\bullet^P)^\Delta = \mathrm{conv}(\mathit{row}(A^\bullet)^T)$, but this does not mean that the vertices are given by $\mathit{row}(A^\bullet)^T$, unfortunately! A row vector of $A^\bullet$ might be a convex combination of the other row vectors of $A^\bullet$, in which case it is redundant, as it does not contribute to the convex hull. The corresponding element of $\mathit{row}(A^\bullet)^T$ is then no vertex of $(\mathrm{B}_\bullet^P)^\Delta$.

Recall that each vertex of $(\mathrm{B}_\bullet^P)^\Delta$ corresponds with a facet of $\mathrm{B}_\bullet^P$, and each facet of $\mathrm{B}_\bullet^P$ corresponds with a linear constraint, i.e., with a row of $A^\bullet$. So the problem of enumerating all vertices of $(\mathrm{B}_\bullet^P)^\Delta$ corresponds with identifying all redundant linear constraints (redundant in the sense that removing the constraint-defining row from $A^\bullet$ would still lead to the same set $\{f \in \mathbb{R}^n : A^\bullet f \leq 1\}$). This problem has been widely studied. Solving techniques can be found in [TTZ66] and [Mat73]. However, solving the problem will of course add even more computations to our method via the polar.

All in all, the polar provides a geometric picture, but for practical applications, it is more efficient to stick to the simplex algorithm described in Section 4.4.

Remark 4.5.5. *In Example 2.5.4, we came across another famous problem related to enumerating vertices of polytopes, when we considered the extreme points of a specific* $\mathrm{B}_{\mathrm{BL}}^{P}$. *As we mentioned there, it is extremely difficult to find and enumerate all extreme points (i.e., vertices) of a polytope given the polytope-defining constraints. Now we have introduced polytopes, we elaborate on this a bit more.*

There does exist a brute force way to determine all vertices: for each selection of n *rows of* $A^{\bullet}$, *one can verify whether the* $n \times n$*-matrix consisting of these* n *rows is invertible. If it is invertible, then the intersection of the* n *boundaries of the halfplanes corresponding to the* n *rows will define a vertex (this vertex can be found as was done in* (4.17)*). Going through all* $\binom{m}{n}$ *choices of* n *rows, one precisely finds all extreme points in this way, as follows from [Ber97, Theorem 2.3, Definition 2.9, Theorem 2.2]. However,* $m = n^2 + n$ *for the* FM*-norm and* $m = 2n(n-1)^2$ *for the* BL*-norm, so going through* $\binom{m}{n}$ *selections of rows will get completely out of hand.*

A lot of research has been done on more efficient methods to determine all extreme points. However, the problem remains extremely hard. A historical overview and a comparison of algorithms that do find the extreme points can be found in [KBB^{+}*08] and [MR80].*

Chapter 5

Approximations by measures with finite support

We have described various ways to compute Fortet-Mourier and bounded Lipschitz distances between finite positive measures of which one is a linear combination of Dirac measures. We now study related approximation questions. As motivated in the introduction, we are interested in approximating a probability measure μ with positive linear combinations of at most N Dirac measures. Ultimately, we would like to find a best approximation for μ.

In this chapter, we examine whether such a best approximation exists with respect to the FM-norm and BL-norm. In Section 5.1, we prove an affirmative answer when the underlying metric space S is compact. For non-compact S, we make the conjecture that a best approximation exists as well. This is motivated by the examples we encounter in Sections 5.2 and 5.3. In the examples, we focus on the FM-norm.

In Section 5.2, we study best approximations for the case $N = 1$ and μ of specific forms, using the new expressions for Fortet-Mourier distances derived in Section 4.1. It turns out that a best approximation exists for the studied examples, including settings with non-compact S. However, even for $N = 1$, the nature of best approximations can vary a lot.

In Section 5.3, we show that for a slightly more general, but still very simple example, finding a best approximation is equivalent to solving the so-called *Fermat-Weber problem*. The name already suggests that finding a best approximation is not an easy task. However, using theory for the Fermat-Weber problem, we do obtain the existence of a best approximation for this example, provided that S is a so-called *Hadamard space*.

Although the examples give hope, proving the general statement of our conjecture seems highly complicated. In Section 5.4, we elaborate on the complexity of the problem. We sketch some possible proof strategies and outline some of the obstacles that need to be overcome in order to prove our conjecture. Finally, we give some ideas that might help to do so. These ideas are worth exploring in a further research.

We now give the definitions of the sets of measures from which we will take the approximations. Throughout the chapter, we let (S, d) be a Polish space, where d is an admissible metric. We consider the set of positive sums of at most N Dirac measures

$$\mathcal{D}_N^{\mathbb{R}_+}(S) := \{\sum_{i=1}^{N} \lambda_i \delta_{x_i} : x_i \in S, \lambda_i \geq 0\}.$$

Since (S, d) is assumed to be Polish, it is separable. By Lemma 1.2.5, the elements of $\mathcal{D}_N^{\mathbb{R}_+}(S)$ are thus precisely all finitely supported, finite positive measures with a support consisting of at most N points. First, we show that in the context of approximating a probability measure, we could as well look at the elements in $\mathcal{D}_N^{\mathbb{R}_+}(S)$ with a total mass of at most 2.

Lemma 5.0.1. *For any* $\mu \in \mathcal{P}(S)$ *and* $\bullet = \mathrm{FM}, \mathrm{BL}$*, it holds that*

$$\inf_{\nu \in \mathcal{D}_N^{\mathbb{R}_+}(S)} \|\nu - \mu\|_\bullet^* = \inf_{\substack{\nu \in \mathcal{D}_N^{\mathbb{R}_+}(S) \\ \nu(S) \leq 2}} \|\nu - \mu\|_\bullet^*.$$

Proof. Let 0 be the zero measure. We always have $0 \in \mathcal{D}_N^{\mathbb{R}_+}(S)$, $0(S) = 0 \leq 2$ and $\|0 - \mu\|_\bullet^* = \mu(S) = 1$. Let $\nu \in \mathcal{D}_N^{\mathbb{R}_+}(S)$ with $\nu(S) > 2$. Then

$$\|\nu - \mu\|_\bullet^* = \sup_{g \in \mathrm{B}_\bullet} \langle\, \nu - \mu, g\,\rangle \geq \langle\, \nu - \mu, 1\,\rangle = \nu(S) - \mu(S) > 2 - 1 = 1 = \|0 - \mu\|_\bullet^*,$$

implying the desired result. ☐

In view of Lemma 5.0.1, we can equivalently look for best approximations within the following subset:

$$\mathcal{D}_N(S) := \{\sum_{i=1}^N \lambda_i \delta_{x_i} : x_i \in S, \lambda_i \geq 0, \sum_{i=1}^N \lambda_i \leq 2\}.$$

The set $\mathcal{D}_N(S)$ is slightly more convenient than $\mathcal{D}_N^{\mathbb{R}_+}(S)$, since it is $\|\cdot\|_\bullet^*$-bounded.

We consider yet another subset of $\mathcal{D}_N^{\mathbb{R}_+}(S)$, motivated by the following. Physical and chemical phenomena often satisfy the law of conservation of mass. When describing these phenomena in a mathematical model using finitely supported measures, it can be desirable to capture this essential mass conservation property in the model. Then, it is natural to impose that the approximations are probability measures, just like the approximated probability measure μ.

With this in mind, we define

$$\mathcal{P}_N(S) := \{\sum_{i=1}^N \lambda_i \delta_{x_i} : x_i \in S, \lambda_i \geq 0, \sum_{i=1}^N \lambda_i = 1\} = \mathcal{D}_N(S) \cap \mathcal{P}(S),$$

and consider the problem of finding a best approximation of μ within $\mathcal{P}_N(S)$.

One could expect that any best approximation of a probability measure μ automatically has the same total mass 1 as μ. In that case, the best approximation within $\mathcal{D}_N(S)$ would in fact lie in $\mathcal{P}_N(S)$. However, this is generally not true, as we will see in Section 5.2. Example 5.2.4 shows that in some cases, best approximations necessarily have a total mass that is strictly smaller than 1.

5.1 Existence of a best approximation

In this section, we prove the existence of a best approximation in $\mathcal{D}_N(S)$, when S is compact. Also, we pose a conjecture for the case in which S is not compact.

Best approximation existence questions have often been asked in history and there are quite a few general results for Banach spaces. Especially, when a Banach space X is reflexive, some useful sufficient conditions are known for existence of best approximations within a subset. For example, when a Banach space X is reflexive and $A \subset X$ is closed and convex, then for each element in X, there exists a best approximation in A (see [Deu80]). In our case, we are working in the Banach space $\overline{\mathrm{Mol}}(S)_\bullet = \overline{\mathcal{M}}(S)_\bullet$. Unfortunately, this space is not reflexive. Indeed, the dual space is isomorphic to $\mathrm{BL}(S)_\bullet$ by Lemma 2.2.2 and Lemma 2.2.1, so $\overline{\mathcal{M}}(S)_\bullet^{**} \cong \mathrm{BL}(S)_\bullet^* \ncong \overline{\mathcal{M}}(S)_\bullet$. Thus, we cannot use results for reflexive Banach spaces. Instead, we start by proving a useful property of $\mathcal{D}_N(S)$ and $\mathcal{P}_N(S)$ from scratch, namely, weak closedness.

Remark 5.1.1. *We note that* $\mathcal{D}_N(S), \mathcal{P}_N(S) \subset \mathcal{M}^+(S)$*, so the weak topology on* $\mathcal{D}_N(S)$ *and* $\mathcal{P}_N(S)$ *coincides with the topology induced by the Dudley norm and the Fortet-Mourier norm by Theorem 1.2.13. Therefore, we will gratefully switch between these topologies in the upcoming proofs. Note that, since the weak topology on these sets is metrizable via the Dudley norm and Fortet-Mourier norm, we can use sequences instead of nets when proving closedness or compactness.*

Proposition 5.1.2. *For all $N \in \mathbb{N}$, the set $\mathcal{D}_N(S)$ is weakly closed.*

Proof. Recall that $\mathcal{M}^+(S)$ is weakly closed by Proposition 1.2.14. Let $(\mu_n) \subset \mathcal{D}_N(S)$ be such that $\mu_n \to \mu \in \mathcal{M}^+(S)$ weakly. We prove that $0 \leq \mu(S) \leq 2$ and $\#\operatorname{supp}(\mu) \leq N$. This together with Lemma 1.2.5 implies that $\mu \in \mathcal{D}_N(S)$, proving that $\mathcal{D}_N(S)$ is sequentially weakly closed. From Remark 5.1.1, we then conclude that $\mathcal{D}_N(S)$ is also weakly closed.

We have $\mu_n(S) \in [0, 2]$ for all n and $1 \in C_b(S)$ so by the weak convergence:

$$\mu(S) = \int_S 1 \, d\mu = \lim_{n\to\infty} \int_S 1 \, d\mu_n = \lim_{n\to\infty} \mu_n(S) \in [0, 2]. \tag{5.1}$$

It remains to show that $\#\operatorname{supp}(\mu) \leq N$. If $\mu = 0$, then $\#\operatorname{supp}(\mu) = 0$ so we are done immediately. Therefore, we assume that $\mu(S) > 0$. From (5.1) it follows that $\mu_n(S) > 0$ for all large enough $n \in \mathbb{N}$. Since we are taking the limit $n \to \infty$, we can thus assume that $\mu_n(S) > 0$ for all $n \in \mathbb{N}$.

Suppose that $\#\operatorname{supp}(\mu) > N$. We will derive a contradiction. Pick $\{x_1, \dots, x_{N+1}\} \subset \operatorname{supp}(\mu)$ with $x_i \neq x_j$ for all $i \neq j$. Define

$$\varepsilon := \frac{1}{2} \min\{d(x_i, x_j) : i \neq j, 1 \leq i, j \leq N+1\} > 0$$

and let $B_k := B(x_k, \varepsilon)$ for $k = 1, \dots, N+1$. Note that the B_k are open, pairwise disjoint and satisfy $\mu(B_k) > 0$, since $x_k \in \operatorname{supp}(\mu)$ (see Lemma 1.2.4 (*iii*)). By the weak convergence of (μ_n) and by (5.1), we can apply Alexandrov's Theorem (Theorem 1.2.11). This yields

$$\liminf_{n\to\infty} \mu_n(B_k) \geq \mu(B_k) > 0, \qquad \text{for all } \ k \in \{1, \dots, N+1\}.$$

In particular, for all $k \in \{1, \dots, N+1\}$, there exists $M_k \in \mathbb{N}$ such that $\inf_{n \geq M_k} \mu_n(B_k) > \frac{1}{2}\mu(B_k) > 0$. Hence,

$$\mu_n(B_k) > \frac{1}{2}\mu(B_k) > 0, \qquad \text{for all } \ n \geq M_k.$$

Let $M := \max\{M_1, \dots, M_{N+1}\}$ and consider $\mu_M \in \mathcal{D}_N(S) \cap \mathcal{P}(S)$. It holds that

$$\mu_M(B_k) > \frac{1}{2}\mu(B_k) > 0, \qquad \text{for all } \ k \in \{1, \dots, N+1\}.$$

Recall that $0 < \#\operatorname{supp} \mu_M \leq N$, so we can write $\operatorname{supp}(\mu_M) = \{y_1, \dots, y_N\}$ (the y_j not necessarily different). Since $\mu_M(B_k) > 0$, by Lemma 1.2.4 (iii), we can pick $y_{i_k} \in \operatorname{supp}(\mu_M) \cap B_k$ for all $k \in \{1, \dots, N+1\}$. Then, $d(x_k, y_{i_k}) < \varepsilon = \frac{1}{2} \min\{d(x_i, x_j) : i \neq j, 1 \leq i, j \leq N+1\}$, so whenever $k \neq \tilde{k}$, we have

$$d(y_{i_k}, y_{i_{\tilde{k}}}) \geq d(x_k, y_{i_{\tilde{k}}}) - d(x_k, y_{i_k}) \geq d(x_k, x_{\tilde{k}}) - d(x_{\tilde{k}}, y_{i_{\tilde{k}}}) - d(x_k, y_{i_k}) > 2\,\varepsilon - \varepsilon - \varepsilon = 0,$$

so $y_{i_k} \neq y_{i_{\tilde{k}}}$. Therefore,

$$N + 1 = \#\{y_{i_1}, \dots, y_{i_{N+1}}\} \leq \#\operatorname{supp}(\mu_M) \leq N.$$

This is a contradiction, hence $\#\operatorname{supp}(\mu) \leq N$.

□

Corollary 5.1.3. *For all $N \in \mathbb{N}$, the set $\mathcal{P}_N(S)$ is weakly closed.*

Proof. It holds that $\mathcal{P}_N(S) = \mathcal{D}_N(S) \cap \mathcal{P}(S)$. The sets $\mathcal{D}_N(S)$ and $\mathcal{P}(S)$ are weakly closed by Proposition 5.1.2 and Proposition 1.2.14, respectively. Thus, $\mathcal{P}_N(S)$ is an intersection of two weakly closed sets and therefore itself weakly closed in $\mathcal{D}_N(S)$. □

Proposition 5.1.4. *For all $N \in \mathbb{N}$, the set $\mathcal{D}_N(S)$ is weakly compact (or equivalenty, $\|\cdot\|_\bullet^*$-compact for $\bullet = \mathrm{FM}, \mathrm{BL}$), if and only if S is compact. If S is compact, then there exists $\nu_0 \in \mathcal{D}_N(S)$ such that*

$$\|\nu_0 - \mu\|_\bullet^* = \inf_{\nu \in \mathcal{D}_N(S)} \|\nu - \mu\|_\bullet^*.$$

Proof. If S is compact, then $\mathcal{D}_N(S)$ is uniformly tight: for the compact set $K := S$ we trivially have $|\nu|(S \setminus K) = 0 < \varepsilon$, for all $\varepsilon > 0$ and $\nu \in \mathcal{D}_N(S)$. Also, $|\nu|(S) \leq 2$ for all $\nu \in \mathcal{D}_N(S)$. So by Prohorov's Theorem ([Bog07, II, Theorem 8.6.2]), every sequence in $\mathcal{D}_N(S)$ has a weakly convergent subsequence. The limit of this subsequence lies in $\mathcal{D}_N(S)$, since $\mathcal{D}_N(S)$ is weakly closed by Proposition 5.1.2. Hence, $\mathcal{D}_N(S)$ is weakly sequentially compact. On account of Remark 5.1.1, we conclude that $\mathcal{D}_N(S)$ is weakly compact.

On the other hand, if $\mathcal{D}_N(S)$ is weakly compact, then $\mathcal{D}_N(S)_{\mathrm{BL}}$ is also compact. Moreover, $\mathcal{P}_1(S) = \{\delta_x : x \in S\}$ is a weakly closed subset of $\mathcal{D}_N(S)$ by Corollary 5.1.3. Therefore, it is also closed in the compact space $\mathcal{D}_N(S)_{\mathrm{BL}}$. So $\mathcal{P}_1(S)_{\mathrm{BL}}$ is compact.

We now show that S is compact. The map

$$\phi : S \hookrightarrow \mathcal{D}_N(S)_{\mathrm{BL}} : x \mapsto \delta_x$$

is a homeomorphism onto its range $\phi(S) = \mathcal{P}_1(S)$, since $\|\delta_x - \delta_y\|^*_{\mathrm{BL}} = \frac{2d(x,y)}{2+d(x,y)}$ ([HW09, Lemma 3.5]). Indeed, from the expression it follows immediately that

$$\|\delta_{x_n} - \delta_x\|^*_{\mathrm{BL}} \to 0 \iff d(x_n, x) \to 0 \quad \text{and} \quad \|\delta_x - \delta_y\|^*_{\mathrm{BL}} = 0 \iff d(x,y) = 0 \iff x = y$$

so ϕ is a homeomorphism between S and $\mathcal{P}_1(S)$. Now, since $\mathcal{P}_1(S)_{\mathrm{BL}}$ is compact, S is compact as well, proving the other implication.

The second statement of this proposition is in fact an example of a general result in compact metric spaces. Again, let S be compact. One can pick $(\nu_n)_n \subset \mathcal{D}_N(S)$ with $\lim_{n\to\infty} \|\nu_n - \mu\|^*_\bullet = \inf_{\nu \in \mathcal{D}_N(S)} \|\nu - \mu\|^*_\bullet$. By the above obtained weak compactness of $\mathcal{D}_N(S)$, this sequence has a convergent subsequence (ν_{n_k}) with a limit $\nu_0 \in \mathcal{D}_N(S)$, which satisfies

$$\|\nu_0 - \mu\|^*_\bullet = \lim_{k\to\infty} \|\nu_{n_k} - \mu\|^*_\bullet = \lim_{n\to\infty} \|\nu_n - \mu\|^*_\bullet = \inf_{\nu \in \mathcal{D}_N(S)} \|\nu - \mu\|^*_\bullet.$$

□

Corollary 5.1.5. *For all $N \in \mathbb{N}$, the set $\mathcal{P}_N(S)$ is weakly compact, if and only if S is compact. If S is compact, then for $\bullet = \mathrm{FM}, \mathrm{BL}$, there exists $\nu_0 \in \mathcal{P}_N(S)$ such that*

$$\|\nu_0 - \mu\|^*_\bullet = \inf_{\nu \in \mathcal{P}_N(S)} \|\nu - \mu\|^*_\bullet.$$

Proof. If S is compact, then $\mathcal{D}_N(S)$ is weakly compact by Proposition 5.1.4. Also, $\mathcal{P}_N(S)$ is a weakly closed subset by Corollary 5.1.3 and therefore, weakly compact. For the other implication, we can mimic the proof of Proposition 5.1.4, since $\mathcal{P}_1(S)$ is also a weakly closed subset of $\mathcal{P}_N(S)$.

The second statement can be proved similarly as in Proposition 5.1.2. □

For compact S, Proposition 5.1.4 provides the existence of a minimizer in $\mathcal{D}_N(S)$. On the other hand, for non-compact S it is in no way obvious that there exists a minimizer, as $\mathcal{D}_N(S)$ is not weakly compact. Still, we do think that also for non-compact S, there should exist a best approximation. In the next two sections, we provide several examples of measures μ for which best approximations do exist, also if S is non-compact. This is a motivation for our conjecture:

Conjecture 5.1.6. *Let (S, d) be a Polish space (not necessarily compact). Then, for $\bullet = \mathrm{FM}, \mathrm{BL}$, for any $N \in \mathbb{N}$ and for any $\mu \in \mathcal{M}^+(S)$, there exists $\nu_0 \in \mathcal{D}_N(S)$ such that*

$$\|\nu_0 - \mu\|^*_\bullet = \inf_{\nu \in \mathcal{D}_N(S)} \|\nu - \mu\|^*_\bullet.$$

We have not succeeded in proving the above conjecture yet. However, the efforts did produce many insights. In the next two sections, we study some examples of the approximation problem for specific measures μ. The examples give an idea of what best approximations can be like. We will see that even for a very simple example, certain properties of best approximations (such as the total mass or the support) can be very diverse, making best approximations hard to grasp.

We conclude this section with a functional analytic result that is a by-product of one of our proving attempts. We find the result worth mentioning since it provides more knowledge about the peculiar set $\mathcal{D}_N(S)$. Our idea was to consider a weaker topology on $\mathcal{M}(S)$ for which $\mathcal{D}_N(S)$ is compact, even for non-compact S. A natural weaker topology on $\mathcal{M}(S)$ is the functional analytic 'weak topology' $\sigma(\mathcal{M}(S)_\bullet, \mathcal{M}(S)_\bullet^*)$, for $\bullet = \mathrm{FM}, \mathrm{BL}$. We note that $\mathcal{M}(S)_\bullet^* \cong \overline{\mathcal{M}(S)}_\bullet^* \cong \mathrm{BL}(S)_\bullet$. The first equality holds since the dual of a normed space equals the dual of its completion (see [Con90, §III.2, Exercise 2]). The second equality follows from Corollary 1.2.20 combined with Lemma 2.2.1 and Lemma 2.2.2. The identification $\mathcal{M}(S)_\bullet^* \cong \mathrm{BL}(S)_\bullet$ yields

$$\mu_\alpha \to \mu \text{ wrt } \sigma(\mathcal{M}(S)_\bullet, \mathcal{M}(S)_\bullet^*) \iff \langle\, \mu_\alpha, f \,\rangle \to \langle\, \mu, f \,\rangle \text{ for all } f \in \mathrm{BL}(S). \tag{5.2}$$

As an immediate consequence of the characterization on the right-hand side, convergence in $\mathcal{M}(S)_\bullet = (\mathcal{M}(S), \|\cdot\|_\bullet^*)$ implies convergence with respect to the topology $\sigma(\mathcal{M}(S)_\bullet, \mathcal{M}(S)_\bullet^*)$. Therefore, $\sigma(\mathcal{M}(S)_\bullet, \mathcal{M}(S)_\bullet^*)$ is indeed a weaker topology than the topology induced by $\|\cdot\|_\bullet^*$.

Unfortunately, it turned out that $\mathcal{D}_N(S)$ is not compact with respect to $\sigma(\mathcal{M}(S)_\bullet, \mathcal{M}(S)_\bullet^*)$ in general, so the topology was not useful for the intended proof. However, we were able to prove that also for the topology $\sigma(\mathcal{M}(S)_\bullet, \mathcal{M}(S)_\bullet^*)$, $\mathcal{D}_N(S)$ is compact precisely when S is compact.

Corollary 5.1.7. *Consider the functional analytic 'weak topology' $\sigma(\mathcal{M}(S)_\bullet, \mathcal{M}(S)_\bullet^*)$, for which convergence is characterized by (5.2). It holds that $\mathcal{D}_N(S)$ is $\sigma(\mathcal{M}(S)_\bullet, \mathcal{M}(S)_\bullet^*)$-compact if and only if S is compact.*

Proof. If S is compact, then $\mathcal{D}_N(S)_\bullet$ is compact by Proposition 5.1.4. Now, since the norm topology induced by $\|\cdot\|_\bullet$ is stronger than the $\sigma(\mathcal{M}(S)_\bullet, \mathcal{M}(S)_\bullet^*)$-topology by (5.2), it follows that $\mathcal{D}_N(S)$ is $\sigma(\mathcal{M}(S)_\bullet, \mathcal{M}(S)_\bullet^*)$-compact (every open cover in a weaker topology is also an open cover in the stronger topology).

Next, suppose that $\mathcal{D}_N(S)$ is $\sigma(\mathcal{M}(S)_\bullet, \mathcal{M}(S)_\bullet^*)$-compact. We first show that $\mathcal{D}_N(S)_\bullet$ is compact. Let $(\mu_n) \subset \mathcal{D}_N(S)_\bullet$. By the $\sigma(\mathcal{M}(S)_\bullet, \mathcal{M}(S)_\bullet^*)$-compactness, there exists a subsequence (μ_{n_k}) that converges to some $\mu \in \mathcal{D}_N(S)$ in the $\sigma(\mathcal{M}(S)_\bullet, \mathcal{M}(S)_\bullet^*)$-topology. This is not trivial (compactness does not imply sequential compactness in general), but we can use the Eberlein-Šmullian theorem to prove this. As we mentioned above, $\mathcal{M}(S)_\bullet^* \cong \overline{\mathcal{M}}(S)_\bullet^*$, so when viewing $\mathcal{D}_N(S)$ as a subset of $\overline{\mathcal{M}}(S)$, we also have that $\mathcal{D}_N(S)$ is $\sigma(\overline{\mathcal{M}}(S)_\bullet, \overline{\mathcal{M}}(S)_\bullet^*)$-compact. The space $\overline{\mathcal{M}}(S)_\bullet$ is Banach, so the Eberlein-Šmullian theorem ([Con90, Theorem V.13.1]) gives us a $\sigma(\overline{\mathcal{M}}(S)_\bullet, \overline{\mathcal{M}}(S)_\bullet^*)$-convergent subsequence (μ_{n_k}). This sequence converges with respect to $\sigma(\mathcal{M}(S)_\bullet, \mathcal{M}(S)_\bullet^*)$ as well, since $\mathcal{M}(S)_\bullet^* \cong \overline{\mathcal{M}}(S)_\bullet^*$. Also, its limit must be in $\mathcal{D}_N(S)$, since $\mathcal{D}_N(S)$ is $\sigma(\mathcal{M}(S)_\bullet, \mathcal{M}(S)_\bullet^*)$-compact and Hausdorff, hence closed. We denote this limit by μ.

Now, by (5.2), we have $\langle\, \mu_{n_k}, f \,\rangle \to \langle\, \mu, f \,\rangle$ for all $f \in \mathrm{BL}(S)$. Combining [Bog07, II, Corollary 8.6.3] and Prohorov's Theorem (see [Bog07, II, Theorem 8.6.7], note that $\nu_{n_k}(S) \leq 2$ for all k), it follows that (μ_{n_k}) has a weakly convergent subsequence $(\mu_{n_{k_j}})$ that converges weakly to μ (in the sense of Definition 1.2.10). Since all measures involved are positive, it follows that $\|\mu_{n_{k_j}} - \mu\|_\bullet^* \to 0$, proving that $\mathcal{D}_N(S)_\bullet$ is compact. Consequently, by Proposition 5.1.4, S must be compact, proving the contraposition of the statement.

□

5.2 Best approximations by one Dirac measure

In this section, we consider the case $N = 1$ and $\bullet = \mathrm{FM}$. We study examples of best approximations in $\mathcal{D}_1(S)$ or $\mathcal{P}_1(S)$ for a probability measure μ. In the examples we consider, we always have existence of a best approximation, showing that Conjecture 5.1.6 holds at least for certain specific μ.

Furthermore, we come back to one of the questions raised in the beginning of this chapter: do best approximations have the same total mass 1 as the approximated measure μ? Even for 'simple' examples, we find surprising answers. For example, Proposition 5.2.2, Example 5.2.3 and Example 5.2.4 show that best approximations do generally not need to have the same mass as the approximated measure and that in some cases, best approximations even necessarily have a smaller mass than the approximated measure.

Notice that we have already seen an answer to an approximation question in Proposition 3.1.5. There, we found best approximations in $\mathcal{P}_1(S)$ for probability measures on $[0,1]$ with a density function. The best approximations were given by the median(s).

The next lemma shows that, when searching for best approximations in $\mathcal{D}_1(S)$, one can restrict to the elements in $\mathcal{D}_1(S)$ with total mass at most 1. This is a stronger result than the more general Lemma 5.0.1.

Lemma 5.2.1. *Let* $\mu \in \mathcal{P}(S)$. *Then*

$$\inf_{\nu\in\mathcal{D}_1(S)} \|\nu-\mu\|_{\mathrm{FM}}^* = \inf_{\alpha\in[0,2],x\in S} \|\alpha\delta_x-\mu\|_{\mathrm{FM}}^* = \inf_{\alpha\in[0,1],x\in S} \|\alpha\delta_x-\mu\|_{\mathrm{FM}}^*.$$

Proof. Let $x \in S$ be fixed. Define

$$\psi_x(\alpha) := \alpha\theta_0(\alpha), \quad \phi_x(\alpha) := \langle\, \mu, (-1)\vee(\theta_0(\alpha)-d(x,\cdot))\,\rangle,$$

where $\theta_0(\alpha)=\theta_0$ as defined in Corollary 4.1.5. We have (by the same corollary):

$$\|\alpha\delta_x-\mu\|_{\mathrm{FM}}^* = \psi_x(\alpha)-\phi_x(\alpha), \qquad \text{for all } x\in S.$$

For all $\alpha > 1$ it holds that $\theta_0(\alpha)=1$, because μ is a probability measure. Hence,

$$\psi_x(\alpha)-\phi_x(\alpha) = \alpha - \langle\, \mu, (-1)\vee(1-d(x,\cdot))\,\rangle\,.$$

This expression increases in α. Note that norms are continuous. In particular,

$$\inf_{\alpha>1} \|\alpha\delta_x-\mu\|_{\mathrm{FM}}^* = \lim_{\alpha\downarrow 1} \|\alpha\delta_x-\mu\|_{\mathrm{FM}}^* = \|1\cdot\delta_x-\mu\|_{\mathrm{FM}}^*.$$

Consequently,

$$\inf_{\alpha\geq 0,x\in S} \|\alpha\delta_x-\mu\|_{\mathrm{FM}}^* = \inf_{\alpha\in[0,1],x\in S} \|\alpha\delta_x-\mu\|_{\mathrm{FM}}^*,$$

completing the proof. □

The remainder of this section is devoted to the study of best approximations when μ is a convex combination of two Diracs.

Proposition 5.2.2. *Let* $\mu = b_1\delta_{y_1}+b_2\delta_{y_2} \in \mathcal{P}(S)$, $b_1 = 1-b_2 \in [0,1]$ *and* $y_1, y_2 \in S$. *Then*

$$\inf_{\nu\in\mathcal{D}_1(S)} \|\nu-\mu\|_{\mathrm{FM}}^* = \inf_{\alpha\in[0,2],x\in S} \|\alpha\delta_x-\mu\|_{\mathrm{FM}}^* = \min_{x\in\{y_1,y_2\},\alpha\in\{b_1,b_2,1\}} \|\alpha\delta_x-\mu\|_{\mathrm{FM}}^*.$$

In particular, $\inf_{\nu\in\mathcal{D}_1(S)} \|\nu-\mu\|_{\mathrm{FM}}^* = (b_1\wedge b_2)(1\wedge d(y_1,y_2))$.

Proof. By Lemma 5.2.1, we only have to minimize over $\alpha\in[0,1]$. Let $\alpha\in[0,1]$, $x\in S$ and define $T_x(\alpha) := \|\alpha\delta_x-\mu\|_{\mathrm{FM}}^*$. This defining expression yields that T_x is continuous in α. By Corollary 4.1.5, we have

$$T_x(\alpha) = \alpha\theta_0(\alpha) - b_1\big((-1)\vee(\theta_0(\alpha)-d(x,y_1))\big) - b_2\big((-1)\vee(\theta_0(\alpha)-d(x,y_2))\big), \tag{5.3}$$

where

$$\theta_0(\alpha) := \begin{cases} \inf\{\theta\in[-1,1] : \mu\big(B(x,\theta+1)\big)\geq\alpha\}, & \text{if } \mu\big(B(x,\theta+1)\big)\geq\alpha \text{ for some } \theta\in[-1,1],\\ 1, & \text{otherwise.}\end{cases}$$

First, let us assume that $d(x,y_1)\leq d(x,y_2)$. We determine $\theta_0(\alpha)$. If $\alpha=0$, then $\mu(B(x,-1+1))=\mu(\emptyset)=0\geq\alpha$, so $\theta_0(\alpha)=-1$. Moreover, observe that for $0<\alpha\leq b_1$:

$$\mu(B(x,\theta+1))\geq\alpha \iff y_1\in B(x,\theta+1) \iff d(x,y_1)-1\leq\theta,$$

and for $\alpha > b_1$, we have

$$\mu(B(x,\theta+1)) \geq \alpha \iff y_2 \in B(x,\theta+1) \iff d(x,y_2) - 1 \leq \theta.$$

Now, one can easily derive that

$$\theta_0(\alpha) = \begin{cases} -1, & \alpha = 0, \\ (d(x,y_1)-1) \wedge 1, & 0 < \alpha \leq b_1, \\ (d(x,y_2)-1) \wedge 1, & \alpha > b_1. \end{cases} \tag{5.4}$$

Next, we determine $\inf_{\alpha \geq 0} T_x(\alpha)$ for fixed x, still assuming that $d(x,y_1) \leq d(x,y_2)$. Let us distinguish between three cases:

a) $d(x,y_i) \geq 2$ for $i = 1,2$, i.e., $(d(x,y_i)-1) \wedge 1 = 1$ for $i = 1,2$,

b) $d(x,y_1) < 2, d(x,y_2) \geq 2$, i.e., $(d(x,y_1)-1) \wedge 1 = d(x,y_1) - 1$, $(d(x,y_2)-1) \wedge 1 = 1$,

c) $d(x,y_i) < 2$ for $i = 1,2$, i.e., $(d(x,y_i)-1) \wedge 1 = d(x,y_i) - 1$ for $i = 1,2$.

In what follows, we will be using that

$$(-1) \vee (1 - d(x,y_i)) = -((d(x,y_i)-1) \wedge 1). \tag{5.5}$$

Also, note that we always have $T_x(0) = \|0 - \mu\|^*_{\mathrm{FM}} = \mu(S) = 1$ and recall that T_x is continuous in α. Now we are ready to determine $\inf_{\alpha \geq 0} T_x(\alpha)$ for each of the cases above.

a) For all $\alpha > 0$, we have $\theta_0(\alpha) = 1$ by (5.4). So, using (5.3) and (5.5), we obtain

$$T_x(\alpha) = \alpha \cdot 1 - b_1 \cdot (-1) - b_2 \cdot (-1) = \alpha + 1,$$

which strictly increases in α. Thus,

$$\inf_{\alpha \geq 0} T_x(\alpha) = T_x(0) = 1.$$

b) For $0 < \alpha \leq b_1$, we have $\theta_0(\alpha) = d(x,y_1) - 1$. Observe that in this case, since $d(x,y_1) \leq d(x,y_2)$, we have $\theta_0(\alpha) - d(x,y_2) \leq -1$ and

$$T_x(\alpha) = \alpha(d(x,y_1)-1) - b_1 \cdot (-1) - b_2 \cdot (-1) = \alpha(d(x,y_1)-1) + 1,$$

which strictly decreases in α if $d(x,y_1) \in [0,1)$ and is non-decreasing if $d(x,y_1) \in [1,2)$.

For $\alpha > b_1$, we have $\theta_0(\alpha) = 1$, so

$$T_x(\alpha) = \alpha \cdot 1 - b_1(1 - d(x,y_1)) - b_2 \cdot (-1) = \alpha - b_1(1 - d(x,y_1)) + b_2,$$

which strictly increases in α.

Thus,

$$\inf_{\alpha \geq 0} T_x(\alpha) = \begin{cases} T_x(b_1) = b_1(d(x,y_1)-1)) + 1, & d(x,y_1) \in [0,1), \\ T_x(0) = 1, & d(x,y_1) \in [1,2). \end{cases}$$

c) For $0 < \alpha \leq b_1$, we have $\theta_0(\alpha) = d(x,y_1) - 1$. Since $d(x,y_1) \leq d(x,y_2)$, this yields as in b):

$$T_x(\alpha) = \alpha(d(x,y_1)-1) - b_1 \cdot (-1) - b_2 \cdot (-1) = \alpha(d(x,y_1)-1) + 1,$$

which strictly decreases in α if $d(x,y_1) \in [0,1)$ and is non-decreasing if $d(x,y_1) \in [1,2)$.

For $\alpha > b_1$, we have $\theta_0(\alpha) = d(x,y_2) - 1$, so

$$\begin{aligned} T_x(\alpha) &= \alpha(d(x,y_2)-1) - b_1(d(x,y_2) - 1 - d(x,y_1)) - b_2 \cdot (-1) \\ &= (\alpha - b_1)d(x,y_2) - \alpha + 1 + b_1 d(x,y_1), \end{aligned}$$

which strictly decreases in α if $d(x,y_2)\in[0,1)$ and is non-decreasing if $d(x,y_2)\in[1,2)$. We note that $d(x,y_1)\geq 1$ implies $d(x,y_2)\geq 1$. Thus,

$$\inf_{\alpha\geq 0} T_x(\alpha)=\begin{cases} T_x(1)=b_2d(x,y_2)+b_1d(x,y_1), & d(x,y_1),d(x,y_2)\in[0,1),\\ T_x(b_1)=b_1(d(x,y_1)-1))+1, & d(x,y_1)\in[0,1),d(x,y_2)\in[1,2),\\ T_x(0)=1, & d(x,y_1),d(x,y_2)\in[1,2).\end{cases}$$

Summarizing, we have six cases:

$$\inf_{\alpha\geq 0} T_x(\alpha)=\begin{cases} T_x(0)=1, & d(x,y_1),d(x,y_2)\geq 2, & \text{(a)}\\ T_x(b_1)=b_1(d(x,y_1)-1))+1, & d(x,y_1)\in[0,1),d(x,y_2)\geq 2, & \text{(b1)}\\ T_x(0)=1, & d(x,y_1)\in[1,2),d(x,y_2)\geq 2, & \text{(b2)}\\ T_x(1)=b_1d(x,y_1)+b_2d(x,y_2), & d(x,y_1),d(x,y_2)\in[0,1), & \text{(c1)}\\ T_x(b_1)=b_1(d(x,y_1)-1))+1, & d(x,y_1)\in[0,1),d(x,y_2)\in[1,2), & \text{(c2)}\\ T_x(0)=1, & d(x,y_1),d(x,y_2)\in[1,2), & \text{(c3)}\end{cases}$$

which can be reduced to

$$\inf_{\alpha\geq 0} T_x(\alpha)=\begin{cases} T_x(0)=1, & d(x,y_1)\geq 1, & \text{(A1)}\\ T_x(b_1)=b_1d(x,y_1)+b_2, & d(x,y_1)\in[0,1),d(x,y_2)\geq 1, & \text{(B1)}\\ T_x(1)=b_1d(x,y_1)+b_2d(x,y_2), & d(x,y_1),d(x,y_2)\in[0,1). & \text{(C1)}\end{cases}$$

Next, suppose that $d(x,y_1)\geq d(x,y_2)$. Then, the above analysis can be applied when we interchange the pairs (b_1,y_1) and (b_2,y_2), and we immediately obtain

$$\inf_{\alpha\geq 0} T_x(\alpha)=\begin{cases} T_x(0)=1, & d(x,y_2)\geq 1, & \text{(A2)}\\ T_x(b_2)=b_1+b_2d(x,y_2), & d(x,y_2)\in[0,1),d(x,y_1)\geq 1, & \text{(B2)}\\ T_x(1)=b_1d(x,y_1)+b_2d(x,y_2), & d(x,y_1),d(x,y_2)\in[0,1). & \text{(C2)}\end{cases}$$

Combining these results, we obtain an expression for all $x\in S$:

$$\inf_{\alpha\geq 0} T_x(\alpha)=\begin{cases} T_x(0)=1, & d(x,y_1),d(x,y_2)\geq 1, & \text{(A)}\\ T_x(b_1)=b_1d(x,y_1)+b_2, & 0\leq d(x,y_1)<1\leq d(x,y_2), & \text{(B1)}\\ T_x(b_2)=b_1+b_2d(x,y_2), & 0\leq d(x,y_2)<1\leq d(x,y_1), & \text{(B2)}\\ T_x(1)=b_1d(x,y_1)+b_2d(x,y_2), & 0\leq d(x,y_1),d(x,y_2)<1. & \text{(C)}\end{cases}$$

In particular, the value of the infimum is given by the following single expression:

$$\inf_{\alpha\geq 0} T_x(\alpha)=b_1(1\wedge d(x,y_1))+b_2(1\wedge d(x,y_2)). \tag{5.6}$$

Our next goal is to determine $\inf_{x\in S}\inf_{\alpha\geq 0}T_x(\alpha)$. In what follows, we distinguish between many cases, and by 'x belongs to (X)' for some X$\in$ {A, B1, B2, C}, we will indicate that x satisfies the conditions on $d(x,y_1)$ and $d(x,y_2)$ that are written on the right-hand side of case (X).

For x belonging to (B1), we have:

$$\inf_{\alpha\geq 0} T_x(\alpha)=T_x(b_1)=b_1d(x,y_1)+b_2.$$

This expression grows in $d(x,y_1)$, so the choice $x=y_1$ gives the minimal value, provided that $x=y_1$ belongs to (B1). Note that $x=y_1$ gives $d(x,y_1)=0\in[0,1)$ and $d(x,y_1)=0<d(x,y_2)$ as required for (B1). But we also need $d(y_1,y_2)\geq 1$, since otherwise we are in case (C) instead of (B1). However, if $x=y_1$ does belong to (B1), this yields $\inf_{\alpha\geq 0}T_{y_1}(\alpha)=T_{y_1}(b_1)$. Thus,

$$\inf_{x\in B(y_1,1)\cap B(y_2,1)^c}\ \inf_{\alpha\geq 0} T_x(\alpha)=T_{y_1}(b_1),$$

and by symmetry, provided that $d(y_1, y_2) \geq 1$, for (B2) we obtain

$$\inf_{x \in B(y_2,1) \cap B(y_1,1)^c} \inf_{\alpha \geq 0} T_x(\alpha) = T_{y_2}(b_2).$$

In case (C), we have

$$\inf_{\alpha \geq 0} T_x(\alpha) = T_x(1) = b_1 d(x, y_1) + b_2 d(x, y_2), \tag{5.7}$$

which grows in both $d(x, y_1)$ and $d(x, y_2)$. However, a global minimum is always attained at $x = y_1$ or $x = y_2$. Indeed, let $i \in \{1, 2\}$ be such that $b_i = \min(b_1, b_2)$ and let $j = (i + 1) \bmod 2$, i.e., $b_j = \max(b_1, b_2)$. Then we have for all $x \in S$:

$$\begin{aligned} b_1 d(x, y_1) + b_2 d(x, y_2) &= b_i \big(d(x, y_i) + d(x, y_j)\big) + (b_j - b_i) d(x, y_j) \\ &\geq b_i d(y_i, y_j) + (b_j - b_i) d(x, y_j) \\ &\geq b_i d(y_i, y_j) + 0 \\ &= b_i d(y_j, y_i) + b_j d(y_j, y_j) \\ &= T_{y_j}(1), \end{aligned} \tag{5.8}$$

so

$$\inf_{x \in B(y_1,1) \cap B(y_2,1)} \inf_{\alpha \geq 0} T_x(\alpha) = T_{y_j}(1).$$

In the remainder of the proof, let $b_i = \min(b_1, b_2)$ and $j = (i + 1) \bmod 2$. We argue that case (A) can be discarded in our search for a minimizer. According to (5.6), $\inf_{\alpha \geq 0} T_{y_j}(\alpha) \leq b_i < 1$. Hence,

$$\inf_{x \in S} \inf_{\alpha \geq 0} T_x(\alpha) \leq \min(b_1, b_2) < 1, \tag{5.9}$$

so minimizers cannot belong to case (A). Therefore, they must belong to the case (B1), (B2) or (C). We now distinguish between $d(y_1, y_2) < 1$ and $d(y_1, y_2) \geq 1$.

If $d(y_1, y_2) < 1$, then we have for $k = 1, 2$ and x belonging to (Bk):

$$d(x, y_k) \geq d(x, y_{(k+1) \bmod 2}) - d(y_1, y_2) > 0.$$

Hence,

$$T_x(b_k) = b_k d(x, y_k) + b_{(k+1) \bmod 2} > b_{(k+1) \bmod 2} \geq \min(b_1, b_2). \tag{5.10}$$

By (5.9), it follows that the cases (Bk) can be discarded, i.e., minimizers belong to (C).

Now suppose that $d(y_1, y_2) \geq 1$. From (5.8), we see that for all x belonging to (C):

$$T_x(1) \geq b_i d(y_1, y_2) \geq b_i = T_{y_j}(b_j).$$

And for x belonging to case (Bi), by (5.10) we have $\inf_{\alpha \geq 0} T_x(\alpha) \geq b_j \geq b_i = T_{y_j}(b_j)$. So if $d(y_1, y_2) \geq 1$, we can discard cases (A), (Bi) and (C).

We have shown the following:

$$\begin{aligned} \inf_{x \in S} \inf_{\alpha \geq 0} T_x(\alpha) &= \begin{cases} T_{y_1}(1), & b_1 \geq b_2, d(y_1, y_2) < 1, \\ T_{y_2}(1), & b_1 < b_2, d(y_1, y_2) < 1, \\ T_{y_1}(b_1), & b_1 \geq b_2, d(y_1, y_2) \geq 1, \\ T_{y_2}(b_2), & b_1 < b_2, d(y_1, y_2) \geq 1, \end{cases} \\ &= (b_1 \wedge b_2)(1 \wedge d(y_1, y_2)). \end{aligned} \tag{5.11}$$

In particular, $\inf_{x \in S} \inf_{\alpha \geq 0} T_x(\alpha) = \min_{x \in \{y_1, y_2\}, \alpha \in \{b_1, b_2, 1\}} T_x(\alpha)$, concluding the proof.

□

Example 5.2.3. Best approximations in $\mathcal{D}_1(S)$ do not have to be unique, nor do all best approximations need to have the same total mass.

Consider $S = [0,1]$ *and let* $\mu = \frac{1}{2}\delta_0 + \frac{1}{2}\delta_1$. *Note that* $d(y_1, y_2) = 1$. *By Proposition 5.2.2, at least one of* $\frac{1}{2}\delta_0$, $\frac{1}{2}\delta_1$, δ_0 *and* δ_1 *is a best approximation. We have*

$$\|\frac{1}{2}\delta_0 - \mu\|^*_{\mathrm{FM}} = \|\frac{1}{2}\delta_1 - \mu\|^*_{\mathrm{FM}} = \frac{1}{2}.$$

Also, in fact for all $x \in [0,1]$, *we have*

$$\|\delta_x - \mu\|^*_{\mathrm{FM}} = \frac{1}{2}d(x,0) + \frac{1}{2}d(x,1) = \frac{1}{2}.$$

So there are uncountably many best approximations, and they do not all have the same total mass.

Example 5.2.4. In some cases, best approximations necessarily have a strictly smaller total mass than the total mass 1 of the approximated probability measure μ.

We now consider general S, *with Diam*$(S) > 1$. *Let* $\mu = b_1\delta_{y_1} + b_2\delta_{y_2}$, $b_1 = 1 - b_2 \in (0,1)$ *and* $y_1, y_2 \in S$ *with* $d(y_1, y_2) > 1$. *By* (5.11) *it holds that*

$$\inf_{x\in S}\inf_{\alpha\geq 0} T_x(\alpha) = T_{y_j}(b_j) = \min(b_1, b_2),$$

where j *is such that* $b_j = \max(b_1, b_2)$.

We show that $\inf_{x\in S} T_x(1)$ *is strictly larger. For all* $x \in S$, *we have*

$$\begin{aligned} b_1 d(x,y_1) + b_2 d(x,y_1) \geq \min(b_1,b_2)\big(d(x,y_1) + d(x,y_2)\big) &\geq \min(b_1,b_2)d(y_1,y_2) \\ &> \min(b_1,b_2). \end{aligned} \tag{5.12}$$

Using Proposition 3.1.2, we thus derive

$$\begin{aligned} T_x(1) = \langle\, \mu, 2\wedge d(x,\cdot)\,\rangle &= b_1\langle 2\wedge d(x,y_1)\,\rangle + b_2\langle 2\wedge d(x,y_2)\,\rangle \\ &= \begin{cases} 2, & d(x,y_1), d(x,y_2) \geq 2, \\ 2b_1 + b_2 d(x,y_2), & d(x,y_1) \geq 2, d(x,y_2) < 2, \\ 2b_2 + b_1 d(x,y_1), & d(x,y_1) < 2, d(x,y_2) \geq 2, \\ b_1 d(x,y_1) + b_2 d(x,y_2), & d(x,y_1), d(x,y_2) < 2, \end{cases} && (5.13) \\ &\geq \min\big(2, 2b_1, 2b_2, \min(b_1,b_2)d(y_1,y_2)\big) && (5.14) \\ &> \min(b_1,b_2) \\ &= T_{y_j}(b_j), \end{aligned}$$

using (5.12) *to estimate the last case of* (5.13). *Since* (5.14) *is independent of* x, *we conclude that*

$$\inf_{\nu\in\mathcal{D}_1(S)} \|\nu - \mu\|^*_{\mathrm{FM}} = \min(b_1, b_2) < \inf_{\nu\in\mathcal{P}_1(S)} \|\nu - \mu\|^*_{\mathrm{FM}}.$$

Example 5.2.5. In some cases, best approximations necessarily have the same total mass 1 as the approximated probability measure μ.

Let $\mu = b_1\delta_{y_1} + b_2\delta_{y_2}$, $b_1 = 1 - b_2 \in (0,1)$ *and* $y_1, y_2 \in S$ *with* $d(y_1,y_2) < 1$. *Then the choices* $x = y_k$ *for* $k = 1,2$ *belong to* (C) *and yield*

$$\inf_{x\in S} T_x(1) \leq T_{y_k}(1) = b_{(k+1)\bmod 2}\, d(y_1,y_2) < b_{(k+1)\bmod 2} \leq T_z(b_k),$$

for all z *belonging to case* (Bk) *(*$k = 1,2$*). We conclude that best approximations in* $\mathcal{D}_1(S)$ *cannot belong to* $\mathcal{D}_1(S) \setminus \mathcal{P}_1(S)$ *and that*

$$\inf_{\nu\in\mathcal{D}_1(S)} \|\nu - \mu\|^*_{\mathrm{FM}} = \min_{x\in\{y_1,y_2\},\alpha\in\{1\}} \|\alpha\delta_x - \mu\|^*_{\mathrm{FM}} = \inf_{\nu\in\mathcal{P}_1(S)} \|\nu - \mu\|^*_{\mathrm{FM}}.$$

5.3 Fermat-Weber problem

We consider μ of the form $\sum_{i=1}^{M} \alpha_i \delta_{x_i}$, with $M \in \mathbb{N}$, $\alpha_i \geq 0$, $\sum_{i=1}^{M} \alpha_i = 1$ and $x_i \in S$. In the previous section, we explicitly found a best approximation in $\mathcal{D}_1(S)$ for the case $M = 2$. Even this simple example cost quite some effort. We now study the problem of finding a best approximation of μ within $\mathcal{P}_1(S) = \{\delta_x : x \in S\}$, for general $M \in \mathbb{N}$. Again, we only use the FM-norm.

Let us rewrite the approximation problem. We turn to a setting with friendlier expressions by assuming that $\mathrm{Diam}(S) := \sup\{d(x, y) : x, y \in S\} \leq 2$. By Proposition 3.1.2, we have for any $x \in S$:

$$\|\delta_x - \mu\|_{\mathrm{FM}}^* = \langle\, \mu, 2 \wedge d(x, \cdot)\, \rangle = \langle\, \mu, d(x, \cdot)\, \rangle = \sum_{i=1}^{M} \alpha_i d(x, x_i). \tag{5.15}$$

Notice that we encountered a similar expression for $\inf_{\alpha \geq 0} T_x(\alpha)$ in (5.6).

Our goal is to find $\arg\min_{x \in S} \|\delta_x - \mu\|_{\mathrm{FM}}^*$, i.e.,

$$\arg\min_{x \in S} \sum_{i=1}^{M} \alpha_i d(x, x_i). \tag{5.16}$$

We demonstrate that solving (5.16) is equivalent to solving the *Fermat-Weber problem.* Alternative names for this problem are the *Weber problem*, the *Steiner problem* and variations on these. Note that the problem (5.16) is only a slight generalization of the problem studied in the previous section ($M = 2$). However, when a problem bears the names Fermat, Weber and Steiner, one knows it cannot be easy to solve the problem, let alone further generalizations of the problem.

Let us pose the Fermat-Weber problem. There exist different formulations. Some authors state the problem on $\mathbb{R}^2$, but we adopt the more general formulation on $\mathbb{R}^n$, following [Eck80] among others.

Definition 5.3.1. The *Fermat-Weber problem* in classical form is as follows. Let $M, n \in \mathbb{N}$ and let $x_i \in \mathbb{R}^n$ and $w_i \geq 0$ for all $i \in \{1, \ldots, M\}$. Find

$$\arg\min_{y \in \mathbb{R}^n} \sum_{i=1}^{M} w_i d(y, x_i), \tag{5.17}$$

where d is the Euclidean metric on $\mathbb{R}^n$, i.e., $d(y, z) = \sqrt{(y_1 - z_1)^2 + \ldots + (y_n - z_n)^2}$.

The similarity between (5.16) and (5.17) is obvious. The only difference is the more general Polish space setting in (5.16). The requirement $\sum_{i=1}^{M} \alpha_i = 1$ does not alter the problem, because the object function has the same minimizing points when multiplied by a positive scalar.

Would we have recognized the famous Fermat-Weber problem at an earlier stage, then we might have been less optimistic to explicitly find best approximations within $\mathcal{D}_N(S)$ and $\mathcal{P}_N(S)$. The Fermat-Weber problem is difficult, and cannot be solved exactly for $M > 3$, though it has been intensively studied. So even for μ of the simple form above (finitely supported), and for $N = 1$, finding a best approximation in $\mathcal{P}_N(S)$ does not seem feasible.

Let us sketch some of the history of the study of the Fermat-Weber problem. The first version of the problem was the special case $n = 2$, $M = 3$ and $w_i = 1$ for $i = 1, 2, 3$, and is called the *Fermat problem.* The problem was posed by Fermat (1601-1665) himself in the beginning of the 17th century. In a famous essay on maxima and minima, Fermat posed the problem as a challenge to the reader ([Kuh67]):

> "Let he who does not approve of my method attempt the solution of the following problem: given three points in a plane, find a fourth point such that the sum of its distances to the three given points is a minimum!"

The problem was solved quite soon afterwards. There has been a lot of discussion about who solved the problem first, but it seems most likely that it was Torricelli (1608-1647), a mathematician and student of Galileo ([DKSW02, p. 3]). Torricelli presented a geometrical construction to find a minimizing point. Simpson (1710-1761) later provided an alternative geometrical method and suggested to generalize the problem by including different weights ([DKSW02, p. 3]). In this way, the Fermat-Weber problem arose.

In the 20th century, the above defined Fermat-Weber problem became widely studied. This was partly due to its natural appearance in continuous location theory. For example, the problem appears when one wants to determine the optimal location for a single central facility that serves a number of demand centers. Here, a location is optimal if it minimizes the total cost associated with serving the demand centers, under the assumption that the associated service costs are directly proportional to the (Euclidean) distances between the demand centers and the central facility ([MF94]).

For more than three points ($M > 3$), an exact geometrical solution such as Torricelli's solution (for $M = 3$) does not exist. However, there do exist well-developed algorithms for numerical approximation of a minimizing point. Weiszfeld (1916–2003) invented an efficient numerical method for approximating a solution to (5.17) with equal weights w_i. Weiszfeld's algorithm was generalized for different weights in [KK62] by Kuhn and Kuenne. Many improved and further generalized algorithms have been proposed afterwards, by numerous authors ([DKSW02, p. 5]). Even now, the research continues ([CDT22]).

When $S = \mathbb{R}^n$ and d is the Euclidean metric, we can choose one of the Fermat-Weber problem algorithms for an approximation of a solution to our own problem (5.16). However, we originally posed (5.16) in a general Polish space setting. There are no algorithms that apply to every Polish space (yet), but there do exist algorithms that solve (5.16) for classes of more general, non-Euclidean spaces. Among others, [Eck80] offers an algorithm for a generalized problem in reflexive Banach spaces and [Bač14a] provides algorithms for *Hadamard spaces*. The latter are a class of complete metric spaces that are also known as *complete* $CAT(0)$ *spaces*. They include Hilbert spaces, some Riemannian manifolds, and the rather exotic *Euclidean buildings* and *BHV tree space* ([Bač14a, p. 1]).

Remark 5.3.2. *The existence of a (not necessarily unique) solution to the Fermat-Weber problem for Hadamard spaces is guaranteed by [Bač14b, Lemma 2.2.19]. In particular, there exists a solution in the Euclidean space setting of* (5.17)*.*

We now consider an example in which we use available knowledge about the Fermat-Weber problem to find a best approximation in $\mathcal{P}_1(S)$. Recall Proposition 5.2.2, which shows that for $\mathcal{D}_1(S)$ and $M = 2$, there always exists a best approximation $\alpha\delta_x \in \mathcal{D}_1(S)$ with $x \in \operatorname{supp}(\mu)$. Similarly, for $\mathcal{P}_1(S)$ and $M = 2$, (5.13) and (5.8) together yield the existence of a best approximation $\delta_x \in \mathcal{P}_1(S)$ with $x \in \operatorname{supp}(\mu)$ (the last three expressions of (5.13) are all minimal at $x = y_1$ or $x = y_2$). The next example shows that this is not the case for $M > 2$ in general.

Example 5.3.3. *Let* $S = \mathbb{R}^2$ *and let* $\mu = \sum_{i=1}^{3} \frac{1}{3}\delta_{x_i}$*, with* $x_1 = (0,0)$*,* $x_2 = (1,0)$ *and* $x_3 = (\frac{1}{2}, \frac{1}{2}\sqrt{3})$ *being the vertices of an equilateral triangle. Let* $x_{mid} = (\frac{1}{2}, \frac{1}{\sqrt{12}})$ *be the midpoint of the triangle. From Torricelli's solution (see [DKSW02, p. 6]), one can easily derive that* x_{mid} *is a minimizing point. By* (5.15)*, we have*

$$\|\delta_{x_{mid}} - \mu\|_{\mathrm{FM}}^* = \sum_{i=1}^{3} \frac{1}{3} d(x_{mid}, x_i) = 3\frac{1}{3}\sqrt{(\frac{1}{2})^2 + (\frac{1}{\sqrt{12}})^2} = \frac{1}{\sqrt{3}},$$

while for $j \in \{1,2,3\}$*:*

$$\|\delta_{x_j} - \mu\|_{\mathrm{FM}}^* = \sum_{i=1}^{3} \frac{1}{3} d(x_j, x_i) = 2\frac{1}{3}1 = \frac{2}{3} > \frac{1}{\sqrt{3}}.$$

Therefore, best approximations in $\mathcal{P}_1(S)$ *necessarily have support in* $S \setminus \operatorname{supp}(\mu)$*.*

Now consider $\mathcal{D}_1(S)$ instead of $\mathcal{P}_1(S)$. Using Corollary 4.1.5, one can derive that for all $\alpha \in [0,2]$ and $j \in \{1,2,3\}$:

$$\|\alpha\delta_{x_j} - \mu\|^*_{\mathrm{FM}} = \|\alpha\delta_{x_1} - \mu\|^*_{\mathrm{FM}} = \alpha\theta_0 - \langle\, \mu, (-1) \vee (\theta_0 - d(x_1,\cdot))\,\rangle, \qquad \textit{with } \theta_0 = \begin{cases} -1, & \alpha \le \frac{1}{3}, \\ 0, & \frac{1}{3} < \alpha \le 1, \\ 1, & \alpha > 1. \end{cases}$$

This yields

$$\begin{aligned} \|\alpha\delta_{x_j} - \mu\|^*_{\mathrm{FM}} &= \begin{cases} -\alpha - \langle\, \mu, -1\,\rangle, & \alpha \le \frac{1}{3}, \\ 0 - \langle\, \mu, (-1) \vee (-d(x_1,\cdot))\,\rangle, & \frac{1}{3} < \alpha \le 1, \\ \alpha - \langle\, \mu, (-1) \vee (1 - d(x_1,\cdot))\,\rangle, & \alpha > 1, \end{cases} \\ &= \begin{cases} 1-\alpha, & \alpha \le \frac{1}{3}, \\ \frac{2}{3}, & \frac{1}{3} < \alpha \le 1, \\ \alpha - \frac{1}{3}, & \alpha > 1, \end{cases} \\ &\ge \frac{2}{3} > \frac{1}{\sqrt{3}} = \|\delta_{x_{mid}} - \mu\|^*_{\mathrm{FM}}. \end{aligned}$$

Hence, all best approximations in $\mathcal{D}_1(S)$ have support in $S \setminus \operatorname{supp}(\mu)$.

5.4 Discussion

In the previous sections, we gathered insights about best approximations in $\mathcal{D}_1(S)$ and $\mathcal{P}_1(S)$ for specific examples. The examples revealed that finding a best approximation is very complex, although existence is guaranteed when S is a Hadamard space (Remark 5.3.2).

We now turn back to general $\mu \in \mathcal{P}(S)$ and reflect on Conjecture 5.1.6 and its possible proofs for the FM-norm. We shortly outline some ideas that we wanted to exploit in our own proving attempts thus far and pose some challenges and recommendations for further research.

To start with, we had some hopes that a minimax theorem would allow us to interchange the infimum and supremum in the left-hand side of

$$\inf_{\nu \in \mathcal{D}_N(S)} \sup_{g \in \mathrm{B}_{\mathrm{FM}}} \langle\, \mu - \nu, g\,\rangle = \inf_{\nu \in \mathcal{D}_N(S)} \|\nu - \mu\|^*_{\mathrm{FM}}. \tag{5.18}$$

In most minimax theorems, the infimum and supremum both need to be taken over compact and convex sets. This is not the case in (5.18): $\mathcal{D}_N(S)$ is not convex, nor compact in general (Proposition 5.1.4), and B_{FM} is not compact either, at least in the $\|\cdot\|^*_{\mathrm{FM}}$-topology. However, we found a promising minimax theorem in [Sio58], which we discuss here.

Unfortunately, it turned out that interchanging the infimum and supremum in (5.18) leads to a contradiction (Lemma 5.4.4). Nevertheless, we find it useful to reflect on the almost-applicable minimax theorem in [Sio58, Theorem 4.2]. To do so, we first need some definitions given in [Sio58, p. 172].

Definition 5.4.1. Let X and Y be sets and let ϕ be a function on $X \times Y$. We call ϕ *concavelike* in X if for every $g_1, g_2 \in X$ and $0 \le t \le 1$, there is a $g \in X$ such that

$$t\phi(g_1,\nu) + (1-t)\phi(g_2,\nu) \le \phi(g,\nu), \qquad \text{for all } \nu \in Y. \tag{5.19}$$

The function ϕ is *convexlike* in Y if for every $\nu_1, \nu_2 \in Y$ and $0 \le t \le 1$, there is a $\nu \in Y$ such that

$$t\phi(g,\nu_1) + (1-t)\phi(g,\nu_2) \ge \phi(g,\nu), \qquad \text{for all } g \in X. \tag{5.20}$$

Finally, ϕ is called *concave-convexlike* if it is concavelike in X and convexlike in Y.

The next minimax theorem can be found in [Sio58, Theorem 4.2]. The original version is due to [Fan53, Theorem 2].

Theorem 5.4.2. *Let X be a compact Hausdorff space, let Y be any set and let ϕ be a function on $X \times Y$ that is concave-convexlike. If $\phi(g,\nu)$ is upper semicontinuous in g for each $\nu \in Y$, then* $\sup_X \inf_Y \phi = \inf_Y \sup_X \phi$.

Remark 5.4.3. *Define $X := \mathrm{B}_{\mathrm{FM}}$, $Y := \mathcal{D}_N(S)$ and $\phi : X \times Y \to \mathbb{R} : (g,\nu) \mapsto \langle\, \nu - \mu, g \,\rangle$. Equip $X = \mathrm{B}_{\mathrm{FM}} \subset \mathrm{BL}(S)$ with the $\sigma(\mathrm{BL}(S), \overline{\mathrm{Mol}}(S))$-topology. It can be shown that all conditions of Theorem 5.4.2 are satisfied, except the convexlikeness in Y.*

Compactness of X follows from Theorem 2.2.1 and the Banach-Alaoglu Theorem. Note that $\sigma(\mathrm{BL}(S), \overline{\mathrm{Mol}}(S))$-convergence implies pointwise convergence (for $x \in S$, $\iota(\delta_x) \in \overline{\mathrm{Mol}}(S)$ satisfies $\iota(\delta_x)(f) = f(x)$) and note that X is Hausdorff. The pointwise convergence and the Lebesgue Dominated Convergence Theorem yield the upper semicontinuity of $\phi(\cdot,\nu)$ for each $\nu \in Y$. Also, ϕ is linear in the convex set X, implying concavelikeness in X immediately (take $g = tg_1 + (1-t)g_2$ in (5.19)).

The only condition that is not satisfied, is the convexlikeness in Y. Note that $\phi(-g,\cdot) = -\phi(g,\cdot)$. So if (5.20) were satisfied, then by applying it to $\pm g$, one can derive that

$$\phi(g,\nu) = t\phi(g,\nu_1) + (1-t)\phi(g,\nu_2) = \phi(g, t\nu_1 + (1-t)\nu_2), \tag{5.21}$$

for all $g \in X$. Extend ϕ to a function $\tilde{\phi}$ on $\mathrm{BL}(S) \times Y$ in the obvious way, i.e., $\tilde{\phi}(g,\nu) := \langle\, \nu - \mu, g \,\rangle$ for all $g \in \mathrm{BL}(S)$ and $\nu \in Y$. Since $\tilde{\phi}$ is positive homogeneous in g (linear even), (5.21) also holds for $\tilde{\phi}$ instead of ϕ, for all $g \in \mathrm{BL}(S)$. From the injectivity of the embedding ι, defined in Lemma 1.2.7, we obtain $\nu = t\nu_1 + (1-t)\nu_2$.

Now apply this reasoning to any choice of ν_1, ν_2 and t with $\#\,\mathrm{supp}(\nu_i) = N$ for $i = 1,2$, $\mathrm{supp}(\nu_1) \neq \mathrm{supp}(\nu_2)$ and $t \notin \{0,1\}$. Of course, S needs to contain at least $N+1$ points to do so. Then we arrive at the contradiction $\mathrm{supp}(\nu) = \mathrm{supp}(t\nu_1 + (1-t)\nu_2) \geq N+1$, i.e., $\nu \notin Y$. Thus, ϕ is not convexlike when $\#S \geq N+1$.

The next lemma reconfirms that ϕ cannot be convexlike in general. All other conditions of Theorem 5.4.2 were already satisfied, so if ϕ would have been convexlike, then we could have interchanged the infimum and supremum. The latter is not possible by the next lemma. In addition, the lemma shows that other minimax theorems could not have worked either.

Lemma 5.4.4. *Let X, Y and ϕ be as in Remark 5.4.3 and let $\mu \in \mathcal{P}(S)$. Then*

$$\sup_{g\in X} \inf_{\nu\in Y} \langle\, \nu - \mu, g \,\rangle = 0.$$

Consequently, whenever $\mu \in \mathcal{P}(S) \setminus \mathcal{D}_N(S)$, it does not *hold that*

$$\sup_{g\in X} \inf_{\nu\in Y} \langle\, \nu - \mu, g \,\rangle = \inf_{\nu\in Y} \sup_{g\in X} \langle\, \nu - \mu, g \,\rangle .$$

Proof. Fix $g \in X$ and let $\inf(g) := \inf_{x\in S} g(x)$. We have

$$\begin{aligned}\inf_{\nu\in\mathcal{D}_N(S)} \langle\, \nu - \mu, g \,\rangle = \inf_{\nu\in\mathcal{D}_N(S)} \langle\, \nu, g \,\rangle \quad - \langle\, \mu, g \,\rangle &= \inf_{\substack{x_i\in S\\ \alpha_i\geq 0\\ \sum_{i=1}^N \alpha_i \leq 2}} \sum_{i=1}^N \alpha_i g(x_i) \quad - \langle\, \mu, g \,\rangle \\ &= 2(\inf(g) \wedge 0) - \langle\, \mu, g \,\rangle .\end{aligned} \tag{5.22}$$

To see why (5.22) holds, consider the cases $\inf(g) \geq 0$ and $\inf(g) < 0$ separately. If $\inf(g) \geq 0$, then $g(x_i) \geq 0$ for any $x_i \in S$, so the infimum over the x_i and α_i equals 0 (pick $\alpha_i = 0$ for all i). Also, $\inf(g) \wedge 0 = 0$, proving (5.22). Now suppose that $\inf(g) < 0$. For any choice of $x_i \in S$ and $\alpha_i \geq 0$ with $\sum_{i=1}^N \alpha_i \leq 2$, we have $\sum_{i=1}^N \alpha_i g(x_i) \geq \sum_{i=1}^N \alpha_i \inf(g) \geq 2\inf(g) \geq 2(\inf(g) \wedge 0)$. This proves '$\geq$'. For the other inequality, pick a sequence $(y_n) \subset S$ with $\lim_{n\to\infty} g(y_n) = \inf(g)$ and let

$\nu_n := 2\delta_{y_n} \in \mathcal{D}_N(S)$. We have $\langle\, \nu, g \,\rangle = 2g(y_n) \to 2\inf(g)$ as $n \to \infty$. Thus, $\inf_{\nu\in\mathcal{D}_N(S)} \langle\, \nu, g \,\rangle \leq 2\inf(g) = 2(\inf(g) \wedge 0)$. This establishes '$\leq$'.

Now we determine

$$\sup_{g\in X} \inf_{\nu\in Y} \langle\, \nu - \mu, g \,\rangle = \sup_{g\in X} \Big(2(\inf(g) \wedge 0) - \langle\, \mu, g \,\rangle \Big). \tag{5.23}$$

Suppose that $g \in X$ is such that $I := \inf(g) < 0$. It can easily be shown that $h := (g - I) \wedge 1$ is an element of X with $h \geq 0$, $\inf(h) = 0$ and $h \leq g - I$. We have

$$\begin{aligned} 2(\inf(h) \wedge 0) - \langle\, \mu, h \,\rangle = 0 - \langle\, \mu, h \,\rangle \geq - \langle\, \mu, g - I \,\rangle = I - \langle\, \mu, g \,\rangle &\geq 2I - \langle\, \mu, g \,\rangle \\ &= 2(\inf(g) \wedge 0) - \langle\, \mu, g \,\rangle . \end{aligned}$$

Therefore,

$$\sup_{g\in X} \Big(2(\inf(g) \wedge 0) - \langle\, \mu, g \,\rangle \Big) = \sup_{g\in X, g\geq 0} \Big(2(\inf(g) \wedge 0) - \langle\, \mu, g \,\rangle \Big). \tag{5.24}$$

But for any $g \geq 0$, we have $-\langle\, \mu, g \,\rangle \leq 0 = -\langle\, \mu, 0 \,\rangle$ and $\inf(g) \wedge 0 = 0$, so

$$\sup_{g\in X, g\geq 0} \Big(2(\inf(g) \wedge 0) - \langle\, \mu, g \,\rangle \Big) = \sup_{g\in X, g\geq 0} -\langle\, \mu, g \,\rangle = -\langle\, \mu, 0 \,\rangle = 0. \tag{5.25}$$

Combining (5.23), (5.24) and (5.25), we conclude that

$$\sup_{g\in X} \inf_{\nu\in Y} \langle\, \nu - \mu, g \,\rangle = 0.$$

Now let $\mu \in \mathcal{P}(S)\backslash\mathcal{D}_N(S)$. Recall that $\mathcal{D}_N(S)$ is $\|\cdot\|^*_{\mathrm{FM}}$-closed (Proposition 5.1.2). An elementary property of metric spaces (see [Men90, Chapter 2, Theorem 6.9]), is that the distance from an element x to a closed subset A is zero, if and only if $x \in A$. As a result, we have

$$\inf_{\nu\in Y} \sup_{g\in X} \langle\, \nu - \mu, g \,\rangle = \inf_{\nu\in Y} \|\nu - \mu\|^*_{\mathrm{FM}} > 0.$$

We conclude that

$$\inf_{\nu\in Y} \sup_{g\in X} \langle\, \nu - \mu, g \,\rangle \neq \sup_{g\in X} \inf_{\nu\in Y} \langle\, \nu - \mu, g \,\rangle = 0.$$

☐

Now that we have excluded the application of minimax theorems to (5.18), we outline some other ideas for proving Conjecture 5.1.6.

An obvious strategy is to somehow reduce the set S in Conjecture 5.1.6 to suitable compact subsets K_i. Natural contenders for compact subsets can be found by exploiting for example the tightness of μ (recall Proposition 1.2.16). Once we have compact subsets K_i, Proposition 5.1.4 provides the existence of a best approximation for $\mu|_{K_i}$ in $\mathcal{D}_N(K_i) \subset \mathcal{M}(K_i)$. These best approximations should then be linked to a best approximation in $\mathcal{D}_N(S)$ somehow. Finding this link is difficult. Still, the next lemma provides some relation between the FM-norm on $\mathcal{M}(S)$ and the FM-norm on $\mathcal{M}(K_i)$.

Lemma 5.4.5. *Let $\emptyset \neq K \subset S$ and $\nu, \mu \in \mathcal{M}(S)$. Then for $\bullet = \mathrm{FM}, \mathrm{BL}$, we have*

$$\|\nu|_K - \mu|_K\|^*_{\bullet,S} = \|\nu|_K - \mu|_K\|^*_{\bullet,K}. \tag{5.26}$$

Here, $\nu|_K$ is defined by $\nu|_K(A) := \nu(K \cap A)$ for $A \in \mathcal{B}(S)$ or $A \in \mathcal{B}(K)$. It can be seen as an element of both $\mathcal{M}(S)$ and $\mathcal{M}(K)$ (and the same holds for $\mu|_K$, defined analogously).

Proof. We have $\langle\, \nu|_K - \mu|_K, f \,\rangle = \langle\, \nu|_K - \mu|_K, f|_K \,\rangle$ for all $f \in \mathrm{B}^S_\bullet$. Corollary 1.1.7 now immediately implies the result. ☐

Lemma 5.4.5 is useful, but a main difficulty remains. When we replace $\nu|_K$ by ν on the left-hand side of (5.26), we do not have a similar relation. Say, for example, an inequality version of (5.26) cannot be derived. So given μ with $K := \operatorname{supp}(\mu)$, it is unclear how the support of a best approximation ν_0 relates to K. We could only prove one modest relation, stated in the following lemma.

Lemma 5.4.6. *Let $\mu \in \mathcal{M}^+(S)$ and define $K_1^\mu := \{s \in S : d(s, \operatorname{supp}(\mu)) \leq 1\}$, where $d(s,E) := \inf_{x\in E} d(s,x)$ for $E \subset S$. Then*

$$\inf_{\nu\in\mathcal{D}_N(S)} \|\nu-\mu\|_{\mathrm{FM}}^* = \inf_{\substack{\nu\in\mathcal{D}_N(S),\\ \operatorname{supp}(\nu)\subset K_1^\mu}} \|\nu-\mu\|_{\mathrm{FM}}^*. \tag{5.27}$$

Proof. Consider the following map:

$$T : \mathrm{B}_{\mathrm{FM}}^{\operatorname{supp}(\mu)} \to \mathrm{B}_{\mathrm{FM}} : Tg^*(s) := (-1) \vee \sup\{g^*(x) - d(x,s) : x \in \operatorname{supp}(\mu)\}.$$

One can show that $Tg^* \in \mathrm{B}_{\mathrm{FM}}$ for any $g^* \in \mathrm{B}_{\mathrm{FM}}^{\operatorname{supp}(\mu)}$ using a similar argument as in Proposition 1.1.5 (we do not have $|g^*|_L = 1$ necessarily, but we do have $|g^*|_L \leq 1$ and the argument in the proof still applies with $C = 1$). So T is well-defined.

Let $g \in \mathrm{B}_{\mathrm{FM}}$ and $\nu \in \mathcal{M}^+(S)$. Define $g^* := g|_{\operatorname{supp}(\mu)} \in \mathrm{B}_{\mathrm{FM}}^{\operatorname{supp}(\mu)}$. We show that $Tg^* \leq g$. Since $|g|_L \leq 1$, we have $g^*(x) - g(s) = g(x) - g(s) \leq d(x,s)$ for all $x \in \operatorname{supp}(\mu)$, i.e., $g^*(x) - d(x,s) \leq g(s)$. Taking the supremum over $\operatorname{supp}(\mu)$ and noting that $g \geq -1$, we obtain $Tg^* \leq g$. Next, we show that $Tg^* = g$ on $\operatorname{supp}(\mu)$. For $x \in \operatorname{supp}(\mu)$, we have by definition of Tg^*: $Tg^*(x) \geq g^*(x) - d(x,x) = g(x)$. Together with the fact that $Tg^* \leq g$, this proves that $Tg^* = g$ on $\operatorname{supp}(\mu)$.

Using the latter, together with $Tg^* \leq g$ and $\nu \geq 0$, we obtain

$$\langle\, \mu-\nu, Tg^* \,\rangle = \langle\, \mu, Tg^*\, \mathbb{1}_{\operatorname{supp}(\mu)} \,\rangle - \langle\, \nu, Tg^* \,\rangle \geq \langle\, \mu, g\, \mathbb{1}_{\operatorname{supp}(\mu)} \,\rangle - \langle\, \nu, g \,\rangle = \langle\, \mu-\nu, g \,\rangle. \tag{5.28}$$

Now define

$$T_\mu := \{Tg^* : g^* \in \mathrm{B}_{\mathrm{FM}}^{\operatorname{supp}(\mu)}\} \subset \mathrm{B}_{\mathrm{FM}}.$$

From (5.28), it follows that

$$\begin{aligned} \|\nu-\mu\|_{\mathrm{FM}}^* = \sup_{g\in\mathrm{B}_{\mathrm{FM}}} \langle\, \mu-\nu, g \,\rangle &= \sup_{h\in T_\mu} \langle\, \mu-\nu, h \,\rangle \\ &= \sup_{h\in T_\mu} \big(\langle\, \mu, h \,\rangle - \langle\, \nu|_{K_1^\mu}, h|_{K_1^\mu} \,\rangle - \langle\, \nu|_{(K_1^\mu)^c}, h|_{(K_1^\mu)^c} \,\rangle \big). \end{aligned} \tag{5.29}$$

Note that for all $g^* \in \mathrm{B}_{\mathrm{FM}}^{\operatorname{supp}(\mu)}$, $s \in (K_1^\mu)^c$ and $x \in \operatorname{supp}(\mu)$, we have $d(x,s) \geq d(s, \operatorname{supp}(\mu)) > 1$, so $g^*(x) - d(x,s) \leq 1 - d(x,s) < 0$. Consequently, $Tg^*(s) \leq 0$. This shows that $h|_{(K_1^\mu)^c} \leq 0$ for all $h \in T_\mu$, so $-\langle\, \nu|_{(K_1^\mu)^c}, h|_{(K_1^\mu)^c} \,\rangle \geq 0$. Equality holds when $\nu|_{(K_1^\mu)^c} = 0$. Hence, by (5.29):

$$\|\nu-\mu\|_{\mathrm{FM}}^* \geq \sup_{h\in T_\mu} \langle\, \mu - \nu|_{K_1^\mu}, h \,\rangle = \|\nu|_{K_1^\mu} - \mu\|_{\mathrm{FM}}^*. \tag{5.30}$$

Note that $\operatorname{supp}(\nu|_{K_1^\mu}) \subset K_1^\mu$. Applying (5.30) to all $\nu \in \mathcal{D}_N(S)$ yields (5.27). ☐

Unfortunately, the set K_1^μ in Lemma 5.4.6 is not compact generally, even when $\operatorname{supp}(\mu)$ itself is compact. For example, let S be an infinite dimensional normed linear space and let $\mu = \delta_x$ for some $x \in S$. Then it holds that $\operatorname{supp}(\mu) = \{x\}$, but K_1^μ is the closed unit ball with center x and radius 1, which is not compact (see [RY08, Theorem 2.26]).

To reduce the set S to a compact subset, one could exploit tightness of μ to approximate S by compact K_i in μ-measure. As mentioned already, one can then let $\nu_i \in \mathcal{D}_N(K_i)$ be (best) approximations for $\mu|_{K_i}$. But without more information on $\operatorname{supp}(\nu_i)$, it is hard to find a convergent (diagonal) sequence converging to a best approximation in $\mathcal{D}_N(S)$. On the other hand, one can start with a sequence $(\nu_n) \subset \mathcal{D}_N(S)$ with $\lim_{n\to\infty} \|\nu_n - \mu\|_{\mathrm{FM}}^* = \inf_{\nu\in\mathcal{D}_N(S)} \|\nu-\mu\|_{\mathrm{FM}}^*$ and take weakly convergent subsequences of $(\nu_n|_{K_i}) \subset \mathcal{D}_N(K_i)$ for $i \in \mathbb{N}$, followed by a diagonal sequence. But then, one will encounter similar norm estimation obstacles. Things would be simpler when we could assume that $\mathrm{supp}(\nu_0) \subset \mathrm{supp}(\mu)$. But this is generally not true, as follows from Example 5.3.3. Therefore, it seems very difficult to exploit tightness.

A solution could be to make extra assumptions on S. It is worth noting that existence of a solution to the related Fermat-Weber problem was obtained in [Bač14b, Lemma 2.2.19] in the context of Hadamard spaces. These are metric spaces with a particular, generalized convexity structure. Therefore, it may be fruitful to first consider classes of metric spaces with such properties. *Menger convex metric spaces* are among these. Approximation results for Menger convex metric spaces can be found in [BA05, Theorem 25] and [Kha88], although not immediately useful for proving Conjecture 5.1.6. Still, in view of the mentioned result for Hadamard spaces, we believe that exploring other classes of metric spaces with additional structure could well provide new insights.

Outlook

As always happens when studying something closely, many discoveries and observations lead to new questions. In this thesis, we have described many new perspectives to look at Fortet-Mourier and Dudley distances between measures. Some of these perspectives led to elegant and useful, new expressions and algorithms. For other perspectives, we feel that there might be even more to gain in a further study. Therefore, we conclude this thesis by making a few suggestions for further research.

In Chapter 5, we formulated Conjecture 5.1.6 that has yet to be proved or disproved. Possible approaches for a proof were mentioned in Section 5.4. In our opinion, the most important suggestion is to first consider classes of metric spaces with additional generalized convexity structures such as Hadamard spaces, motivated by Remark 5.3.2. In Sections 5.2 and 5.3, we came across some interesting examples that showed diverse behavior of best approximations in $\mathcal{D}_N(S)$ and $\mathcal{P}_N(S)$. Getting more grip on this behavior, we deem a suitable objective for future research. In particular, it could be useful to get a better understanding on the support of best approximations, related to support of the approximated measure μ.

In earlier chapters, we discovered some other interesting things that deserve a further investigation. In Section 4.2, we proved that computing a distance $\|\nu-\mu\|_{\mathrm{FM}}^*$ with $\nu \in \mathcal{D}_N(S)$, $\mu \in \mathcal{M}^+(S)$ is equivalent to minimizing the convex and Lipschitz continuous functional $-\psi$:

$$\|\nu - \mu\|_{\mathrm{FM}}^* = \inf_{f \in \mathrm{B}_{\mathrm{FM}}^P} -\psi(f), \qquad \psi : \mathrm{B}_{\mathrm{FM}}^P \to \mathbb{R} : f \mapsto \left\langle\, \nu - \mu, (-1) \vee \bigvee_{i=1}^N (f_i - d(x_i, \cdot)) \,\right\rangle .$$

When S is a straightforward subset of $\mathbb{R}^n$ and when μ allows a density with respect to the Borel-Lebesgue measure, we demonstrated that $-\psi$ can efficiently be minimized numerically. Nevertheless, it would be worth exploring whether analytic properties of the minimum can be derived, using the specific structure of $\mathrm{B}_{\mathrm{FM}}^P$. This might allow to compute norms faster numerically, or to extend the applicability to general $\mu \in \mathcal{M}^+(S)$ in non-Euclidean settings. Also, it would be interesting to explore whether more exact expressions for distances can be derived, using the minimization of $-\psi$. For example, it might be that our exact expressions from Proposition 3.1.2 and Proposition 4.1.2 for $\nu \in \mathcal{P}_1(S)$, can be generalized for $\nu \in \mathcal{P}_N(S)$ for $N \in \mathbb{N}$. However, we do know that generalizing these expressions is not an easy task.

In the light of applications (see Introduction), it would also be interesting to consider the specific setting $S = \mathbb{R}$ and $\mu \in \mathcal{P}(S)$ of the form $hd\lambda$, with $h \in L^1(\mathbb{R}, \mathcal{B}(\mathbb{R}), \lambda)$ and λ the Borel-Lebesgue measure on $\mathbb{R}$ (and later generalize to $S = \mathbb{R}^n$). Then, one could investigate whether more explicit expressions or improved algorithms can be derived for $\|\nu - \mu\|_{\mathrm{FM}}^*$, with $\nu \in \mathcal{D}_N(S)$. Possibly, one can impose more conditions on f (smoothness or $f \in L^p$ for some $p > 1$), if required. Also, one could impose in addition that ν is an empirical measure (i.e., all weights before the Dirac measures are equal). This is a rather specific choice, but useful for applications to modeling with measures as described in the Introduction.

Another idea is to study $\|hd\lambda\|_{\mathrm{FM}}^*$ or $\|hd\lambda\|_{\mathrm{BL}}^*$. This norm cannot be computed yet, when f takes both positive and negative values in $\mathbb{R}$. However, using the partly new knowledge from Chapter 2, we do know that

$$\|hd\lambda\|_{\bullet}^* = \sup_{g \in \mathrm{E}_{\bullet}} \langle\, hd\lambda, g \,\rangle = \sup_{g \in \mathrm{E}^{\bullet}} \langle\, hd\lambda, g \,\rangle,$$

as was proved in Corollary 2.6.1 and Remark 2.6.2. Here, $\mathrm{E}^{\bullet}$ is completely determined by the extreme points of balls $\mathrm{B}_{\bullet}^{P}$ with $P \subset S$ finite. Thus, studying $\mathrm{ext}(\mathrm{B}_{\bullet}^{P})$ could also give useful insights. Recall that for $\bullet = \mathrm{BL}$, we already proved a remarkable necessary condition for every element f of $\mathrm{ext}(\mathrm{B}_{\mathrm{BL}}^{P})$: f must attain both $+\|f\|_\infty$ and $-\|f\|_\infty$ by Lemma 2.5.2.

Related to extreme points, a final suggestion would be to have another look at the connectedness assumption on S in the proofs for the dense subsets $\mathrm{E}_{\bullet}$ of $\mathrm{ext}(\mathrm{B}_{\bullet})$ (Theorem 2.4.7 and Theorem 2.5.10). The connectedness seems a rather technical, unnatural condition. It would be worthwhile to investigate whether this condition could be omitted. Especially, since the majority of the results in Chapters 3 and 4 were derived using functions in E_{FM}, and the results applied to disconnected metric spaces as well.

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Appendix A

MATLAB algorithms for norms of measures

A.1 FM-norm of a linear combination of Dirac measures

```
function [norm,f] = FMdualnorm(a,dist)
%a=[a_1 a_2 ... a_n], mu=sum_i=1^n a_i delta_s_i, dist=[d_ij]_i,j=1^n matrix
%norm =||mu||_FM^*, f=ext pt for which <mu,f>=norm
n=length(a);
A=[];
for i=1:n
    for j=i+1:n
    B=zeros(1,n);
    B(i)=dist(i,j)^(-1);
    B(j)=-B(i);
    A=[A;B];
    end
end
A=[A;eye(n)];
A=[A;-A];
b=ones(n^2+n,1); %m=#rows of A=2n+2(n choose 2)=2n+n(n-1)=n^2+n
minus_a=-a;
f=linprog(minus_a,A,b);
norm=a*f;
```

A.2 BL-norm of a linear combination of Dirac measures

```
function [norm,f] = BLdualnorm(a,dist)
%a=[a_1 a_2 ... a_n], mu=sum_i=1^n a_i delta_s_i, dist=[d_ij]_i,j=1^n matrix
%norm =||mu||_BL^*, f=ext pt for which <mu,f>=norm
n=length(a);
A=[];
for k=1:n
    for i=1:n
        if k~=i
            for j=i+1:n
                if j~=k
                B=zeros(1,n);
```

```
                B(k)=1;
                B(i)=dist(i,j)^(-1);
                B(j)=-dist(i,j)^(-1);
                A=[A;B];
                B([i j])=-B([i j]);
                A=[A;B];
                end
            end
        end
    end
end
for k=1:n
    for i=k+1:n
    B=zeros(1,n);
    B(k)=1+dist(k,i)^(-1);
    B(i)=-dist(k,i)^(-1);
    A=[A;B];
    B([k i])=B([i k]);
    A=[A;B];
    end
end
A=[A;-A];
b=ones(2*n*(n-1)^2,1);
minus_a=-a;
f=linprog(minus_a,A,b);
norm=a*f;
```

A.3 FM-distance between a positive linear combination of Dirac measures and a positive measure

```
% Computes ||\nu-\mu||_FM^* for \nu in Mol^+(S), \mu in M^+(S),
% S=(Smin, Smax)\subset\R (possibly Smin=-Inf, Smax=+Inf)
% \mu=h d\lambda, \mu abs ct wrt Lebesgue measure, \nu=sum a_i delta_{s_i}

Smin = 0;
Smax = Inf;
a = [1/2 2 1/5 1/3]; % a=[a_1,...,a_n]
n = length(a);
P = [0 1/3 1/2 3]; %=supp(\nu)=[s_1,...,s_n]

h = @(s) exp(-s^2);
integrand = @(s,f)h(s)*max(-1,max(f-abs(P-s)));
psi = @(f) -dot(a,f)+integral(@(s) integrand(s,f),Smin,Smax,'ArrayValued',true);

A = [];
for i = 1:n
    for j = i+1:n
    B = zeros(1,n);
    B(i) = abs(P(i)-P(j))^(-1);
    B(j) = -B(i);
    A = [A;B];
    end
```

```
end
A = [A;eye(n)];
A = [A;-A];

b = ones(n^2+n,1);
f0 = zeros(1,n);

[f,val] = fmincon(psi,f0,A,b);
f
norm = -val
```