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Volumen 1

Metrization

Hugo Aimar - Ivana Gómez

2023

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Prefacio de la Serie Monografías

Con este volumen iniciamos **Publicaciones del IMAL. Serie Monografías.** Esta serie está pensada para comunicar exposiciones de temas específicos de las áreas de investigación afines a las del IMAL, notas breves de cursos y/o seminarios de posgrado avanzados, entre otras.

Sobre los autores de este primer volumen: actualmente, Hugo Aimar es Investigador Superior ad-honorem del CONICET en el IMAL, e Ivana Gómez es Investigadora Independiente del CONICET en el IMAL. Ambos son miembros del grupo LABRA-IMAL dedicado a la investigación en temas relacionados con el análisis en espacios métricos, wavelets, probabilidad y ecuaciones en derivadas parciales, incluyendo aplicaciones a Big-data y Deep-learning.

Estefanía Dalmasso.
Santa Fe, julio de 2023

With this volume we launch **IMAL Publications. Monographs Series.** This series is designed to communicate presentations on specific topics in research areas related to those of the IMAL, short notes on advanced postgraduate courses or seminars, among others.

About the authors of this first volumen: Currently, Hugo Aimar is an ad-honorem Senior Researcher of CONICET at IMAL, and Ivana Gómez is an Independent Researcher of CONICET at IMAL. Both are members of the LABRA-IMAL group dedicated to research on topics related to analysis in metric spaces, wavelets, probability and partial differential equations, including applications to Big-data and Deep-learning.

Estefanía Dalmasso.
Santa Fe, July 2023.

METRIZATION

Hugo Aimar – Ivana Gómez

Grupo LABRA-IMAL

Preface

These notes are based in a graduate level course for Doctoral students in Mathematics at the Universidad Nacional del Litoral in Santa Fe, Argentina. The acronym LABRA for our group translates to ALORA, Analysis of Lower Regularity and Applications. The birth of this group in our institute IMAL goes back to the early eighties with the research on harmonic analysis on metric measure spaces. In particular in spaces of homogeneous type that was also a good general framework for the analysis related to general elliptic and parabolic operators. The comparatively more recent work on learning and data analysis, gave a rather important dynamics to the general needs for metrics and distances on general sets.

The title *Metrization* is expected to reflect action. The outstanding "Encyclopedia of Distances" by Michele Marie Deza and Elena Deza [**DD16**], prevents us from the use of "Metrics" as a title. On the other hand, the classical results of general topology prevents us from using "Metrizability". Also, we pretend that most of the results and examples presented here take the form of algorithms. Here the word algorithm has to be understood in a general sense. But in some particular subjects we shall provide also `Python` scripts for computation and visualization of examples of particular situations.

Since we clearly know that the complement of our subject index is much larger that our index itself, we do not claim for completeness. Moreover we do not even try to save the bias produced by our own construction and contributions to the subject. Even so, we expect our results and points of view could be of some help to our students and to the interested reader. We hope also that our constructions and results will contribute to M. Gromov's claim in the introduction of this book [**Gro07**] titled "Metrics Everywhere".

We shall left comments and references for the end of each chapter in order to avoid interruptions in the main text. There is no way to find a unified notation and terminology in the subject. Nevertheless these different languages are quite inessential and irrelevant. In particular we shall keep using the analysts names for quasi-metrics or quasi-distances instead of near-metrics. In any case we shall be precise at defining each concept.

Contents

CHAPTER 1

Quasi-distances and balls

1.1. Introduction and basic definitions

Let X be a set. A real function d defined on $X \times X$ is said to be a quasi-metric or a quasi-distance on X if d is symmetric, nonnegative, vanishing on the diagonal of $X \times X$ and only on the diagonal, such that there exists a positive constant K such that the inequality

$$d(x, z) \leq K(d(x, y) + d(y, z))$$

holds for every x, y and z in X. Notice first that if X has at least two elements, then $K \geq 1$. In fact, $d(x, z) \leq K(d(x, z) + d(z, z)) = Kd(x, z)$. When $K = 1$ the quasi-metric space (X, d) is a metric space in the standard sense. Given a quasi-metric space (X, d) we have a well defined family of subsets of X, that we call the family of balls of d on X given by

$$B(x, r) = \{y \in X : d(x, y) < r\}$$

for every $x \in X$ and every $r > 0$. A caveat is in order. Since we do not have a priori a natural topology defined in X by d when $K > 1$ even when $B(x, r)$ is defined by the strict inequality $d(x, y) < r$, the expression "open balls" has no meaning. In fact, as we shall see later, with the neighborhood or uniform topologies induced in X by d, it can happen that some d-balls are not open sets. Nevertheless we are not considering topological properties at this point. Instead we ask for properties of some families of subsets of X that qualify as families of balls for some quasi-metric d in X. In this chapter we aim to characterize these families of sets up to equivalences that we shall precisely define.

1.2. Some properties of the family of quasi-metric balls on a set X

Let (X, d) be a quasi-metric space with triangle constant $K \geq 1$. Let $B : X \times \mathbb{R}^+ \to \mathcal{P}(X)$ be the function that to each pair (x, r) in $X \times \mathbb{R}^+$ assigns the part of X defined by $B(x, r) = \{y \in X : d(x, y) < r\}$, i.e. the d-ball centered at $x \in X$ with radius $r > 0$. The next proposition collects the relevant properties of the function B.

Proposition 1.1. *Let (X, d) be a quasi-metric space with constant $K \geq 1$. Let B as before. Then*

(a) *for every $x \in X$ fixed, the function $B(x, \cdot) : \mathbb{R}^+ \to \mathcal{P}(X)$ is nondecreasing with the usual order in $\mathbb{R}^+$ and $\mathcal{P}(X)$;*

(b) *for every $x \in X$ we have that $\bigcup_{r>0} B(x, r) = X$;*

(c) *for every $x \in X$, $\bigcap_{r>0} B(x, r) = \{x\}$;*

(d) *for every choice of x and y in X and $r > 0$ such that $x \in B(y, r)$, we have*

(d.i) *$B(y, r) \subseteq B(x, 2Kr)$, and*

(d.ii) *$B(x, r) \subseteq B(y, 2Kr)$.*

Proof. To prove (a) notice that for $0 < r_1 < r_2$, the inequality $d(x, y) < r_1$ implies $d(x, y) < r_2$. Item (b) is a consequence of the fact that d is finite for every $(x, y) \in X \times X$. Property (c) follows from the fact that $d(x, y) = 0$ if and only if $x = y$. To prove (d.i) take $z \in B(y, r)$, then $d(x, z) \leq K(d(x, y) + d(y, z)) < 2Kr$, since $x \in B(y, r)$ and $z \in B(y, r)$. □

The above result shows that every quasi-metric on X with triangle constant K induces a family of subsets of X, which we call the balls, satisfying properties (a), (b), (c) and (d). In the next section we prove a converse; if a family of subsets of X satisfies properties (a), (b), (c) and (d), then there exists a quasi-metric d on X such that the d-balls are almost the given family of subsets of X.

1.3. From balls to quasi-metrics

In this section we consider the converse of the result in Section 1.2 above. Now we start with a set X and a function $B : X \times \mathbb{R}^+ \to \mathcal{P}(X)$ and we prove that if the family of subsets of X given by $\{B(x, r) : x \in X, r > 0\}$ satisfies (a), (b), (c) and (d) of Proposition 1.1, then there exists a quasi-distance d on X such that the d-balls are "almost the same" as the sets $B(x, r)$. In order to precise the idea of "almost the same", let us define equivalence of two functions B_1 and B_2 assigning to each $x \in X$ and each $r > 0$ a subset of X. Let $B_i : X \times \mathbb{R}^+ \to \mathcal{P}(X)$, $i = 1, 2$. We say that B_1 is equivalent to B_2 and we write $B_1 \sim B_2$ if there exist positive constants γ and Γ such that

$$B_1(x, \gamma r) \subseteq B_2(x, r) \subseteq B_1(x, \Gamma r),$$

for every $x \in X$ and every $r > 0$. It is easy to check that $\sim$ is an equivalence relation in $\mathcal{P}(X)$.

We are now in position to state and prove the main result of this chapter.

THEOREM 1.2. *Let X be a set. Let $B : X \times \mathbb{R}^+ \to \mathcal{P}(X)$ be a function satisfying the following properties*

(a) *for each $x \in X$, $B(x, \cdot)$ is a nondecreasing function of r;*

(b) $\bigcup_{r>0} B(x,r) = X$*, for every $x \in X$;*

(c) $\bigcap_{r>0} B(x,r) = \{x\}$*, for every $x \in X$;*

(d) *there exists a constant $c > 0$ such that for every $x, y \in X$ and $r > 0$ with $x \in B(y,r)$ we have*

  (d.i) $B(y,r) \subseteq B(x,cr)$*, and*

  (d.ii) $B(x,r) \subseteq B(y,cr)$.

Then, there exists a quasi-metric d on X such that $B \sim B_d$, with B_d the family of d-balls in X, i.e. $B_d(x,r) = \{y \in X : d(x,y) < r\}$.

PROOF. Take x and y two points in X. From (b) applied twice, we see that there exist r_1 and r_2 such that $y \in B(x,r_1)$ and $x \in B(y,r_2)$. With $r = \sup\{r_1, r_2\}$ and property (a) of the function B, we have that $x \in B(y,r)$ and $y \in B(x,r)$. Hence the set $\{r > 0 : x \in B(y,r) \text{ and } y \in B(x,r)\}$ is non-empty. So that

$$d(x,y) = \inf\{r > 0 : x \in B(y,r) \text{ and } y \in B(x,r)\}$$

is a well defined nonnegative valued function on $X \times X$. From (c) we have that $x \in B(x,r)$ for every $r > 0$, hence $d(x,x) = 0$. On the other hand, if $d(x,y) = 0$, then there exists a sequence r_n of positive real numbers such that $r_n \to 0$ and $x \in B(y,r_n)$ for every n. Notice that from (a), property (c) gives $\bigcap_n B(y,r_n) = \{y\}$. Hence, since $x \in \bigcap_n B(y,r_n)$, necessarily $x = y$. Let us now check that $d(x,z) \leq c(d(x,y) + d(y,z))$ for every choice of x, y and $z \in X$, where c is the constant in (d). In fact, for $\varepsilon > 0$ take $r_1 > 0$ and $r_2 > 0$ such that

(1) $r_1 < d(x,y) + \varepsilon$;

(2) $x \in B(y,r_1)$;

(3) $y \in B(x,r_1)$

(4) $r_2 < d(y,z) + \varepsilon$;

(5) $y \in B(z,r_2)$;

(6) $z \in B(y,r_2)$.

Let us first show that $x \in B(z, c(r_1 + r_2))$. From (5) $y \in B(z, r_2) \subseteq B(z, r_1 + r_2)$. From (d.ii), $B(y, r_1 + r_2) \subseteq B(z, c(r_1 + r_2))$. Now, from (2),

$$x \in B(y, r_1) \subseteq B(y, r_1 + r_2) \subseteq B(z, c(r_1 + r_2)),$$

as desired. Applying (6) and (3) we have in a similar way that $z \in B(x, c(r_1 + r_2))$. Hence, from (1) and (4), we have also

$$d(x, z) \leq c(r_1 + r_2) \leq c(d(x, y) + d(y, z)) + 2c\varepsilon,$$

for every $\varepsilon > 0$. So that d is a quasi-metric on X.

Let us finally show that the family B_d of d-balls in X and the given B are equivalent. Notice first that $B_d(x, r) \subseteq B(x, r)$. Take $y \in B_d(x, r)$, then $d(x, y) < r$. So that, from the definition of $d(x, y)$, there exists $0 < s < r$ such that $x \in B(y, s)$ and $y \in B(x, s) \subseteq B(x, r)$ from (a), so $B_d(x, r) \subseteq B(x, r)$. Take now $y \in B(x, r)$, from (d) we have $B(x, r) \subseteq B(y, cr)$ and $B(y, r) \subseteq B(x, cr)$. Then $x \in B(y, cr)$ and $y \in B(x, cr)$, hence $d(x, y) \leq cr < (c + \varepsilon)r$ and $y \in B_d(x, (c + \varepsilon)r)$ for every $\varepsilon > 0$. □

1.4. Some applications and examples

1.4.1. Dyadic metrics. Let $X = \mathbb{R}^+_0 = \{x \in \mathbb{R} : x \geq 0\}$. The dyadic intervals in $\mathbb{R}^+$ are given by $I^j_k = [k2^{-j}, (k + 1)2^{-j})$ for $j \in \mathbb{Z}$ and k a nonnegative integer. Since for each $j \in \mathbb{Z}$ fixed $\{I^j_k : k \geq 0\}$ is a partition of $\mathbb{R}^+_0 = X$, for every $x \in \mathbb{R}^+_0$ and every $j \in \mathbb{Z}$ there exists one and only one interval I^j_k in this family, that we denote $I^j(x)$, containing x.

Let $B : \mathbb{R}^+_0 \times \mathbb{R}^+ \to \mathcal{P}(\mathbb{R}^+_0)$ be given by

$$B(x, r) = I^{\left[\log_2 \frac{1}{r}\right]}(x),$$

where $[\cdot]$ denotes the integer part function. Let us check that the function B satisfies properties (a), (b), (c) and (d) in Theorem 1.2.

If $0 < r_1 \leq r_2$, then $\left[\log_2 \frac{1}{r_1}\right] \geq \left[\log_2 \frac{1}{r_2}\right]$ and $I^{\left[\log_2 \frac{1}{r_1}\right]}(x) \subseteq I^{\left[\log_2 \frac{1}{r_2}\right]}(x)$. This proves (a). Properties (b) and (c) are also clear.

To check (d) take $x, y \in \mathbb{R}^+_0$ and $r > 0$ with $x \in B(y, r) = I^{\left[\log_2 \frac{1}{r}\right]}(y)$. Set $j = \left[\log_2 \frac{1}{r}\right]$. Then x and y belong to the same dyadic interval of level j, say $x, y \in I^j_k$. In order to prove (d.i), take $z \in B(y, r) = I^{\left[\log_2 \frac{1}{r}\right]}(y) = I^j_k$, then z and x belong both to I^j_k. Hence $z \in B(x, r)$. Which is (d.i) with $c = 1$. The same argument shows (d.ii). Hence, from Theorem 1.2, we have a quasi-metric in $\mathbb{R}_0^+$ given by

$$
\begin{aligned}
\delta(x,y) &= \inf\{r>0 : x\in B(y,r) \text{ and } y \in B(x,r)\} \\
&= \inf\left\{r>0 : x \in I^{\left[\log_2 \frac{1}{r}\right]}(y) \text{ and } y \in I^{\left[\log_2 \frac{1}{r}\right]}(x)\right\} \\
&= \inf\left\{r>0 : x \text{ and } y \text{ belong to the same dyadic interval of length } 2^{-\left[\log_2 \frac{1}{r}\right]}\right\} \\
&= 2\left|I(x,y)\right|,
\end{aligned}
$$

where $I(x,y)$ is the smallest dyadic interval containing x and y. Actually, $\delta(x,y)$ is an ultra-metric in $X=\mathbb{R}^+$ called the dyadic metric.

1.4.2. Balls as sections of convex functions. Suppose that $\varphi:\mathbb{R}^n\to\mathbb{R}$ is a smooth convex function on $\mathbb{R}^n$. Given a positive number t and a point $x_0\in\mathbb{R}^n$, the section of φ at x_0 of height t is defined by

$$S_\varphi(x_0,t)=\{x\in\mathbb{R}^n : \varphi(x)<\varphi(x_0)+\nabla\varphi(x_0)\cdot(x-x_0)+t\}$$

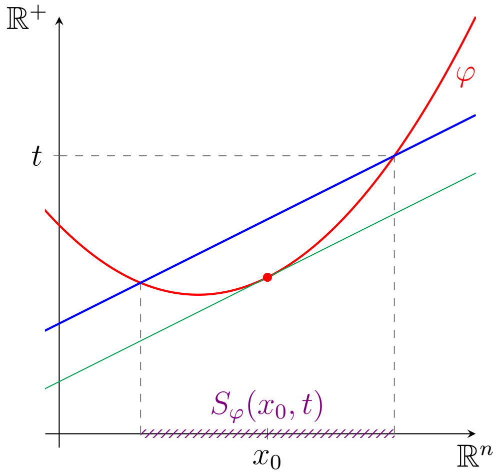


FIGURE 1. The sections of the convex function φ.

How do this sections behave? Let us consider the most classical case. Let

$$\varphi(x)=\frac{|x|^2}{2}=\frac{1}{2}\sum_{i=1}^n x_i^2.$$

Then $\nabla\varphi(x_0)=x_0$. Hence

$$S_\varphi(x_0,t)=\{x\in\mathbb{R}^n : \varphi(x)<\varphi(x_0)+\nabla\varphi(x_0)\cdot(x-x_0)+t\}$$

$$= \left\{ x \in \mathbb{R}^n : \frac{|x|^2}{2} < \frac{|x_0|^2}{2} + x_0 \cdot (x - x_0) + t \right\}$$
$$= \left\{ x \in \mathbb{R}^n : |x|^2 + |x_0|^2 - 2x_0 \cdot x < 2t \right\}$$
$$= \left\{ x \in \mathbb{R}^n : |x - x_0|^2 < 2t \right\}.$$

In other words, the section of φ at x_0 with height t is the Euclidean ball centered at x_0 with radius $\sqrt{2t}$. Also, $S_\varphi(x_0, t)$ is the d-ball centered at x_0 with radius t if d is the quasi-metric $d(x, y) = \frac{1}{2} |x - y|^2$ in $\mathbb{R}^n$.

An important fact regarding the application of Theorem 1.2 to the harmonic analysis setting for Monge-Ampère equation, is that some basic assumptions on a convex function φ imply that the family of sections of φ satisfy properties (a), (b), (c) and (d) in Theorem 1.2. So that there is a quasi-metric in $\mathbb{R}^n$ describing the sections as metric balls. See [**AFT98**].

1.4.3. Metrization of data affinities. Let X be a given set. Assume that an affinity kernel $\mathcal{K}$ is defined on the pairs of points in X. Precisely, suppose that

$$\mathcal{K} : X \times X \to \mathbb{R}^+$$

satisfies the following natural properties for a measure of the affinity of two data points in X:

(K1) $\mathcal{K}(x, x) = +\infty$;

(K2) $\mathcal{K}(x, y) = +\infty$, implies $x = y$;

(K3) $\mathcal{K}(x, y) = \mathcal{K}(y, x)$ for every $x, y \in X$;

(K4) there exists a constant $\gamma \in (0, 1)$ such that the inequalities $\mathcal{K}(x, y) > s$ and $\mathcal{K}(y, z) > s$ imply the inequality $\mathcal{K}(x, z) > \gamma s$, for every $s > 0$.

The kernel $\mathcal{K}$ has some natural properties of what we could expect to be a measure of affinity between data points in X. In particular, the only quantitative property of $\mathcal{K}$ is given by (K4) which has a simple interpretation. In fact, if the affinity between x and y is larger than s and the affinity between y and z is also larger than s, then the affinity between x and z is larger than a half of s (when $\gamma = 1/2$).

Assume, then, that X is given and $\mathcal{K}$ is an affinity kernel satisfying (K1) to (K4). Define the function

$$B : X \times \mathbb{R}^+ \to \mathcal{P}(X)$$

by

$$B(x,r)=\left\{y\in X:\mathcal{K}(x,y)>\frac{1}{r}\right\}.$$

Properties (a), (b) and (c) in Theorem 1.2 are easy to check. Property (d) holds with constant $c=\gamma^{-1}$. In fact, take $x,y\in X$ and $r>0$ with $x\in B(y,r)$, then for $z\in B(y,r)$ we have both $\mathcal{K}(x,y)>\frac{1}{r}$ and $\mathcal{K}(y,z)>\frac{1}{r}$. Hence, from (K4) we get that $\mathcal{K}(x,z)>\frac{\gamma}{r}$. In other words, $z\in B(x,\frac{r}{\gamma})$. This means that $B(y,r)\subseteq B(x,\frac{1}{\gamma}r)$. In a similar way we obtain (d.ii), $B(x,r)\subseteq B(y,\frac{1}{\gamma}r)$. So that (d) holds with $c=\frac{1}{\gamma}$. Applying Theorem 1.2 we obtain a quasi-metric d on X such that the family of d-balls is equivalent to the family B of the level sets of the affinity kernel $\mathcal{K}$.

1.5. Comments, problems and further results

(1) If (X,τ) is a topological space and $x\in X$, a subset V of X is said to be a neighborhood of x if there exists $A\in\tau$ such that $x\in A\subseteq V$. Set $\mathcal{N}_x$ to denote the family of all the neighborhoods of $x\in X$. Prove that
   - (a) if $U\in\mathcal{N}_x$, then $x\in U$;
   - (b) if $U\in\mathcal{N}_x$ and if $V\in\mathcal{N}_x$, then $U\cap V\in\mathcal{N}_x$;
   - (c) if $U\supset V$ and $V\in\mathcal{N}_x$, then $U\in\mathcal{N}_x$;
   - (d) if $U\in\mathcal{N}_x$ then, there exists $V\in\mathcal{N}_x$ with $V\subset U$ and $V\in\mathcal{N}_y$ for every $y\in V$.

(2) Let X be a set. Let $\mathcal{N}:x\to\mathcal{N}_x$ be a function assigning to each $x\in X$ a family of parts of X satisfying properties (a), (b) and (c) in (1) above. Prove that the family $\tau=\{U:U\in\mathcal{N}_x$ for every $x\in U\}$ is a topology on X. See the book of Kelley [**Kel62**].

(3) Let (X,d) be a quasi-metric space. Define

$$\mathcal{N}_x=\{U:B_d(x,r)\subset U\text{ for some }r>0\}$$

for every $x\in X$. Show that $\mathcal{N}_x$ satisfies properties (a), (b) and (c) in (1) above. Hence

$$\tau=\{U:\text{ for every }x\in U\text{ there exists }r>0\text{ with }B_d(x,r)\subset U\}$$

is a topology on X. Call this topology the quasi-metric topology on X.

(4) Prove that d-balls may not be open sets in the quasi-metric topology when d is a quasi-metric that is not a metric.

CHAPTER 2

Quasi-metrics in X and bands in $X \times X$

2.1. Introduction and basic facts

The robustness of the concept of quasi-metric with respect to the family of balls, considered in the previpus chapter, can also be witnessed from the properties of the diagonal bands in $X \times X$. We shall explore this approach in this chapter. By the way, we introduce some basic notation needed to face the metrization of quasi-metrics through the structures of uniform spaces, that we shall consider in forthcoming chapters. Here, instead of balls in X we consider families of relations on $X \times X$ that describe the behavior of metric bands. For the sake of completeness let us introduce the basic notation and definitions.

Let X be a set and let U and V be two subsets of $X \times X$. The composition is defined by

$$V \circ U = \{(x, z) \in X \times X : \text{ such that there exists } y \in X \text{ with } (x, y) \in U \text{ and } (y, z) \in V\}.$$

This definition is consistent with the composition of functions. With $\triangle$ we denote the diagonal of $X \times X$, i.e. $\triangle = \{(x, x) : x \in X\}$. For $U \subseteq X \times X$, U^{-1} is defined by $U^{-1} = \{(x, y) : (y, x) \in U\}$. A set U in $X \times X$ is said to be symmetric if $U^{-1} = U$.

For a given quasi-metric on X we shall provide some basic properties on the family of metric bands

$$V(r) = \{(x, y) \in X \times X : d(x, y) < r\}$$

in $X \times X$ that characterize the existence of a quasi-metric in X with metric bands equivalent to the given family.

2.2. Some properties of the family of quasi-metric bands on $X \times X$

Let (X, d) be a quasi-metric space with triangle constant K. For each $r > 0$ define

$$V_d(r) = \{(x, y) \in X \times X : d(x, y) < r\},$$

where V_d can be seen as a function from $\mathbb{R}^+$ to $\mathcal{P}(X \times X)$, the family of subsets of $X \times X$.

The next result contains some basic properties of the function V_d which in turn shall suffice to build a quasi-metric on X.

PROPOSITION 2.1. *Let (X, d) be a quasi-metric space with triangle constant equal to K. Let V_d be defined as before. Then*

(a) *each $V_d(r)$ is symmetric;*

(b) *$\triangle \subset V_d(r)$, for every $r > 0$;*

(c) *$V_d(r_1) \subseteq V_d(r_2)$, for $0 < r_1 < r_2$;*

(d) *$\bigcup_{r>0} V_d(r) = X \times X$;*

(e) *$\bigcap_{r>0} V_d(r) \subseteq \triangle$;*

(f) *$V_d(r) \circ V_d(r) \subseteq V_d(2Kr)$, for every $r > 0$.*

PROOF. Item (a) follows from the symmetry of d. Since $d(x, x) = 0$ for every x, we see that $\triangle \subset V_d(r)$ for every $r > 0$. Property (c) is clear. Since $d(x, y) < \infty$ for every $(x, y) \in X \times X$ we have (d). On the other hand, if (x, y) belongs to every $V_d(r)$ we have that $0 \leq d(x, y) < r$ for every $r > 0$. Hence $d(x, y) = 0$ and $x = y$. So that $(x, y) \in \triangle$, and we have (e). In order to prove (f), take $(x, z) \in V_d(r) \circ V_d(r)$, then there exists $y \in X$ such that $(x, y) \in V_d(r)$ and $(y, z) \in V_d(r)$. This means $d(x, y) < r$ and $d(y, z) < r$. From the triangle inequality for d we have

$$d(x, z) \leq K(d(x, y) + d(y, z)) < 2Kr.$$

In other words, $(x, z) \in V_d(2Kr)$ and we have (f). □

2.3. From bands to quasi-metrics

Properties (a) to (f) in Proposition 2.1, proved in the above section, for a general function $V : \mathbb{R}^+ \to \mathcal{P}(X \times X)$ are sufficient in order to have a quasi-metric in X such that the families $\{V(r) : r > 0\}$ and $\{V_d(r) : r > 0\}$ are "almost" the same. Let us precise the meaning of "almost" in this setting. Given two functions V_1 and V_2 defined in $\mathbb{R}^+$ with values in $\mathcal{P}(X \times X)$, we say that V_1 and V_2 are equivalent, and we write $V_1 \sim V_2$, if there exist constants $0 < \gamma \leq \Gamma < \infty$ such that

$$V_1(\gamma r) \subseteq V_2(r) \subseteq V_1(\Gamma r)$$

for every $r > 0$. The result of this section is the following statement.

THEOREM 2.2. *Let X be a set. Let $V : \mathbb{R}^+ \to \mathcal{P}(X \times X)$ satisfying*

(a) $V(r) = V^{-1}(r)$ *for every* $r > 0$*;*

(b) $\triangle \subset V(r)$ *for every* $r > 0$*;*

(c) V *is nondecreasing with respect to the usual orders in* $\mathbb{R}^+$ *and* $\mathcal{P}(X \times X)$*;*

(d) $X \times X = \bigcup_{r>0} V(r)$*;*

(e) $\triangle = \bigcap_{r>0} V(r)$*;*

(f) *there exists a positive constant* c *such that* $V(r) \circ V(r) \subseteq V(cr)$ *for every* $r > 0$.

Then, there exists a quasi-metric d *on* X *with constant for the triangle inequality bounded above by* c*, such that* $V \sim V_d$*. Where* $V_d(r) = \{(x, y) : d(x, y) < r\}$*.*

PROOF. Notice that from (d) we know that given any couple $(x, y) \in X \times X$ we have a positive r such that $(x, y) \in V(r)$. Hence $d(x, y) = \inf\{r > 0 : (x, y) \in V(r)\}$, is a well defined nonnegative function. The symmetry of d follows from (a). From (b), we have that $(x, x) \in V(r)$ for every $r > 0$. Hence $d(x, x) = 0$. On the other hand, if $d(x, y) = 0$ we have that $(x, y) \in V(r)$ for every $r > 0$. So that from (e) we have that $(x, y) \in \triangle$, which means $x = y$.

Let us check that d satisfies the triangle inequality. Take $x, y, z \in X$. For any given positive ε we have that there exist positive numbers r_1 and r_2 satisfying

(i) $r_1 < d(x, y) + \varepsilon$;

(ii) $(x, y) \in V(r_1)$;

(iii) $r_2 < d(y, z) + \varepsilon$;

(iv) $(y, z) \in V(r_2)$.

Set $r = \sup\{r_1, r_2\}$. Then from (c) and (f), $(x, z) \in V(r_2) \circ V(r_1) \subseteq V(r) \circ V(r) \subseteq V(cr)$. Hence

$$\begin{aligned} d(x, z) &\le cr \\ &\le c(r_1 + r_2) \\ &< c(d(x, y) + d(y, z)) + 2c\varepsilon, \end{aligned}$$

for every $\varepsilon > 0$. So that c is a triangle constant for d.

Let us finally check that $V_d \sim V$. In fact, from (c) we have that $V_d(r) \subseteq V(r)$ for every $r > 0$. On the other hand, given $(x, y) \in V(r)$ we have that $d(x, y) \le r < 2r$. Hence $V(r) \subseteq V_d(2r)$ for every $r > 0$. □

2.4. Applications and examples

2.4.1. Dyadic metrics and bands. Let $X=\mathbb{R}^+$. The family of dyadic intervals

$$\mathcal{D}=\{I_k^j=[k2^{-j},(k+1)2^{-j}):j\in\mathbb{Z},k\geq 0\}$$

is the disjoint union $\mathcal{D}=\bigcup_{j\in\mathbb{Z}}\mathcal{D}^j$, where $\mathcal{D}^j=\{I_k^j:k\geq 0\}$ are the dyadic intervals of level $j\in\mathbb{Z}$ and length 2^{-j}.

Given $I\in\mathcal{D}$ we write I^- and I^+ to denote the left and right halves of I, respectively. Hence $I=I^-\cup I^+$ with I^- and I^+ in $\mathcal{D}^{j+1}$ when $I\in\mathcal{D}^j$. For each $j\in\mathbb{Z}$ consider the following subset of $X\times X=\mathbb{R}_0^+\times\mathbb{R}_0^+$,

$$W_j=\bigcup_{I\in\mathcal{D}^j}\left[(I^-\times I^+)\cup(I^+\times I^-)\right].$$

The following figure depicts schematically the basic shapes of the sets W_j

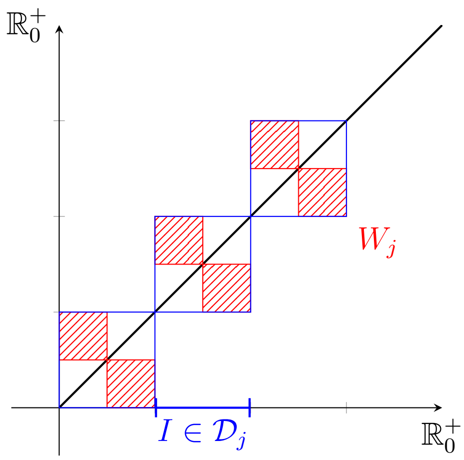


FIGURE 2. The set W_j.

Define $V:\mathbb{R}^+\to\mathcal{P}(\mathbb{R}_0^+\times\mathbb{R}_0^+)$ by

$$V(r)=\bigcup_{j\geq\left[\log\frac{1}{r}\right]}W_j.$$

We leave as an exercise to check that the function V satisfies properties (a) to (f) in Theorem 2.2. Moreover, the quasi-metric obtained is the same $\delta(x,y)$ given as an example in Section 1.4.1 of the previous chapter.

2.4.2. Affinity kernels. In this section we consider, as in Section 1.4.3, the problem of metrization of data sets on which we have a transitive kernel $\mathcal{K}$. Let us state the result of this sub-section.

PROPOSITION 2.3. *Let X be a set and $\mathcal{K} : X \times X \to \mathbb{R}^+ \cup \{+\infty\}$ be a symmetric kernel satisfying the following properties*

(K1) $\mathcal{K}(x, y) = \mathcal{K}(y, x)$, $x \in X$, $y \in X$;

(K2) $\mathcal{K}(x, y) = +\infty$ *if and only if* $x = y$;

(K3) *there exists* $0 < \nu < 1$ *such that* $\mathcal{K}(x, y) > \lambda$ *and* $\mathcal{K}(y, z) > \lambda$ *imply* $\mathcal{K}(x, z) > \nu\lambda$.

Then, there exist a quasi-metric d on X and a positive real number β such that $\mathcal{K}(x, y)$ has the Newtonian form

$$\mathcal{K}(x, y) \simeq \frac{1}{d^\beta(x, y)},$$

for every $x \in X$ and $y \in X$ in the sense that

$$\frac{1}{d^\beta(x, y)} \le \mathcal{K}(x, y) \le \frac{2^\beta}{d^\beta(x, y)}.$$

PROOF. Let $\alpha = \frac{\log 2}{\log \nu}$. Notice that $\alpha < 0$. Define

$$V(r) = \{(x, y) \in X \times X : \mathcal{K}(x, y) > r^{1/\alpha}\}.$$

The function V satisfies (a) to (f) in Theorem 2.2. Properties (a) to (e) are straightforward consequences of (K1) and (K2). Let us deal with the quantitative estimate (f). Take a couple $(x, z) \in V(r) \circ V(r)$. Let $y \in X$ be such that $(x, y) \in V(r)$ and $(y, z) \in V(r)$. Then $\mathcal{K}(x, y) > r^{1/\alpha}$ and $\mathcal{K}(y, z) > r^{1/\alpha}$. Hence, from (K3) we also have that

$$\mathcal{K}(x, z) > \nu r^{1/\alpha} = \nu r^{\frac{\log \nu}{\log 2}} = (2r)^{\frac{\log \nu}{\log 2}}.$$

In other words $(x, z) \in V(2r)$. Then, from Theorem 2.2, we have

$$d(x, y) = \inf\{r > 0 : (x, y) \in V(r)\}$$

is a quasi-metric on X with triangle constant bounded above by 2. And, for every $r > 0$

$$\{(x, y) : d(x, y) < r\} \subseteq V(r) \subseteq \{(x, y) : d(x, y) < 2r\},$$

which is equivalent to

$$\left\{(x, y) : d^{\frac{1}{\alpha}}(x, y) > s\right\} \subseteq \{(x, y) : \mathcal{K}(x, y) > s\} \subseteq \left\{(x, y) : d^{\frac{1}{\alpha}}(x, y) > 2^{\frac{1}{\alpha}} s\right\}$$

for every $s > 0$. Set $A(s) = \{(x,y) : d^{1/\alpha}(x,y) > s\}$, $B(s) = \{(x,y) : \mathcal{K}(x,y) > s\}$ and $C(s) = \{(x,y) : d^{1/\alpha}(x,y) > 2^{1/\alpha}s\}$. Then $A(s) \subseteq B(s) \subseteq C(s)$ for every $s > 0$. Hence with $s = \mathcal{K}(x,y)$ we have that $(x,y) \notin B(\mathcal{K}(x,y))$ then $(x,y) \notin A(\mathcal{K}(x,y))$, so $d^{1/\alpha}(x,y) \leq \mathcal{K}(x,y)$.

On the other hand, since $(x,y) \notin C\left(\frac{d^{1/\alpha}(x,y)}{2^{1/\alpha}}\right)$, we also have $(x,y) \notin B\left(\frac{d^{1/\alpha}(x,y)}{2^{1/\alpha}}\right)$, which means that $\mathcal{K}(x,y) \leq \frac{d^{1/\alpha}(x,y)}{2^{1/\alpha}}$. Hence

$$d^{\frac{1}{\alpha}}(x,y) \leq \mathcal{K}(x,y) \leq 2^{\frac{1}{|\alpha|}} d^{\frac{1}{\alpha}}(x,y),$$

for every $(x,y) \in X \times X$. These estimates are the desired with $\beta = -\frac{1}{\alpha} = \frac{\log \nu^{-1}}{\log 2}$. $\square$

2.5. Comments, problems and further results

(1) A family $\mathcal{U}$ of parts of $X \times X$ is said to be a uniform structure on X if
   (a) $\triangle \subset U$ for every $U \in \mathcal{U}$;
   (b) $U \in \mathcal{U}$ if and only if $U^{-1} \in \mathcal{U}$;
   (c) for each $U \in \mathcal{U}$ there exists $V \in \mathcal{U}$ such that $V \circ V \subseteq U$;
   (d) for U and V in $\mathcal{U}$, we have $U \cap V \in \mathcal{U}$;
   (e) for U in $\mathcal{U}$ and $V \supset U$ we have $V \in \mathcal{U}$.

   We also say that $(X,\mathcal{U})$ is a uniform space. Prove that

$$\tau = \{S \subset X : \text{ for every } x \in S \text{ there exists } U \in \mathcal{U} \text{ such that } U(x) \subset S\}$$

   is a topology on X, where $U(x) = \{y \in X : (x,y) \in U\}$ is the section of U at x.

(2) Let d be a quasi-distance on X. For each $r > 0$ define $V_r = \{(x,y) : d(x,y) < r\}$ and

$$\mathcal{U}_d = \{U \in \mathcal{P}(X \times X) : \text{ there exists } r > 0 \text{ with } V_r \subset U\}.$$

   Prove that $\mathcal{U}_d$ is a uniform structure on X. Prove that the d-balls centered at x provide a neighborhood basis for the topology τ_d induced by $\mathcal{U}_d$ on X. These neighborhoods are not necessarily τ_d-open sets.

(3) The introduction of the uniform structures and their metrization can be found in [**Kel62**]. Their use to produce metrics starts with the results in [**Fri37**]. We shall see in the next chapter the metrization of quasi-metrics whose pioneer contributions are given in [**Gus74**] and [**MS79**]. The approach provided in this chapter for the metrization of affinity kernels is contained in [**AG18a**].

CHAPTER 3

Metrization of quasi-metrics

3.1. Introduction

In this chapter we provide a metrization result for quasi-metric spaces, which can actually be extended to triangular inequalities of more general type than those considered in the previous chapters. The starting point for this approach is the basic remark contained in the following statement.

PROPOSITION 3.1. *Let (X, ρ) be a metric space. Then, for every choice of $x \in X$ and $y \in X$ we have that*

$$\rho(x, y) = \inf \left\{ \sum_{i=1}^{n} \rho(x_i, x_{i+1}) : x_1 = x, x_2, \ldots, x_n, x_{n+1} = y; n \in \mathbb{N} \right\}.$$

In other words $\rho(x, y)$ coincides with the infimum of the sums $\sum_{i=1}^{n} \rho(x_i, x_{i+1})$ over all chains of points joining x with y.

PROOF. If $x_1 = x, x_2, x_3, \ldots, x_n, x_{n+1} = y$ is any chain of points in X joining x with y, from the triangle inequality ($K = 1$) for ρ we have that $\rho(x, y) \leq \sum_{i=1}^{n} \rho(x_i, x_{i+1})$. Hence $\rho(x, y)$ is a lower bound for the set

$$\left\{ \sum_{i=1}^{n} \rho(x_i, x_{i+1}) : x_1 = x, x_2, \ldots, x_n, x_{n+1} = y; n \in \mathbb{N} \right\}.$$

On the other hand, clearly $\rho(x, y)$ belongs to this set. And we are done. □

With the above observation in mind we shall search for some positive real number less than one, that we denote by β, such that for a given quasi-metric d on X we have a non-trivial behavior of the infimum of the set

$$\left\{ \sum_{i=1}^{n} d^{\beta}(x_i, x_{i+1}) : x_1 = x, x_2, \ldots, x_n, x_{n+1} = y; n \in \mathbb{N} \right\}.$$

At this point some example helps to understand the role of the parameter β. Consider in $X = \mathbb{R}$, the quasi-distance $d(x, y) = |x - y|^2$. Take $0 < \beta < 1$, and assuming $y > x$, take $h = \frac{y-x}{n}$, $n \in \mathbb{N}$. Then for $x_i = x + (i-1)h$, $i = 1, 2, \dots, n+1$, we have

$$\sum_{i=1}^{n} d^{\beta}(x_i, x_{i+1}) = \sum_{i=1}^{n} \left(|x_i - x_{i+1}|^2\right)^{\beta} = \sum_{i=1}^{n} h^{2\beta} = n\left(\frac{y-x}{n}\right)^{2\beta} = n^{1-2\beta}(y-x)^{2\beta}.$$

Hence the infimum of $\left\{\sum_{i=1}^{n} |x_i - x_{i+1}|^{2\beta} : x_1, \dots, x_{n+1}; x_1 = x, x_{n+1} = y; n \in \mathbb{N}\right\}$ vanishes for $\beta > \frac{1}{2}$. Nevertheless for $\beta = \frac{1}{2}$ we recover the underlying metric structure on $X = \mathbb{R}$ given by $|x - y|$.

3.2. Metrization of quasi-metric

In this section we prove the following result.

THEOREM 3.2. *Let X be a set and let d be a quasi-distance on X with triangle constant equal to K. Then there exists a positive constant β less than or equal to one, depending only on K, such that the function*

$$\rho(x, y) = \inf\left\{\sum_{i=1}^{n} d^{\beta}(x_i, x_{i+1}) : x_1, x_2, \dots, x_{n+1}; x_1 = x, x_{n+1} = y; n \in \mathbb{N}\right\}$$

is a metric on X and $\rho^{1/\beta} \sim d$ in the sense that for $x \neq y$ in X,

$$0 < c_1 \leq \frac{\rho^{1/\beta}(x, y)}{d(x, y)} \leq c_2 < \infty$$

for some constants c_1 and c_2. Moreover, the constant β can be taken to be less than or equal to $\frac{\log 2}{\log 2K}$.

The proof of Theorem 3.2 will be a consequence of the next two lemmas.

LEMMA 3.3. *Let X be a set. Let g be a nonnegative symmetric function defined on $X \times X$ vanishing on the diagonal $\triangle$. Then the function*

$$\rho(x, y) = \inf \sum_{i=1}^{n} g(x_i, x_{i+1})$$

is a pseudo-metric bounded above by $g(x, y)$, where the infimum is taken over all finite chains $x = x_1, x_2, \dots, x_{n+1} = y$ joining x with y.

PROOF. Notice first that since $g(x, x) = 0$ we have that $\rho(x, x) = 0$ by taking the trivial chain joining x with x. The symmetry of ρ follows from the symmetry of g. Given $x, y, z \in X$ and $\varepsilon > 0$, take

$$x_1 = x, x_2, \dots, x_n, x_{n+1} = y$$

and

$$y_1 = y = x_{n+1}, y_2, \dots, y_m, y_{m+1} = z$$

such that

$$\sum_{i=1}^{n} g(x_i, x_{i+1}) < \rho(x, y) + \varepsilon$$

and

$$\sum_{j=1}^{m} g(y_j, y_{j+1}) < \rho(y, z) + \varepsilon.$$

Since $x = x_1, x_2, \dots, x_n, x_{n+1} = y = y_1, y_2, \dots, y_m, y_{m+1} = z$ is a chain joining x and z, we have

$$\begin{aligned}\rho(x, y) &\leq \sum_{i=1}^{n} g(x_i, x_{i+1}) + \sum_{j=1}^{m} g(y_j, y_{j+1}) \\ &< \rho(x, y) + \rho(y, z) + 2\varepsilon,\end{aligned}$$

for every positive ε. Hence $\rho(x, z) \leq \rho(x, y) + \rho(y, z)$. □

Corollary 3.4. *If d is quasi-distance in X and $\beta > 0$, then*

$$\rho(x, y) = \inf \left\{ \sum_{i=1}^{n} d^{\beta}(x_i, x_{i+1}) : x_1 = x, x_2, \dots, x_n, x_{n+1} = y; n \in \mathbb{N} \right\}$$

is a pseudo-metric on X.

The next result provides at once the remaining property that makes ρ a metric and the equivalence of d to a power of ρ.

Lemma 3.5. *Let (X, d) be a quasi-metric space with constant $K > 1$. Then, for every $0 < \beta \leq \frac{\log 2}{\log 2K}$ and every finite chain $x_1, x_2, \dots, x_{k+1}$ of points in X we have the inequality*

$$d^{\beta}(x_1, x_{k+1}) \leq 2 \sum_{i=1}^{k} d^{\beta}(x_i, x_{i+1}).$$

Let us, assuming Lemma 3.5, prove Theorem 3.2.

Proof of Theorem 3.2. From Corollary 3.4 we know that ρ is a pseudo-metric. From Lemma 3.5 we have

$$\frac{1}{2} d^{\beta}(x, y) \leq \rho(x, y).$$

So that, if $\rho(x, y) = 0$, then $d(x, y) = 0$ and, since d is quasi-metric on X we have that $x = y$ and ρ is a metric. On the other hand, since $\rho(x, y) \leq d^{\beta}(x, y)$ for every $x \in X$

and every $y \in X$, we have

$$\rho^{\frac{1}{\beta}}(x,y) \leq d(x,y) \leq 2^{\frac{1}{\beta}} \rho^{\frac{1}{\beta}}(x,y),$$

or, briefly $d \sim \rho^\alpha$, $\alpha \geq 1$. $\square$

Proof of Lemma 3.5. We shall proceed by induction on the length of the chain, in order to prove the inequality

$$d^\beta(x_1, x_{k+1}) \leq 2 \sum_{i=1}^{k-1} d^\beta(x_i, x_{i+1}). \tag{a}$$

Notice first that inequality (a) is trivial for $k = 2$. Now take n to be an integer larger than two and assume that (a) holds for every $k \leq n$. Let us prove

$$d^\beta(x_1, x_{n+1}) \leq 2 \sum_{i=1}^{n} d^\beta(x_i, x_{i+1}). \tag{b}$$

Notice that if $\sum_{i=1}^n d^\beta(x_i, x_{i+1}) = 0$, then all the x_i's are the same and the inequality is trivial. Assume then that

$$\lambda = \sum_{i=1}^n d^\beta(x_i, x_{i+1}) = \sum_{i=1}^n \Delta_i > 0.$$

With a geometric point of view, we may think that we have a partition of the interval $[0, \lambda]$ into n subintervals with lengths $\Delta_1, \Delta_2, \ldots, \Delta_n$. We need to consider the distribution of these intervals with respect to the middle point $\frac{\lambda}{2}$ of the interval $[0, \lambda]$. Let us plot the possible situations.

- First: $\Delta_1 = d^\beta(x_1, x_2) > \frac{\lambda}{2}$.

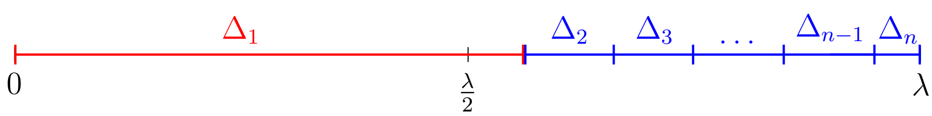


Figure 3. $\Delta_1 > \frac{\lambda}{2}$

- Second: $\sum_{i=1}^{n-1} \Delta_i \leq \frac{\lambda}{2}$.

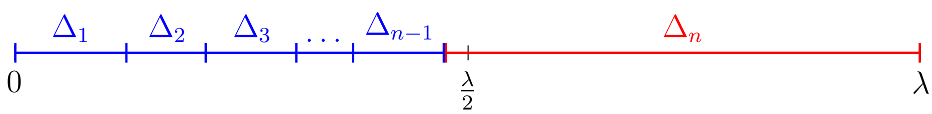


Figure 4. $\sum_{i=1}^{n-1} \Delta_i \leq \frac{\lambda}{2}$

- Third: there exists $k \in \{1, 2, \dots, n-2\}$ such that $\sum_{i=1}^{k} \Delta_i \le \frac{\lambda}{2}$ but $\sum_{i=1}^{k+1} \Delta_i > \frac{\lambda}{2}$.

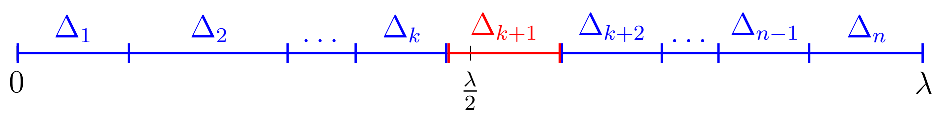


FIGURE 5. $\sum_{i=1}^{k} \Delta_i \le \frac{\lambda}{2}$ and $\sum_{i=1}^{k+1} \Delta_i > \frac{\lambda}{2}$ for some $k \in \{1, 2, \dots, n-2\}$.

Let us start proving (b) in the third case. Recall that we know (a) for every $k \le n$. In fact

$$\begin{aligned}
d^\beta(x_1, x_{n+1}) &\le \{2K \max\left[d(x_1, x_{k+1}), 2K \max(d(x_{k+1}, x_{k+2}), d(x_{k+2}, x_{n+1}))\right]\}^\beta \\
&= (4K^2)^\beta \max\left\{d^\beta(x_1, x_{k+1}), d^\beta(x_{k+1}, x_{k+2}), d^\beta(x_{k+2}, x_{n+1})\right\} \\
&\le (4K^2)^\beta \max\left\{2\sum_{i=1}^{k} \Delta_i, \Delta_{k+1}, 2\sum_{i=k+2}^{n} \Delta_i\right\} \\
&\le (4K^2)^\beta \max\left\{2\frac{\lambda}{2}, \lambda, 2\frac{\lambda}{2}\right\} \\
&\le (4K^2)^\beta \lambda \\
&\le 2\lambda
\end{aligned}$$

since $(4K^2)^\beta \le 2$.

For the first case we proceed in a similar way

$$\begin{aligned}
d^\beta(x_1, x_{n+1}) &\le \{2K \max\left[d(x_1, x_2), d(x_2, x_{n+1})\right]\}^\beta \\
&= (2K)^\beta \max\left[d^\beta(x_1, x_2), d^\beta(x_2, x_{n+1})\right] \\
&\le (2K)^\beta \max\left[\Delta_1, 2\sum_{i=2}^{n} \Delta_i\right] \\
&\le (2K)^\beta \lambda \\
&\le 2\lambda.
\end{aligned}$$

The second case is similar to the first one. And we are done. □

Theorem 3.2 has many important consequences. In particular we have that the quasi-metrization method developed in Chapters 1 and 2 also provide metrization methods. From the general point of view, we also obtain a natural topology on X induced by the quasi-metric d. In fact, there exist constants γ and Γ, positive and finite, such that

$$B_d(x,r) \subseteq B_\rho(x,\gamma r^\beta) \subseteq B_d(x,\Gamma r)$$

for every $r > 0$.

Notice also that the d-balls do not need to be open sets even when they are neighborhoods of their centers. The parameter $\beta > 0$ is relevant and its supremum could not be a maximum. Nevertheless the set of values of $\beta > 0$ that produces a metric ρ as in Theorem 3.2 is an interval with left end point 0.

3.3. Comments, problems and further results

(1) Let $X = \mathbb{R}^n$ and, for $x = (x_1, \dots, x_n)$ and $y = (y_1, \dots, y_n)$, set

$$d(x,y) = \sup\left\{|x_i - y_i|^{\gamma_i} : i = 1, 2, \dots, n\right\},$$

where $\gamma_i > 0$ for each $i \in \{1, \dots, n\}$.

(a) Show that d is a quasi-metric on X.

(b) Find the values of γ_i's such that d becomes a metric on X.

(c) Show that d is translation invariant.

(d) Find the values of $\beta > 0$ for which

$$\triangle_\beta(x,y) = \inf\left\{\sum_{i=1}^{m} d^\beta(x_i, x_{i+1}) : x = x_1, x_2, \dots, x_m, x_{m+1} = y; m \in \mathbb{N}\right\}$$

is identically 0.

(e) Find the values of β for which $\triangle_\beta$ above is not faithful, i.e. there exist x and y with $\triangle_\beta(x,y) = 0$ and $x \neq y$.

(f) For $\lambda > 0$ set

$$A_\lambda = \begin{pmatrix} \lambda^{1/\gamma_1} & 0 & \dots & 0 \\ 0 & \lambda^{1/\gamma_2} & \dots & 0 \\ \vdots & \vdots & \ddots & \vdots \\ 0 & 0 & \dots & \lambda^{1/\gamma_n} \end{pmatrix}$$

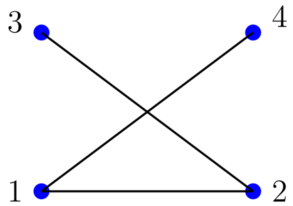
Compute $d(A_\lambda x, A_\lambda y)$ for every $\lambda > 0$ and every choice of x and y in $\mathbb{R}^n$.

(2) Let $X = \{1, 2, \dots, n\}$. Let A be a symmetric $n \times n$ matrix with entries that are only 0 or 1. Assume that the diagonal terms a_{ii} of A are all zero. Consider the

function $\rho : X \times X \to \mathbb{R}$ given by

$$\rho(i,j) = \inf \sum_{l=1}^{m} g(i_l, i_{l+1})$$

where $g(i,j) = a_{ij}$ and the infimum is taken on the family of all finite chains with $i_1 = i$ and $i_{m+1} = j$. When is ρ a metric on $\{1, \ldots, n\}$? Think of A as the adjacency matrix of a graph with vertices $X = \{1, 2, \ldots, n\}$. For instance, when $n = 4$, consider



$$\begin{pmatrix} 0 & 1 & 0 & 1 \\ 1 & 0 & 1 & 0 \\ 0 & 1 & 0 & 0 \\ 1 & 0 & 0 & 0 \end{pmatrix}$$

(3) The results of this chapter are a particular case of those in [**AIN98**]. The general situation is considered in the next chapter.

(4) Some interesting and deep extensions of this basic idea in this chapter can be found in [**PS09**] and in [**MMMM13**].

CHAPTER 4

Metrization of generalized quasi-metrics and generalized affinities

4.1. Introduction

This chapter is devoted to consider some extensions of the previous results when the quasi-triangular inequality or the transitivity of the affinities are nonlinear.

Let us briefly precise the above. Notice first that in metric space theory, a metric d on X is called an ultra-metric if the triangle inequality take the strictly stronger form

$$d(x,z) \leq \sup\{d(x,y), d(y,z)\}.$$

A particular example of ultra-metric is the dyadic metric

$$\delta(x,y) = \inf\{|I| : x, y \in I, I \in \mathcal{D}\},$$

with the notation given in Chapters 1 and 2. Nevertheless, most of the more used and well known metrics are not ultra-metrics. In the context of quasi-metric spaces instead, ultra-quasi-metrics are the same thing as quasi-metrics. In fact, if d is a quasi-metric with constant K, then, for $x, y, z \in X$,

$$d(x,z) \leq K(d(x,y) + d(y,z)) \leq 2K \sup\{d(x,y), d(y,z)\},$$

so that d is an ultra-quasi-metric with constant $\bar{K} = 2K$. On the other hand, if d is an ultra-quasi-metric with constant $\bar{K}$, then

$$d(x,z) \leq \bar{K} \sup\{d(x,y), d(y,z)\} \leq \bar{K}(d(x,y) + d(y,z))$$

and d is a quasi-metric with the same constant $\bar{K}$.

Hence, in this chapter we shall adopt the following equivalent form of the definition of quasi-metric space. Let X be a set. A nonnegative, symmetric function d on $X \times X$ satisfying $d(x,y) = 0$ if and only if $x = y$, is a quasi-metric if there exists a constant K such that $d(x,z) \leq K \sup\{d(x,y), d(y,z)\}$ holds for every $x, y, z \in X$. The right hand side in the triangle inequality above can be seen as a linear operation on $\sup\{d(x,y), d(y,z)\}$. In order to include some interesting nonlinear situations, we define η nonnegative, continuous and increasing defined on the nonnegative real numbers with $\eta(0) = 0$. A function d defined on $X \times X$ is called an η-quasi-metric if

(η-qm-i) $d(x, y) = d(y, x)$ for every x, $y \in X$;

(η-qm-ii) $d(x, y) = 0$ if and only if $x = y$;

(η-qm-iii) $d(x, z) \leq \eta(\sup\{d(x, y), d(y, z)\})$ for every x, y, $z \in X$.

Of course, when $\eta(t) = Kt$ we recover the case of quasi-metrics.

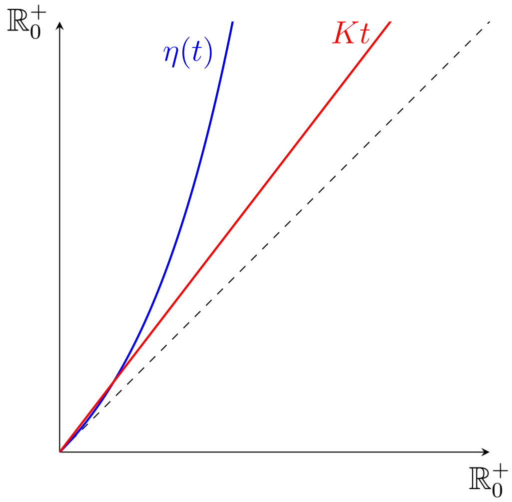


FIGURE 6. The function η.

On the other hand, when we are dealing with the idea underlying affinity of data in a data set X, we consider, as before in Section 1.4.3, affinity kernels $\mathcal{K}$ satisfying properties of type (K1), (K2), (K3) and (K4) in Section 1.4.3, with (K4) with a nonlinear control that is weaker, and hence more realistic than (K4) as stated in Chapter 1. Let us give the precise definition. Let ν be a continuous, concave, increasing and nonnegative function defined on $\mathbb{R}^+$ onto $\mathbb{R}^+$ such that $\nu(t) < t$ for every $t > 0$. Given a set X, a kernel $\mathcal{K} : X \times X \to \mathbb{R}^+ \cup \{+\infty\}$ is said to be a ν-affinity on X if

(ν-af-i) $\mathcal{K}(x, x) = +\infty$, for every $x \in X$;

(ν-af-ii) $\mathcal{K}(x, y) = +\infty$ implies $x = y$;

(ν-af-iii) $\mathcal{K}(x, y) = \mathcal{K}(y, x)$ for every $x \in X$, $y \in X$;

(ν-af-iv) if $\mathcal{K}(x, y) > \lambda$ and $\mathcal{K}(y, z) > \lambda$, then $\mathcal{K}(x, z) > \nu(\lambda)$.

Again, when $\nu(t) = \gamma t$ with $0 < \gamma < 1$ we recover the case introduced in Chapters 1 and 2.

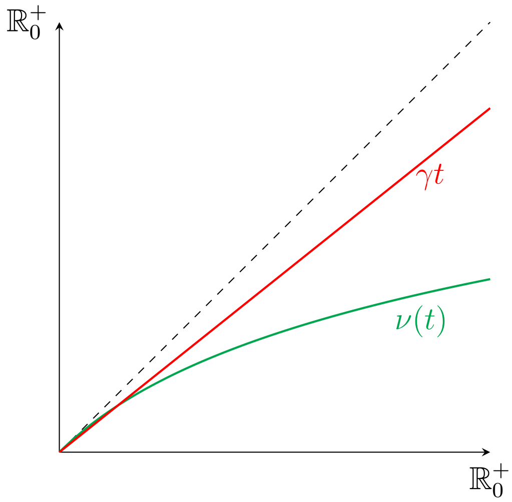


FIGURE 7. The function ν.

4.2. Solving some functional inequalities

In this section we consider some technical lemmas that shall be used on the metrization schemes developed in the next sections. The common theme of these result is the construction of solutions to some functional inequalities for positive functions defined on $\mathbb{R}^+$. To illustrate the idea behind the first result let us recall that we are trying to extend our metrization results to nonlinear controls on the triangle inequality. In the linear case we are dealing with the function $\eta(t) = Kt$ with K the triangle constant for the quasi-metric. In this case the functional equation

$$\psi \circ \eta \circ \eta = 2\psi$$

has a solution ψ of power form, $\psi(t) = t^\gamma$. In fact, for $t > 0$ we have

$$(\psi \circ \eta \circ \eta)(t) = (K^2 t)^\gamma = 2t^\gamma = 2\psi(t),$$

for $\gamma = \frac{\log 2}{2 \log K}$. Notice that when $K^2 > 2$ we have $0 < \gamma < 1$.

For our purposes, with more general convex functions η, we only need to solve inequalities of the form $\psi \circ \eta \circ \eta \leq 2\psi$. The next result provides some sufficient conditions for the existence of concave solutions ψ for this inequality.

LEMMA 4.1. *Let η be a continuous, increasing and convex function defined on $\mathbb{R}_0^+$ with $\eta(0) = 0$ and $\eta(t) > 2t$ for every $t > 0$. Then the functional inequality*

$$\psi \circ \eta \circ \eta \leq 2\psi$$

has at least one solution ψ which is increasing, continuous and concave with $\psi(0) = 0$ and $\psi(1) = 1$.

When dealing with the Newtonian structure of affinity kernels the linear case is given when for the transitivity condition we have a profile $\nu(t)$ of the form $\nu(t) = \delta t$ for some $0 < \delta < 1$. For M larger than one the functional equation

$$\psi \circ \nu = M\psi$$

has now a negative power solution ψ.

In fact, with $\psi(t) = t^\gamma$ we have $\psi \circ \nu(t) = (\delta t)^\gamma = Mt^\gamma$ when $\gamma = \frac{\log M}{\log \delta}$, which is negative. For our purposes we only need to find convex solutions for the inequality

$$\psi \circ \nu \leq M\psi$$

when ν is concave. The result is contained in the next statement.

Lemma 4.2. *Let ν be a concave, continuous, nonnegative and increasing function defined on $\mathbb{R}^+$ onto $\mathbb{R}^+$ such that $\nu(\lambda) < \lambda$ for every $\lambda > 0$. Then, given $M > 1$, there exists a continuous, decreasing and convex function ψ on $\mathbb{R}^+$ with $\psi(1) = 1$ satisfying the inequality*

$$\psi \circ \nu \leq M\psi.$$

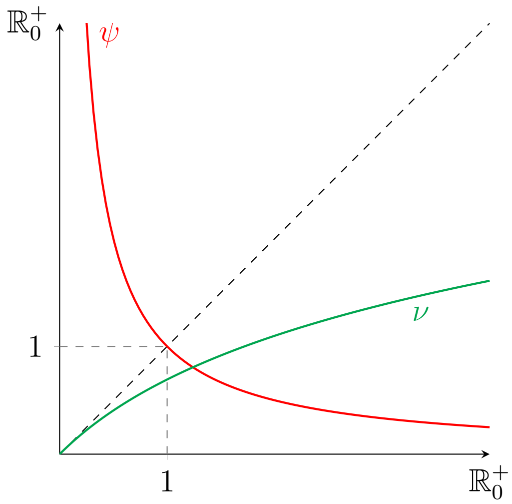


Figure 8. The functions ν and ψ.

Proof Lemma 4.1. Set $\widehat{\eta}$ to denote $\eta \circ \eta$. We need to solve the inequality $\psi \circ \widehat{\eta} \leq 2\psi$ with $\psi(1) = 1$. Notice that $\widehat{\eta}(t) \geq 4t$ for $t > 0$. Since η is one-to-one and onto, so is $\widehat{\eta}$, and $\widehat{\eta}^{-1}$ is well defined. Consider the following sequence of positive real numbers

$$\left\{\widehat{\eta}^{(k)}(1) : k \in \mathbb{Z}\right\}$$

with $\widehat{\eta}^{(1)} = \widehat{\eta}$, $\widehat{\eta}^{(0)}$ the identity, for$k \in \mathbb{Z}^+$, $\widehat{\eta}^{(k)} = \widehat{\eta} \circ \widehat{\eta}^{(k-1)}$, and $\widehat{\eta}^{(k)} = \widehat{\eta}^{(-1)} \circ \widehat{\eta}^{(k+1)}$ for $k \in \mathbb{Z}^-$ and $\widehat{\eta}^{(-1)} = \widehat{\eta}^{-1}$. Notice that $\{\widehat{\eta}^{(k)}(1)\}$ is increasing,

$$\lim_{k\to\infty} \widehat{\eta}^{(k)}(1) = +\infty, \quad \text{and} \lim_{k\to-\infty} \widehat{\eta}^{(k)}(1) = 0.$$

For notational simplicity, let us set $t_k = \widehat{\eta}^{(k)}(1)$, $k \in \mathbb{Z}$.

We proceed to define ψ as a piecewise linear function such that for every $k \in \mathbb{Z}$ satisfies $\psi(t_k) = 2^k$. Let us observe that on the sequence $\{t_k : k \in \mathbb{Z}\}$, ψ solves the equation $\psi \circ \widehat{\eta} = 2\psi$ with $\psi(1) = \psi(\widehat{\eta}^{(0)}(1)) = \psi(t_0) = 2^0 = 1$. Let us check the equation for each t_k,

$$\psi \circ \widehat{\eta}(t_k) = \psi(\widehat{\eta}(\widehat{\eta}^{(k)}(1))) = \psi(\widehat{\eta}^{(k+1)}(1)) = \psi(t_{k+1}) = 2^{k+1} = 2 \cdot 2^k = 2\psi(t_k).$$

Now define $\psi : \mathbb{R}^+ \to \mathbb{R}^+$ as the linear interpolation of the points $(t_k, \psi(t_k)) = (t_k, 2^k)$. Set $I_k = [t_k, t_{k+1}]$. Then, the slope of the line in I_k is given by

$$m_k = \frac{2^{k+1} - 2^k}{t_{k+1} - t_k} = \frac{2^k}{t_{k+1} - t_k}.$$

It is clear from the properties of ψ on the sequence $\{t_k : k \in \mathbb{Z}\}$ that the defined function $\psi : \mathbb{R}^+ \to \mathbb{R}^+$ is strictly increasing, one-to-one and onto $\mathbb{R}^+$. Moreover $\psi(1) = 1$. Hence it only remains to check the concavity of ψ and the inequality $(\psi \circ \widehat{\eta})(t) \leq 2\psi(t)$ for every $t > 0$.

Let us check that ψ is concave. In fact, the concavity is equivalent to the decreasingness of the slopes m_k. In other words, we have to check that $m_{k+1} \leq m_k$. This inequality is equivalent to

$$\frac{2^{k+1}}{t_{k+2} - t_{k+1}} \leq \frac{2^k}{t_{k+1} - t_k},$$

or

$$2(t_{k+1} - t_k) \leq t_{k+2} - t_{k+1},$$

or

$$3t_{k+1} \leq t_{k+2} + t_k.$$

Since $\widehat{\eta}(t) \geq 4t$, we have

$$3t_{k+1} < 4t_{k+1} \leq \widehat{\eta}(t_{k+1}) = t_{k+2} < t_{k+2} + t_k$$

and we are done.

Let us finally check that $(\psi \circ \widehat{\eta})(t) \leq 2\psi(t)$ for every $t > 0$. If $t = t_k$ for some $k \in \mathbb{Z}$ there is nothing to prove. Assume that $t \neq t_k$ for every $k \in \mathbb{Z}$. Let $k \in \mathbb{Z}$ such that $t_k < t < t_{k+1}$. Hence $t_{k+1} = \widehat{\eta}(t_k) < \widehat{\eta}(t) < \widehat{\eta}(t_{k+1}) = t_{k+2}$. Since $\widehat{\eta}$ is convex we have

$$\frac{\widehat{\eta}(t) - \widehat{\eta}(t_k)}{t - t_k} \leq \frac{\widehat{\eta}(t_{k+1}) - \widehat{\eta}(t_k)}{t_{k+1} - t_k} \tag{4.1}$$

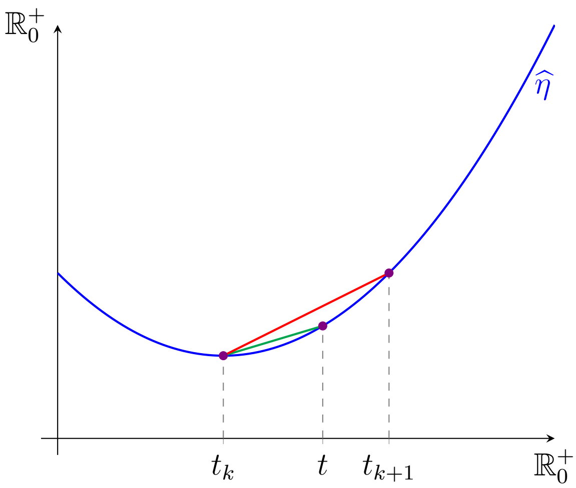


FIGURE 9. The monotonicity of the incremental quotient.

Now, from the definition of $\psi(t)$ we have

$$m_k = \frac{\psi(t) - 2^k}{t - t_k} \tag{4.2}$$

and

$$m_{k+1} = \frac{\psi(\widehat{\eta}(t)) - 2^{k+1}}{\widehat{\eta}(t) - t_{k+1}}. \tag{4.3}$$

Then, applying (4.3), the definition of m_{k+1}, (4.1) and (4.2) we obtain the desired inequality

$$\begin{aligned}
\psi(\widehat{\eta}(t)) &= m_{k+1}(\widehat{\eta}(t) - t_{k+1}) + 2^{k+1} \\
&= \frac{\widehat{\eta}(t) - t_{k+1}}{t_{k+2} - t_{k+1}} 2^{k+1} + 2^{k+1}
\end{aligned}$$

$$\begin{aligned}&\leq (t-t_k).\frac{t_{k+2}-t_{k+1}}{t_{k+1}-t_k}.\frac{2^{k+1}}{t_{k+2}-t_{k+1}}+2^{k+1}\\&=2(t-t_k)m_k+2^{k+1}\\&=2(\psi(t)-2^k)+2^{k+1}\\&=2\psi(t).\end{aligned}$$

□

Proof of Lemma 4.2. We proceed in a similar way as we did in the proof of Lemma 4.1. Let us start by defining a sequence $\{\lambda_k : k \in \mathbb{Z}\}$ in $\mathbb{R}^+$ by the following algorithm. Take $\lambda_0 = 1$, $\lambda_1 = \nu(1)$, $\lambda_{-1} = \nu^{-1}(1)$. Notice that since $\nu(\lambda) < \lambda$ for every $\lambda > 0$, we have

$$\lambda_1 = \nu(1) < 1 = \nu^{-1}(\nu(1)) < \nu^{-1}(1) = \lambda_{-1}.$$

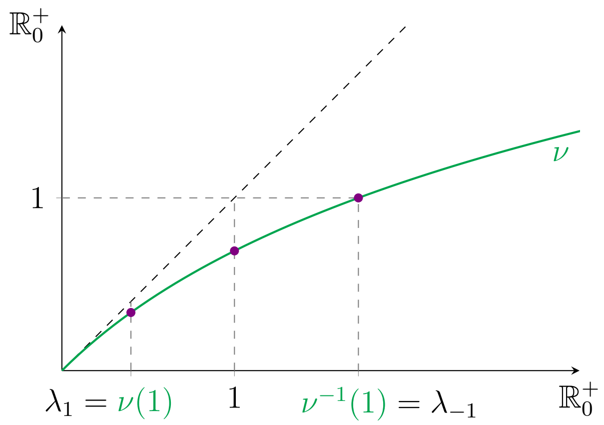


Figure 10. $\nu(1) < 1 < \nu^{-1}(1)$.

For $k \in \mathbb{N}$ define $\lambda_k = \nu(\lambda_{k-1})$ and $\lambda_{-k} = \nu^{-1}(\lambda_{-k+1})$. Hence the monotonicity $\lambda_k < \lambda_{k-1}$ holds for every $k \in \mathbb{Z}$. Moreover, $\lambda_k \to 0$ when $k \to \infty$ and $\lambda_k \to +\infty$ when $k \to -\infty$.

Now, let us proceed to define ψ on the points of the sequence $\{\lambda_k : k \in \mathbb{Z}\}$. Recall that we have a fixed $M > 1$ given in the statement. Set $\psi(\lambda_k) = M^k$. Then

$$(\psi \circ \nu)(\lambda_k) = \psi(\nu(\lambda_k)) = \psi(\lambda_{k+1}) = M^{k+1} = M\psi(\lambda_k),$$

hence, on the sequence $\{\lambda_k : k \in \mathbb{Z}\}$ we have solved the functional equation $\psi \circ \nu = M\psi$. Now, on the interval $[\lambda_{k+1}, \lambda_k]$ we define ψ by linear interpolation. For $\lambda_{k+1} < \lambda < \lambda_k$ we have

$$\frac{M^{k+1}-M^k}{\lambda_k-\lambda_{k+1}}=\frac{M^{k+1}-\psi(\lambda)}{\lambda-\lambda_{k+1}}.$$

Also, since $\lambda_{k+2}=\nu(\lambda_{k+1})<\nu(\lambda)<\nu(\lambda_k)=\lambda_{k+1}$,

$$\frac{M^{k+2}-M^{k+1}}{\lambda_{k+1}-\lambda_{k+2}}=\frac{M^{k+2}-\psi(\nu(\lambda))}{\nu(\lambda)-\lambda_{k+2}}.$$

Hence, we have the two following formulas, the first for $\psi(\lambda)$ and the second for $(\psi\circ\nu)(\lambda)$,

$$\psi(\lambda)=M^{k+1}-M^k(M-1)\frac{\lambda-\lambda_{k+1}}{\lambda_k-\lambda_{k+1}} \tag{4.4}$$

and

(4.5)

$$\psi(\nu(\lambda))=M^{k+2}-M^{k+1}(M-1)\frac{\nu(\lambda)-\lambda_{k+2}}{\lambda_{k+1}-\lambda_{k+2}}=M\left(M^{k+1}-M^k(M-1)\frac{\nu(\lambda)-\lambda_{k+2}}{\lambda_{k+1}-\lambda_{k+2}}\right).$$

Since ν is concave we have

$$\frac{\nu(\lambda)-\nu(\lambda_{k+1})}{\lambda-\lambda_{k+1}}\geq\frac{\nu(\lambda_k)-\nu(\lambda_{k+1})}{\lambda_k-\lambda_{k+1}}.$$

In other words

$$\frac{\nu(\lambda)-\lambda_{k+2}}{\lambda_{k+1}-\lambda_{k+2}}\geq\frac{\lambda-\lambda_{k+1}}{\lambda_k-\lambda_{k+1}},$$

which with (4.4) and (4.5) proves that

$$(\psi\circ\nu)(\lambda)\leq M\psi(\lambda),$$

as desired.

Let us finally check the convexity of ψ. Since ν is concave, we have that for every $0\leq\theta\leq 1$ and every $s,\, t\in\mathbb{R}^+$,

$$\nu(\theta s+(1-\theta)t)\geq\theta\nu(s)+(1-\theta)\nu(t).$$

Hence, for $0<s<u<t$ we have

$$\begin{aligned}\frac{\nu(t)-\nu(u)}{\nu(t)-\nu(s)}&=\frac{\nu(t)-\nu\left(s+\frac{u-s}{t-s}(t-s)\right)}{\nu(t)-\nu(s)}\\&=\frac{\nu(t)-\nu\left((\frac{u-s}{t-s})t+(1-\frac{u-s}{t-s})s\right)}{\nu(t)-\nu(s)}\\&\leq\frac{\nu(t)-(\frac{u-s}{t-s})\nu(t)-(\frac{t-u}{t-s})\nu(s)}{\nu(t)-\nu(s)}\end{aligned}$$

$$= \frac{t-u}{t-s}.$$

Then,

$$\frac{\nu(t)-\nu(u)}{t-u} \leq \frac{\nu(t)-\nu(s)}{t-s}.$$

Since $\nu(0)=0$ and $\nu(t)<t$ we have

$$\frac{\nu(t)-\nu(u)}{t-u} \leq \frac{\nu(t)-\nu(0)}{t-0} < 1$$

for every $0<u<t$. In order to prove the convexity of ψ we only need to check that

$$\frac{M^k-M^{k-1}}{\lambda_{k-1}-\lambda_k} \leq \frac{M^{k+1}-M^k}{\lambda_k-\lambda_{k+1}},$$

or that

$$\frac{\lambda_k-\lambda_{k+1}}{\lambda_{k-1}-\lambda_k} \leq \frac{M^k(M-1)}{M^{k-1}(M-1)} = M.$$

Since

$$\frac{\lambda_k-\lambda_{k+1}}{\lambda_{k-1}-\lambda_k} = \frac{\nu(\lambda_{k-1})-\nu(\lambda_k)}{\lambda_{k-1}-\lambda_k} < 1,$$

we are done, because $M>1$. □

4.3. Metrization of η-quasi-metric spaces

In the introduction above we have defined an η-quasi-metric on a set X for η continuous, increasing, convex with $\eta(0)=0$ by the three basic properties:

(η-1) $d(x,y)=d(y,x)$, x, $y\in X$;

(η-2) $d(x,y)=0$ if and only if $x=y$;

(η-3) $d(x,z)\leq \eta(\sup\{d(x,y),d(y,z)\})$ for every x, y, $z\in X$.

With the ideas of Chapter 3 and Lemma 4.1 from the previous section, we have that every η-quasi-metric is equivalent to a convex function of a metric in the sense explicitly described in the next statement.

Theorem 4.3. *Let η be a nonnegative, continuous, increasing and continuous function defined on the nonnegative real numbers such that $\eta(t)>2t$ and $\psi(0)=0$. Let X be a set and let d be an η-quasi-metric on X. Then for every ψ continuous, increasing and concave solution of the inequality*

$$\psi\circ\eta\circ\eta \leq 2\psi$$

with $\psi(1)=1$ and $\psi(0)=0$, we have

(a) $\rho(x,y) = \inf\{\sum_{i=1}^{n} \psi(d(x_i, x_{i+1})) : x_1 = x, \dots, x_{n+1} = y; n \geq 1\}$ *is a metric on* X*;*

(b) $\psi^{-1} \circ \rho \leq d \leq \psi^{-1} \circ (2\rho)$.

Proof. The proof of (a) follows the lines of Theorem 3.2. Notice first of all that, from Lemma 3.3 we have that ρ is a pseudo-metric on X such that $\rho \leq \psi \circ d$. Which is equivalent to the first inequality $\psi^{-1} \circ \rho \leq d$ in (b). Hence if we prove the second inequality in (b), which is equivalent to

$$\psi \circ d \leq 2\rho,$$

we are done since this inequality also implies the reliability of ρ. In fact, $\rho(x,y) = 0$ implies $\psi(d(x,y)) = 0$ and $d(x,y) = 0$. So that $x = y$. On the other hand, the proof of the inequality $\psi \circ d \leq 2\rho$ follows the lines of those in Lemma 3.5, using here the fact that $\psi \circ \eta \circ \eta \leq 2\psi$ by Lemma 4.1. We have to show that for any $k \geq 1$ and any chain $x_1, x_2, \dots, x_k$ of points in X we have

$$\psi(d(x_1, x_k)) \leq 2 \sum_{i=1}^{k-1} \psi(d(x_i, x_{i+1})). \tag{4.6}$$

We proceed inductively on k. For $k = 2$ the inequality is trivial. In general, we assume that (4.6) holds for every $k \leq n$. Let us prove it for $k = n + 1$. To prove that $\psi(d(x_1, x_{n+1})) \leq 2\sum_{i=1}^{n} \psi(d(x_i, x_{i+1}))$ we proceed as in Lemma 3.5. Now, with the geometric pictures used there, we now have $\Delta_i = \psi(d(x_i, x_{i+1})) > 0$. Doing so we get three possible cases with $\lambda = \sum_{i=1}^{n} \psi(d(x_i, x_{i+1}))$,

- $\Delta_1 = \psi(d(x_1, x_2)) > \frac{\lambda}{2}$;
- $\sum_{i=1}^{n-1} \Delta_i \leq \frac{\lambda}{2}$;
- there exists $k \in \{1, 2, \dots, n-2\}$ such that $\sum_{i=1}^{k} \Delta_i \leq \frac{\lambda}{2}$ and $\sum_{i=1}^{k+1} \Delta_i > \frac{\lambda}{2}$.

In the first case we have, using the inductive hypothesis, that

$$\begin{aligned}
\psi(d(x_1, x_{n+1})) &\leq \psi(\eta(\sup\{d(x_1, x_2), d(x_2, x_{n+1})\})) \\
&\leq (\psi \circ \eta \circ \eta)(\sup\{d(x_1, x_2), d(x_2, x_{n+1})\})) \\
&\leq 2\psi(\sup\{d(x_1, x_2), d(x_2, x_{n+1})\})) \\
&\leq 2\sup\{\psi(d(x_1, x_2)), \psi(d(x_2, x_{n+1}))\} \\
&\leq \sup\{\lambda, 2\sum_{i=1}^{n} \psi(d(x_i, x_{i+1}))\}
\end{aligned}$$

$$< 2\lambda.$$

The second case is similar to the first one. Let us check that the desired estimate holds also in the third case. Notice that in this case we have that $\sum_{i=k+2}^{n} \Delta_i \le \frac{\lambda}{2}$, since

$$\lambda = \sum_{i=1}^{n} \Delta_i = \sum_{i=1}^{k+1} \Delta_i + \sum_{i=k+2}^{n} \Delta_i > \frac{\lambda}{2} + \sum_{i=k+2}^{n} \Delta_i.$$

Hence we can apply two times the triangle inequality using $d(x_1, x_{k+1})$, $d(x_{k+1}, x_{k+2})$ and $d(x_{k+2}, x_{n+1})$, and we get

$$\begin{aligned}
&\psi(d(x_1, x_{n+1})) \le (\psi \circ \eta \circ \eta)(\max\{d(x_1, x_{k+1}), d(x_{k+1}, x_{k+2}), d(x_{k+2}, x_{n+1})\}) \\
&= \left(\psi \circ \eta \circ \eta \circ \psi^{-1}\right)(\max\{\psi(d(x_1, x_{k+1})), \psi(d(x_{k+1}, x_{k+2})), \psi(d(x_{k+2}, x_{n+1}))\}) \\
&\le \left(\psi \circ \eta \circ \eta \circ \psi^{-1}\right)\left(\max\left\{2\sum_{i=1}^{k} \psi(d(x_i, x_{i+1})), \psi(d(x_{k+1}, x_{k+2})), 2\sum_{i=k+2}^{n} \psi(d(x_i, x_{i+1}))\right\}\right) \\
&\le \left(\psi \circ \eta \circ \eta \circ \psi^{-1}\right)(\lambda) = (\psi \circ \eta \circ \eta)(\psi^{-1}(\lambda)) \\
&\le 2\psi(\psi^{-1}(\lambda)) = 2\lambda.
\end{aligned}$$

In the last inequality we used Lemma 4.1. So that $\psi \circ d \le 2\rho$ and the theorem is proved. $\square$

4.4. Metrization of ν-affinities

In this section we aim to use Lemma 4.2 in order to prove the Newtonian structure of affinity kernel with a nonlinear control on the transitive property. The basic context is the following. Let X be a set. A kernel $\mathcal{K} : X \times X \to \mathbb{R}^+ \cup \{+\infty\}$ is said to be a ν-affinity kernel, with ν concave, continuous, increasing, nonnegative onto $\mathbb{R}^+$ with $\nu(\lambda) < \lambda$ for $\lambda > 0$, if

(1) $\mathcal{K}(x, y) = +\infty$ if and only if $x = y$;
(2) $\mathcal{K}(x, y) = \mathcal{K}(y, x)$ for every $x \in X$ and $y \in X$;
(3) if $\mathcal{K}(x, y) > \lambda$ and $\mathcal{K}(y, z) > \lambda$, then $\mathcal{K}(x, z) > \nu(\lambda)$.

Theorem 4.4. *Let X be a set. Let $\mathcal{K}$ be a ν-affinity kernel on $X \times X$. Then, there exist a continuous, decreasing and convex function ψ on $\mathbb{R}^+$ with $\psi(1) = 1$, and a quasi-metric d on X such that*

$$\mathcal{K} \simeq \psi \circ d$$

with constants that shall explicitly be given in the proof.

Proof. Let ψ be the function provided by Lemma 4.2 associated to the control ν on the quantitative transitive property given in the definition of ν-affinity, with $M = 2$. Define $V : \mathbb{R}^+ \to \mathcal{P}(X \times X)$ by

$$V(r) = \{(x, y) \in X \times X : \mathcal{K}(x, y) > \psi^{-1}(r)\}.$$

Let us check that this function satisfies properties (a) to (f) from Theorem 2.2 of Chapter 2. Property (a) is the symmetry of each $V(r)$, which is clear, since $\mathcal{K}$ itself is symmetric. Property (b) holds because $\mathcal{K}(x, x) = +\infty$ for every $x \in X$. To prove property (c) take $0 < r_1 < r_2$, since ψ^{-1} is decreasing, we have that $\psi^{-1}(r_1) > \psi^{-1}(r_2)$. Hence if $\mathcal{K}(x, y) > \psi^{-1}(r_1)$ then $\psi^{-1}(r_2) < \mathcal{K}(x, y)$ and $(x, y) \in V(r_2)$. Since ψ is onto $\mathbb{R}^+$ we have (d). Property (e) follows from the fact that $\mathcal{K}(x, y) = +\infty$ implies $x = y$. Let us check that property (f) in Theorem 2.2 holds with $c = 2$. In fact, for $r > 0$, we have

$$\begin{aligned}
V(r) \circ V(r) &= \{(x, z) : (x, y) \in V(r) \text{ and } (y, z) \in V(r) \text{ for some } y \in X\} \\
&\subseteq \{(x, z) : \mathcal{K}(x, y) > \psi^{-1}(r) \text{ and } \mathcal{K}(y, z) > \psi^{-1}(r) \text{ for some } y \in X\} \\
&\subseteq \{(x, z) : \mathcal{K}(x, z) > \nu(\psi^{-1}(r))\} \\
&= \{(x, z) : \psi(\mathcal{K}(x, z)) < (\psi \circ \nu)(\psi^{-1}(r))\} \\
&\subseteq \{(x, z) : \psi(\mathcal{K}(x, z)) < 2\psi(\psi^{-1}(r))\} \\
&= \{(x, z) : \mathcal{K}(x, z) > \psi^{-1}(2r)\} \\
&= V(2r).
\end{aligned}$$

Then, applying Theorem 2.2 we have a quasi-metric d on $X \times X$ such that

$$V_d(r) \subseteq V(r) \subseteq V_d(2r).$$

Hence $\mathcal{K}(x, y) \simeq \psi^{-1}(d(x, y))$. □

4.5. Comments, problems and further results

(1) Show that the function $\eta : \mathbb{R}_0^+ \to \mathbb{R}_0^+$ given by $\eta(t) = 3(e^t - 1)$ satisfies the hypotheses of Lemma 4.1 What can we say about the growth at infinity of the function ψ provided by Lemma 4.1?

(2) Let $\nu(t) = \log(t+1)$, $t > 0$. Show that ν satisfies the hypotheses of Lemma 4.2. What can we say about the growth at zero of the function ψ provided by Lemma 4.2?

(3) Let $\alpha \in (0, 1]$ and $\psi(t) = t^{-\alpha}$, $t > 0$. Let (X, d) be a metric space and

$$\mathcal{K}(x, y) = \psi(d(x, y)).$$

Then $\mathcal{K}$ satisfies property (3) in Section 4.4, with $\nu(\lambda) = \frac{\lambda}{2}$. What if d is a quasi-metric? What if $\alpha > 1$?

(4) Some of the results of this chapter are contained in [**AIN98**] and [**AG18a**].

CHAPTER 5

An algorithm based on Frink's Lemma for the metrization of weighted undirected graphs

In this chapter we look at Frink's metrization of uniformities with countable bases, from an algorithmic point of view that can help to obtain some natural metrics on weighted undirected graphs. And, as far as possible, to compute those metrics or to build their families of balls. These metric structures on a graph allow the introduction of analytical tools like filtering of signals on nonconvolutional settings. In the first section we introduce Frink's Lemma as stated and proved in the book of Kelley [**Kel62**]. Then we introduce the basic algorithm proving the main properties needed to make it work.

5.1. The basic Frink's Lemma

With the notation introduced in Chapter 2, we have the following result that was first used to show the metrizability of uniform spaces with countable bases.

LEMMA 5.1. *Let X be a set. Let $\{U_m : m = 0, 1, \ldots\}$ be a sequence of subsets of $X \times X$ that satisfy the following properties.*

(i) $U_0 = X \times X$*;*
(ii) $U_n = U_n^{-1}$ *for every* n*;*
(iii) $\triangle \subset U_n$ *for every* n*;*
(iv) $U_{n+1} \circ U_{n+1} \circ U_{n+1} \subseteq U_n$ *for every* n*.*

Then, there exists a pseudo-metric d defined on X such that for every $n = 1, 2, 3, \ldots$

$$U_n \subseteq \{(x, y) \in X \times X : d(x, y) \leq 2^{-n}\} \subseteq U_{n-1}.$$

PROOF. Set $g : X \times X \to \mathbb{R}_0^+$ to denote the function given by $g(x, y) = 0$ if and only if $(x, y) \in \cap_{n \geq 0} U_n$, and $g(x, y) = 2^{-n}$ for $(x, y) \in U_n \setminus U_{n+1}$. Now, as we did in previous chapters, define

$$d(x, y) = \inf \left\{ \sum_{i=1}^{n} g(x_i, x_{i+1}) : x = x_1, x_2, \ldots, x_n, x_{n+1} = y; n \in \mathbb{N} \right\}.$$

Hence $d(x,y)$ is a pseudo-metric on X by Lemma 3.3. Moreover, $d(x,y) \leq g(x,y)$ for every $(x,y) \in X \times X$. Thus if $(x,y) \in U_n$, we have that $g(x,y) \leq 2^{-n}$, so that $d(x,y) \leq 2^{-n}$ and we have the first inclusion in the statement.

On the other hand, if we prove that for every n and every chain joining x_0 with x_{n+1} we have

$$g(x_0, x_{n+1}) \leq 2 \sum_{i=0}^{n} g(x_i, x_{i+1}), \tag{5.1}$$

then $d(x,y) \leq 2^{-n}$ implies $g(x,y) \leq 2^{-n+1}$, hence $(x,y) \in U_{n-1}$. So that we get the second inclusion $\{d(x,y) \leq 2^{-n}\} \subseteq U_{n-1}$.

Now, (5.1) follows from property (iv) as we did before in the previous chapter. In fact, proceeding by induction on the length n of the chain and assuming that

$$g(x_0, x_{n+1}) \leq 2 \sum_{i=0}^{k} g(x_i, x_{i+1}),$$

holds for $k = 0, 1, \ldots, n-1$, let us prove it for $k = n$.

Set $\lambda = \sum_{i=1}^{n} g(x_i, x_{i+1})$. Take k the largest integer such that $\sum_{i=0}^{k-1} g(x_i, x_{i+1}) \leq \frac{\lambda}{2}$. Then $g(x_0, x_k) \leq 2\frac{\lambda}{2} = \lambda$, $g(x_k, x_{k+1}) \leq \lambda$ and $g(x_{k+1}, x_{n+1}) \leq 2\frac{\lambda}{2} = \lambda$. Let m be the smallest integer such that $2^{-m} \leq \lambda$, then we have that $(x_0, x_k) \in U_m$, $(x_k, x_{k+1}) \in U_m$ and $(x_{k+1}, x_{n+1}) \in U_m$. So that, from (iv), $(x_0, x_{n+1}) \in U_{m-1}$. Hence

$$g(x_0, x_{n+1}) \leq 2^{-m+1} = 2 \cdot 2^{-m} \leq 2\lambda,$$

as desired. □

5.2. Composition of subsets of $X \times X$ and matrix multiplication in the finite case

Let n be a large positive integer. Let $X = \{1, 2, \ldots, n\}$ be the set of the n first positive integers. Let U and V be two nonempty subsets of $X \times X$. As before, the composition of U and V is given by

$$V \circ U = \{(i,k) : \text{ there exists } j \in \{1, 2, \ldots, n\} \text{ such that } (i,j) \in U \text{ and } (j,k) \in V\}.$$

We shall also write $V^{(m)}$ to denote the composition of V m-times, for $m \geq 1$. Given a set $V \subset X \times X$, set A_V to denote the indicator $n \times n$ matrix of the set $V \subset X \times X$.

Precisely, if $A_V = (a_{ij}(V))$, then

$$a_{ij}(V) = \begin{cases} 1, & \text{if } (i,j) \in V \\ 0, & \text{if } (i,j) \notin V. \end{cases}$$

PROPOSITION 5.2. *With the notation introduced above, we have*

(a) *given U and V two subsets of $X \times X$, then $V \circ U$ is given by the locations of the nonvanishing entries of the product matrix $A_U A_V$;*

(b) *if V is a subset of $X \times X$ containing the three main diagonals of $X \times X$, i.e.*

$$\{(i,j) \in X \times X : |i-j| \leq 1\} \subset V,$$

then there exists an integer m such that every entry of the matrix $(A_V)^{(m)}$ is positive;

(c) *for V and m as in (b) we have that $V^{(m)} = V \circ V \circ \cdots \circ V$ m times coincides with $X \times X = \{1, 2, \ldots, n\}^2$.*

PROOF.

(a) Set $(a_{ij}(U)) = A_U$, $(a_{ij}(V)) = A_V$ and $(p_{ij}) = A_U A_V$. Recall that $a_{ij} = 1$ if $(i,j) \in U$ and $a_{ij}(U) = 0$ if $(i,j) \notin U$. Also $a_{ij}(V) = 1$ for $(i,j) \in V$ and $a_{ij}(V) = 0$ when $(i,j) \notin V$. Since $p_{ij} = \sum_{k=1}^n a_{ik}(U)a_{kj}(V) > 0$ is equivalent to the existence of $k \in \{1, \ldots, n\}$ such that $a_{ik}(U) = 1$ and $a_{kj}(V) = 1$, we have that $p_{ij} > 0$ if and only if $(i,k) \in U$ and $(k,j) \in V$. So that $p_{ij} > 0$ if and only if $(i,j) = V \circ U$ and (a) is proved.

(b) Let (a_{ij}) be the entries of A_V. Then $a_{ij} > 0$ for $|i-j| \leq 1$. Set (a_{ij}^l) to denote the entries of $A_V^{(l)}$. Then $a_{ij}^l > 0$ for $|i-j| \leq l$. Let us prove it by induction on l.

For $l = 2$, we have

$$a_{i,i+2}^2 = \sum_{k=1}^n a_{ik}a_{k,i+2} \geq a_{i,i+1}a_{i+1,i+2} > 0.$$

Also $a_{i+2,i}^2 > 0$, $a_{ii}^2 > 0$, $a_{i+1,i}^2 > 0$ and $a_{i,i+1}^2 > 0$.

Assume that $a_{ij}^l > 0$ for every $|i-j| \leq l$. Take now (i,j) with $|i-j| \leq l+1$. If $|i-j| < l+1$ we have $a_{ij}^{l+1} = \sum_{k=1}^n a_{ik}^l a_{kj} \geq a_{ij}^l a_{jj} > 0$ from the inductive hypothesis because $|i-j| \leq l$. If $|i-j| = l+1$ we have that $i = j+l+1$

or $i = j - l - 1$. Let us consider only the first case,

$$a_{ij}^{l+1} = a_{j+l+1,j}^{l+1} = \sum_{k=1}^{n} a_{j+l+1,k}^{l} a_{kj} \geq a_{j+l+1,j+1}^{l} a_{j+1,j} > 0,$$

because $|(j+l+1)-(j+1)| = l$ and the induction hypothesis. With $l = n-1$ we have that all the entries of $(A_V)^{(n-1)}$ are positive.

(c) From (a) we have that $V^{(m)}$ is the set of indices of nonvanishing entries of $(A_V)^{(m)}$ which, from (b), coincides with the whole set $\{1, 2, \dots, n\}^2$. □

5.3. Affinity kernels and Frink's Lemma

In the next lemma we obtain a sequence of levels for an affinity kernel on a set X in such way that the corresponding level sets satisfy the hypothesis of Frink's Lemma proved in Section 5.1.

Lemma 5.3. *Let X be a set and let $\mathcal{K}$ be a positive symmetric function defined on $X \times X$ such that*

(i) $\mathcal{K}(x,x) = \sup_{y \in X} \mathcal{K}(x,y)$ *for every* $x \in X$*;*

(ii) $\Lambda_\infty = \sup\{\alpha > 0 : \{\mathcal{K} > \alpha\}^{(m)} = X \times X$ *for some positive integer* $m\} > 0$.

Then, for every $0 < \Lambda < \Lambda_\infty$ *there exists a finite sequence*

$$0 = \lambda(0) < \lambda(1) < \cdots < \lambda(k) = \Lambda$$

such that $\{\mathcal{K} > \lambda(i)\}^{(3)} \subseteq \{\mathcal{K} > \lambda(i-1)\}$*, for every* $i = 1, 2, \dots, k$ *and* $\triangle \subset \{\mathcal{K} > \lambda(i)\}$ *for every* $i = 0, 1, 2, \dots, k$.

Proof. Let us start with two basic observations. First, notice that the set of those $\alpha > 0$ for which $\{\mathcal{K} > \alpha\}^{(m)} = X \times X$ for some m, is the interval $(0, \Lambda_\infty)$ which could be all $\mathbb{R}^+$. Second, observe that if $0 < \alpha < \Lambda_\infty$, then $\triangle \subset \{\mathcal{K} > \alpha\}$. Take $\Lambda_0 \subset (0, \Lambda_\infty)$. We may think to choose it as close to Λ_∞ as desired. Now set $m_0 = \min\{m : \{\mathcal{K} > \Lambda_0\}^{(m)} = X \times X\}$. Then $\{\mathcal{K} > \Lambda_0\}^{(m_0)} = X \times X$ and we may assume $m_0 \geq 3$.

Set $A_1 = \{\alpha > 0 : \{\mathcal{K} > \Lambda_0\}^{(3)} \subseteq \{\mathcal{K} > \alpha\}\}$. If $A_1 = \emptyset$, then the sequence $\lambda(0) = 0$ and $\lambda(1) = \Lambda_0$ satisfies that $\{\mathcal{K} > \lambda(1)\}^{(3)} \subseteq \{\mathcal{K} > \lambda(0)\}$. Assume now that $A_1 \neq \emptyset$. Take $\Lambda_1 > \sup A_1 - \varepsilon$ for $\varepsilon > 0$. Set $A_2 = \{\alpha > 0 : \{\mathcal{K} > \Lambda_1\}^{(3)} \subseteq \{\mathcal{K} > \alpha\}\}$. If $A_2 = \emptyset$ we take the sequence $\lambda(0) = 0$, $\lambda(1) = \Lambda_1$ and $\lambda(2) = \Lambda_0$. If $A_2 \neq \emptyset$ we keep iterating this selection process. Since $\{\mathcal{K} > \Lambda_0\}^{(m_0)} = X \times X$ we see that the procedure stops after a finite number of steps of the order of $\frac{m_0}{3}$. Hence we have a sequence $\Lambda_\infty > \Lambda_0 > \Lambda_1 > \cdots > \Lambda_k$. With $\lambda(i) = \Lambda_{k-i}$ for $i = 0, 1, 2, \dots, k$ we obtain the lemma. $\square$

THEOREM 5.4. *Let X be a a set and let $\mathcal{K}$ be a nonnegative function on $X \times X$ satisfying (i) and (ii) in Lemma 5.3. Then, for every sequence*

$$\vec{\lambda} = \{\lambda(i) : i = 0, 1, 2, \dots, k = k(\vec{\lambda})\}$$

as the one provided in Lemma 5.3, there exists a pseudo-metric $d_{\vec{\lambda}}$ on X such that

(1) $\{\mathcal{K} > \lambda(i)\} \subseteq \{d_{\vec{\lambda}} < 2^{-i}\} \subseteq \{\mathcal{K} > \lambda(i-1)\}$ *for every $i = 1, 2, \dots, k$;*
(2) *the function*

$$\delta_{\vec{\lambda}} = 2^{-\lambda^{-1} \circ \mathcal{K}},$$

where λ^{-1} is the inverse of any increasing extension of $\lambda(i)$ to the whole interval $[0, k(\vec{\lambda})]$, is equivalent to the Frink's pseudo-metric $d_{\vec{\lambda}}$ associated to the family $\{\{\mathcal{K} > \lambda(i)\} : i\}$. Precisely,

$$\frac{1}{4}\delta_{\vec{\lambda}}(x, y) \leq d_{\vec{\lambda}}(x, y) \leq 2\delta_{\vec{\lambda}}(x, y)$$

for every x and y in X such that

$$2^{-k(\vec{\lambda})} \leq d_{\vec{\lambda}}(x, y) < 1.$$

PROOF. From Lemma 5.3 we see that the sequence $U_i = \{\mathcal{K} > \lambda(i)\}$ satisfies properties (i) to (iv) in the hypothesis of Lemma 5.1. Then there exists a pseudo-metric, that we denote by $d_{\vec{\lambda}}$, on X such that

$$\{\mathcal{K} > \lambda(i)\} \subseteq \{d_{\vec{\lambda}} < 2^{-i}\} \subseteq \{\mathcal{K} > \lambda(i-1)\}$$

for every $i = 1, 2, \dots, k$. Let us prove (2). For $x, y \in X$ such that $2^{-k(\vec{\lambda})} \leq d_{\vec{\lambda}}(x, y) < 1$, there exists $i = 0, 1, 2, \dots, k(\vec{\lambda})$ such that

$$2^{-(i+1)} \leq d_{\vec{\lambda}}(x.y) < 2^{-i}.$$

From the second inclusion in (1) we have that $\mathcal{K}(x, y) > \lambda(i-1)$. From the first inclusion in (1) and the first inequality above, $d_{\vec{\lambda}}(x, y) \geq 2^{-(i+1)}$, we see that $(x, y) \notin \{\mathcal{K} > \lambda(i+1)\}$

or that $\mathcal{K}(x,y) \leq \lambda(i+1)$. In other words

$$\lambda(i-1) < \mathcal{K}(x,y) \leq \lambda(i+1)$$

when

$$2^{-(i+1)} \leq d_{\vec{\lambda}}(x,y) < 2^{-i}.$$

Hence

$$i-1 < (\lambda^{-1} \circ \mathcal{K})(x,y) \leq i+1$$

for $2^{-(i+1)} \leq d_{\vec{\lambda}}(x,y) < 2^{-i}$. Then

$$\frac{1}{4} = 2^{-(i+1)}2^{i-1} < d_{\vec{\lambda}}(x,y)2^{(\lambda^{-1}\circ\mathcal{K})(x,y)} \leq 2^{-i}2^{i+1} = 2$$

or

$$\frac{1}{4}\delta_{\vec{\lambda}} < d_{\vec{\lambda}}(x,y) \leq 2\delta_{\vec{\lambda}}(x,y),$$

as desired. Notice that $d_{\vec{\lambda}} \leq 1$ everywhere and we are done. □

The result in (2) of the above theorem can be rephrased as a Newtonian type form for $\mathcal{K}$. In fact

$$\mathcal{K} \simeq \lambda\left(\log_2 \frac{1}{\delta_{\vec{\lambda}}}\right).$$

Notice also that for $2^{-k(\vec{\lambda})} \leq r < 1$ we have, for $x \in X$, that

$$B_{\delta_{\vec{\lambda}}}(x,r) = \left\{y \in X : \mathcal{K}(x,y) > \lambda\left(\log_2 \frac{1}{r}\right)\right\}.$$

5.4. An algorithm for the metrization of weighted undirected graphs based on Frink's Lemma

The above results can be used to produce an explicit an computable algorithm for the metrization of weighted undirected graph. Let $G = (\mathcal{V}, \mathcal{E}, W)$ be a weighted graph. The set $\mathcal{V}$ is the set of vertices. The set $\mathcal{E}$ is the set of all edges joining each vertex $i \in \mathcal{V}$ to each vertex $j \in \mathcal{V}$. The weights W are provided by an $n \times n$ matrix $(w_{ij} : i = 1, \ldots, n; j = 1, \ldots, n)$ where $n = \#(\mathcal{V})$. Each w_{ij} is a positive real number. Since we think that w_{ij} is measuring affinity of the vertices i and j, we naturally assume that $w_{ij} = w_{ji}$. On the other hand, it is also natural to assign to each $i \in \mathcal{V}$ the largest affinity with itself than with each other $j \in \mathcal{V}$ for $j \neq i$. In other words $w_{ii} \geq w_{ij}$ for every $i, j \in \mathcal{V}$.

Taking $X = \mathcal{V}$, $\mathcal{E} = X \times X$, $K = W$ in the above sections we can design the following algorithm to find a sequence $\lambda(i)$, a metric $\delta_{\vec{\lambda}}$ on $\mathcal{V}$ and the family of balls provided by Theorem 5.4.

Step 1. Compute the minimum of W on the three main diagonals, i.e.

$$\min\{w_{i-1,i}; w_{i,i}; w_{i,i+1} : i = 1, \dots, n\} = \Lambda_0;$$

Step 2. build the matrix $A_0 = A_{\{(i,j):w_{ij} \geq \Lambda_0\}}$;
Step 3. compute $A_0^3 = A_0 A_0 A_0 = (a_{ij}^{(3)})$;
Step 4. define $U_0 = \{(i,j) : a_{ij}^{(3)} > 0\}$;
Step 5. find $\Lambda_1 = \max\{\alpha : \{w_{ij} \geq \alpha\} \supseteq U_0\}$;
Step 6. build the matrix $A_1 = A_{\{(i,j):w_{ij} \geq \Lambda_1\}}$;
Step 7. compute A_1^3;
Step 8. define $U_1 = \{(i,j) :$ the (i,j) entry of A_1^3 is positive$\}$;
Step 9. find $\Lambda_2 = \max\{\alpha : \{w_{ij} \geq \alpha\} \supseteq U_1\}$;

$\vdots$

In this way we obtain the sequence $\Lambda_k < \Lambda_{k-1} < \cdots < \Lambda_2 < \Lambda_1 < \Lambda_0$. Set $\lambda(i) = \Lambda_{k-i}$ for $i = 0, \dots, k$. Now compute a version of λ^{-1} and define

$$\delta_{\vec{\lambda}}(i,j) = 2^{-\lambda^{-1}(w_{ij})}.$$

Finally, plot $B_{\delta_{\vec{\lambda}}}(i,r) = \{j : w_{ij} > \lambda(\log_2 \frac{1}{r})\}$, $0 < r < 1$ and $i \in \mathcal{V}$.

5.5. Test and comparison with the diffusive metric for Newtonian type affinities

Proposition 2.3 and Theorem 4.4 suggest testing the algorithm on affinities defined as discretizations of Newtonian type potentials of the form

$$\mathcal{K}_\alpha(x,y) = \frac{1}{|x-y|^\alpha}$$

for α positive. Once a discretization of $\mathcal{K}_\alpha$ is given we may run our algorithm and also the well known diffusion metric introduced in [CL06]. The diffusive metric at time $t > 0$ is given by

$$d_t(i,j) = \left\{ \sum_l e^{2t\nu_l} \left| x_i^l - x^l \right|^2 \right\}^{\frac{1}{2}}$$

where x^l and ν_l, $l = 1, \ldots, L$ are the eigenvectors and the eigenvalues of the Laplace operator on the graph with affinity given by the metric w_{ij}.

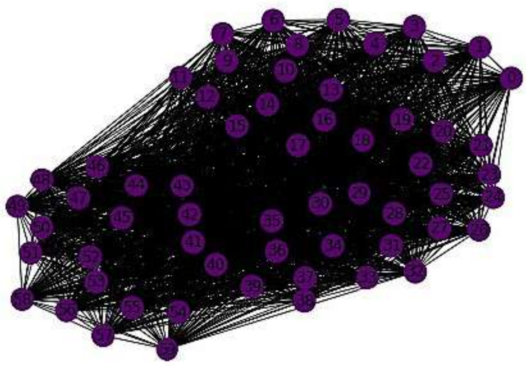


FIGURE 11. Graph.

We shall only write down the comparison of the families of δ_λ-balls, d_t-balls and Euclidean balls for a couple of values of the radii, when we consider the discretization

$$w_{ij} = \begin{cases} 2, & \text{for } i = j \\ |i-j|^{-\alpha}, & \text{for } i \neq j \end{cases}$$

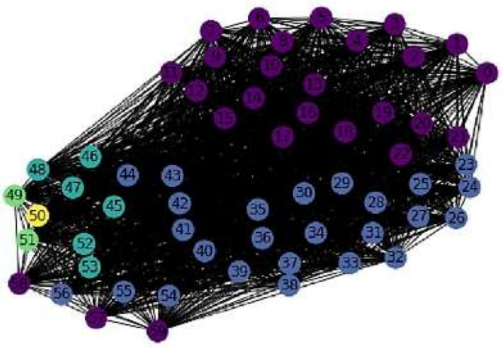
with $i, j = 0, \ldots, 59$.

It is worthy pointing out here that the choice of 60 points of discretization is only taken for the sake of getting better images for the graphs. In particular for the visibility of some edges.

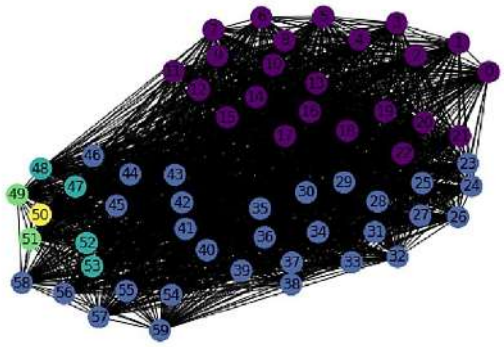
Let us also point out that in the following graphs, the numerical label of each vertex is assigned according to the order of the rows in the affinity matrix, but a priori has nothing to do with distance or affinity.

Figure 11 labels with the integers $0, 1, \ldots, 59$ the 60 vertices of our graph.

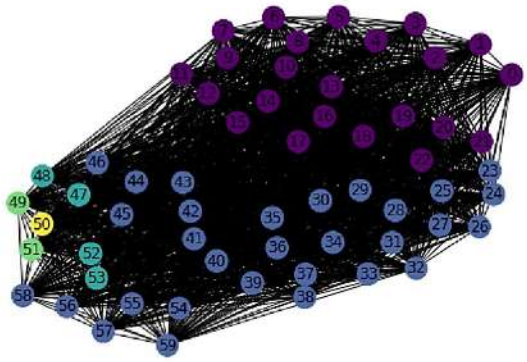
We shall now plot some balls centered at two different vertices, 25 and 50, each for the three metrics, the Euclidean metric **(E)**, the Diffusive metric **(D)** with $t = 0.005$ and Frink's metric **(F)**. The comparison of both, **(D)** and **(F)** with the Euclidean **(E)** is essential because K itself is built in terms of **(E)**. Let us say again that we are interested in the shape of the balls but not in the particular radii for which those balls are attained. This fact is particularly clear in this case where the Euclidean metric is unbounded. Nevertheless we shall write out the values of the radii for which each ball in each metric is plotted. Actually the following pictures show in different colors the annuli between two



(D) Y, G, 0.11, T, 0.135, L, 0.31, P, 0.404327



(F) Y, 0.0169492, G, 0.037037, T, 0.111111, L, 0.333333, P, 1



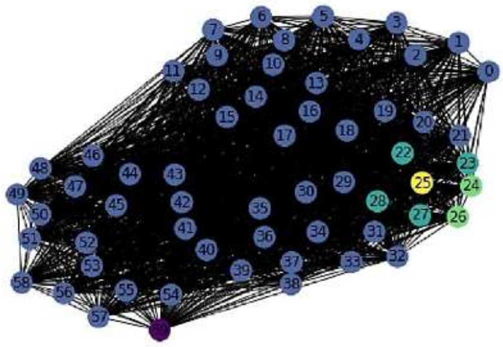
(E) Y, G, 1, T, 3, L, 27, P, 59

FIGURE 12. Center at 50

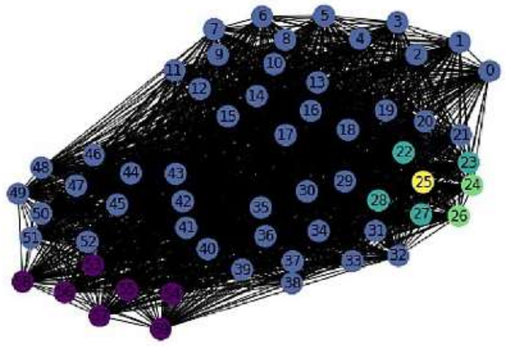
consecutive balls. We use yellow for the center, green for the first annulus, turquoise for the second, lavender for the third and purple for the last annulus.

In Figure 12 above and Figure 13 below we use capital letters, Y, G, T, L and P to denote the colors. The sequences of letters and numbers describe the inner and outer radii of each annulus.

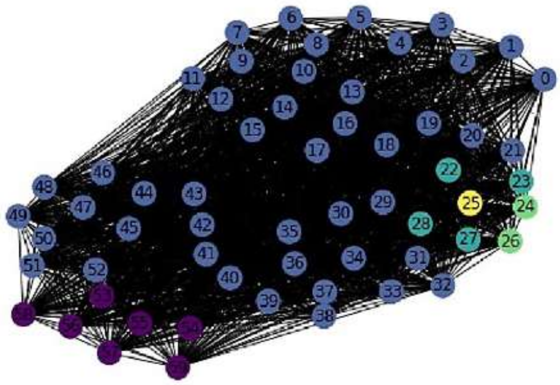
It is worthy noticing that the sequence of radii for **(D)** has been chosen in such a way that the d_t balls become as close as possible to Euclidean balls. At least for this simple situation, of a kernel defined by a metric, the metrization scheme, **(F)**, introduced here seems to reproduce the exact shapes of the balls associated to the metric defining the kernel. It could be argued that the exponential character of Frink's construction provides only a few balls of the graph. Nevertheless we know from the very proof of our main result that we have at hand changing the initial parameter $\Lambda < \Lambda_\infty$ to produce a profuse diversity of sequences $\lambda(i)$.



(D) Y, G, 0.13, T, 0.17, L, 0.212, P, 0.404327



(F) Y, 0.0169492, G, 0.037037, T, 0.111111, L, 0.333333, P, 1



(E) Y, G, 1, T, 3, L, 27, P, 59

FIGURE 13. Center at 25

5.6. Comments, problems and further results

(1) Let X be a set and let U and V be two parts of $X \times X$. Compute $(U \circ V)^{-1}$.

(2) Let (X, d) be a quasi-metric space with triangle constant $K \geq 1$. Find a sequence $\{U_m : m = 0, 1, \ldots\}$ of subsets of $X \times X$ satisfying properties (i) to (iv) in Lemma 5.1. Compare the pseudo-metric provided by Lemma 5.1 with the given d. Show that the pseudo-metric provided by Lemma 5.1 is actually a metric.

(3) Let $X = \{1, 2, \ldots, n\}$ and V be the subset of $X \times X$ given by

$$V = \{(i, j) \in X \times X : j - i > 1\}.$$

Compute $V^{(m)} = V \circ V \circ \cdots \circ V$ m-times for m large.

(4) The results of this chapter are related to those in [AG18a] and [AAG21].

(5) The basic facts regarding Frink's Lemma and its application to the metrization of uniformities with countable basis can be found in [Kel62]. See also the original work of Frink in [Fri37].

CHAPTER 6

Measuring distances with a thermometer. Diffusion distances

6.1. Introduction

In the Euclidean space $\mathbb{R}^n$ the diffusion of thermal energy is governed by the well known heat equation,

$$\frac{\partial u}{\partial t} = \nabla \cdot A \nabla u = \operatorname{div} A \operatorname{grad} u, \tag{6.1}$$

where A is the conductivity matrix which might depend on the point $x \in \mathbb{R}^n$ and even on time t. Of course, the most classical case is the associated to the identity matrix $A = I$,

$$\frac{\partial u}{\partial t} = \Delta u.$$

Let x and y be two points of $\mathbb{R}^n$ and, assuming the standard uniform ellipticity condition for A, set u_x and u_y to denote solutions of

$$(P_x) = \begin{cases} \dfrac{\partial u_x}{\partial t} = \nabla \cdot A \nabla u_x \\ u_x(z, 0) = \delta_x(z) \end{cases}$$

and

$$(P_y) = \begin{cases} \dfrac{\partial u_y}{\partial t} = \nabla \cdot A \nabla u_y \\ u_y(z, 0) = \delta_y(z) \end{cases}$$

respectively, with δ_x and δ_y the Dirac deltas at x and y. Recall that the matrix A collects both the isotropy and homogeneity properties of the material where the diffusion is taking place. Or better, when A is not diagonal neither constant the model contains the information on how heterogeneous and non isotropic is the material. From the point of view of the motion of the thermal energy inside the domain we may think that we have different metric structures on $\mathbb{R}^n$ associated to those matrices A Since no a priori information about this metric structure on $\mathbb{R}^n$ due to A, is known, we may use the temperatures u_x an u_y at some fixed level of time in order to have an insight on how A-far away are the points x and y. Since, for t fixed, u_x and u_y are functions of the space variable z, we may use some norm on the function spaces containing $u_x(t,\cdot)$ and $u_y(t,\cdot)$. For example the $L^2(dz)$ norm to provide, for fixed $t>0$, a quantity

$$d_t(x,y) = \|u_x(t,\cdot) - u_y(t,\cdot)\|_{L^2}\,.$$

Moreover, in any setting where a Laplacian is defined we may solve problems (P_x) and (P_y) and then construct such functions as the above d_t.

This approach in discrete cases is due to Coifman and Lafon [**CL06**], and [**CLL$^+$05**].

In this chapter we aim to explore the basic definitions and properties of the functions of type d_t for different settings.

6.2. The classical heat case

Let us start by the standard homogeneous and isotropic media model provided by the basic heat equation in $\mathbb{R}^n$, $\frac{\partial u}{\partial t} = \Delta u = \operatorname{div}\operatorname{grad} u$. In this simple case, given $x\in\mathbb{R}^n$, the Weierstrass kernel $W_t(x,z) = (4\pi t)^{-\frac{n}{2}} e^{-\frac{|x-z|^2}{4t}}$ solves

$$(P_x) = \begin{cases} \dfrac{\partial}{\partial t} W_t(x,z) = \Delta_z W_t(x,z), & z\in\mathbb{R}^n, t>0;\\ W_0(x,z) = \delta_x(z), \end{cases}$$

in the sense that $\int_{\mathbb{R}^n} W_t(x,z)\varphi(z)dz$ tends to $\varphi(x)$ for every φ smooth and bounded.

Proposition 6.1. *For $t>0$ fixed, the function*

$$d_t(x,y) = \sqrt{\int_{z\in\mathbb{R}^n} |W_t(x,z) - W_t(y,z)|^2\, dz}$$

is a metric defined on $\mathbb{R}^n\times\mathbb{R}^n$.

Proof. Notice first that the Gaussian decay of the Weierstrass kernel guarantees the convergence of the integral. The positivity and symmetry properties of d_t are immediate. On the other hand, if $d_t(x,y)=0$, then $W_t(x,z) = W_t(y,z)$ for every $z\in\mathbb{R}^n$. Hence $|x-z| = |y-z|$ for every $z\in\mathbb{R}^n$, so $x=y$. Now if we write $W_{t,x}(z) = W_t(x,z)$,

$$\begin{aligned} d_t(x,y) &= \|W_{t,x} - W_{t,y}\|_{L^2(\mathbb{R}^n)}\\ &= \|(W_{t,x} - W_{t,\xi}) + (W_{t,\xi} - W_{t,y})\|_{L^2(\mathbb{R}^n)}\\ &\le \|W_{t,x} - W_{t,\xi}\|_{L^2(\mathbb{R}^n)} + \|W_{t,\xi} - W_{t,y}\|_{L^2(\mathbb{R}^n)}\\ &= d_t(x,\xi) + d_t(\xi,y), \end{aligned}$$

and we are done. $\square$

Notice also that $d_t(x,y) \leq \|W_{t,x}\|_{L^2} + \|W_{t,y}\|_{L^2}$. Since $W_{t,x}(z) = (4\pi t)^{-\frac{n}{2}} e^{-\frac{|x-z|^2}{4t}}$, we have that

$$\begin{aligned} d_t(x,y) &\leq 2\frac{1}{(4\pi t)^{n/2}} \left(\int_{\mathbb{R}^n} e^{-\frac{|z|^2}{2t}} dz \right)^{1/2} \\ &= 2\frac{1}{(4\pi t)^{n/2}} \left((2t)^{n/2} \int_{\mathbb{R}^n} e^{-|z|^2} dz \right)^{1/2} \\ &= 2\frac{(2t\pi)^{n/4}}{(4\pi t)^{n/2}} \\ &= 2^{1-\frac{3}{4}n} \pi^{-\frac{n}{4}} t^{-\frac{n}{4}}. \end{aligned}$$

Hence each d_t is bounded above. Moreover this bound tends to zero as $t \to \infty$. So that any of the metrics d_t on $\mathbb{R}^n$ is far from being equivalent to the Euclidean distance. Nevertheless, as we shall prove, the family of d_t-balls coincides with the family of Euclidean balls for every $t > 0$.

Recall that, since the Fourier transform of $e^{-\pi\lambda|x|^2}$ is $\lambda^{-\frac{n}{2}} e^{-\frac{\pi|\xi|^2}{\lambda}}$ for every $\lambda > 0$, the Weierstrass kernel defines a semigroup by convolution. In other words $\mathscr{W}_{t_1} * \mathscr{W}_{t_2} = \mathscr{W}_{t_1+t_2}$, where $\mathscr{W}_t(z) = (4\pi t)^{-\frac{n}{2}} e^{-\frac{|z|^2}{4t}}$, and $\mathscr{W}_{t_1} * \mathscr{W}_{t_2}(x) = \int_{\mathbb{R}^n} \mathscr{W}_{t_1}(x-z)\mathscr{W}_{t_2}(z) dz$.

Let us state and prove the main result of this section.

PROPOSITION 6.2. *Let d_t be defined as before. Then*

(a) *d_t is translation invariant;*
(b) *$d_t(x,y)$ depends only on $|x-y|$, i.e. $d_t(x,y) = \rho_t(|x-y|)$;*
(c) *ρ_t is strictly increasing and continuous, with $\rho_t(0) = 0$;*
(d) *the family of d_t-balls are the Euclidean balls.*

PROOF. To prove (a) we only have to change variables $y - z = u$ in the integral defining $d_t^2(x,y)$. Hence $d_t(x,y) = d_t(x-y,0)$. To prove (b) we have to show that the function of x, $d_t(x,0)$, is rotation invariant. Take a rotation R of $\mathbb{R}^n$. Then, since $\mathscr{W}_t$ is radial

$$\begin{aligned} d_t^2(Rx,0) &= \int_{z\in\mathbb{R}^n} \left|\mathscr{W}_t(Rx-z) - \mathscr{W}_t(z)\right|^2 dz \\ &= \int_{z\in\mathbb{R}^n} \left|\mathscr{W}_t(R(x-R^{-1}z)) - \mathscr{W}_t(R^{-1}z)\right|^2 dz \end{aligned}$$

$$
\begin{aligned}
&= \int_{u\in\mathbb{R}^n} \left|\mathscr{W}_t(R(x-u)) - \mathscr{W}_t(u)\right|^2 du \\
&= d_t^2(x,0).
\end{aligned}
$$

In order to prove (c), notice that since d_t^2 is a radial function of $x-y$, a formula for the profile $\rho_t^2(r)$ is given for $r>0$ by $\rho_t^2(r) = \int_{z\in\mathbb{R}^n} \left|\mathscr{W}_t(r\vec{e_1}-z) - \mathscr{W}_t(z)\right|^2 dz$, with $\vec{e_1}$ the first vector of the canonical basis of $\mathbb{R}^n$. For t fixed, the derivative of ρ_t^2 as a function of $r>0$ is given by

$$
\begin{aligned}
\frac{d\rho_t^2}{dr}(r) &= \frac{1}{(4\pi t)^n}\int_{z\in\mathbb{R}^n} 2\left(e^{-\frac{|r\vec{e}_1-z|^2}{4t}} - e^{-\frac{|z|^2}{4t}}\right)\frac{(-2)(r-z_1)}{4t}\, e^{-\frac{|r\vec{e}_1-z|^2}{4t}}\, dz \\
&= -\frac{4}{(4\pi t)^n}\left[\int_{z\in\mathbb{R}^n} e^{-\frac{2|r\vec{e}_1-z|^2}{4t}}\,\frac{(r-z_1)}{4t}\, dz - \int_{z\in\mathbb{R}^n} e^{-\frac{|z|^2}{4t}} e^{-\frac{|r\vec{e}_1-z|^2}{4t}}\,\frac{(r-z_1)}{4t}\, dz\right] \\
&= -2\int_{z\in\mathbb{R}^n} \frac{e^{-\frac{|z|^2}{4t}}}{(4\pi t)^{-n/2}}\,\frac{e^{-\frac{|r\vec{e}_1-z|^2}{4t}}}{(4\pi t)^{-n/2}}(-2)\frac{(r-z_1)}{4t}\, dz \\
&= -2\left(\mathscr{W}_t * \frac{\partial \mathscr{W}_t}{\partial x_1}\right)(r\vec{e}_1) \\
&= -2\,\frac{\partial}{\partial x_1}\big(\mathscr{W}_t * \mathscr{W}_t\big)(r\vec{e}_1) \\
&= -2\,\frac{\partial}{\partial x_1}\mathscr{W}_{2t}(r\vec{e}_1) \\
&= -2\,\frac{\partial}{\partial x_1}\left(\frac{1}{(8\pi t)^{n/2}} e^{-\frac{|x|^2}{8t}}\right)(r\vec{e}_1) \\
&= \left(\frac{4}{(8\pi t)^{n/2}} e^{-\frac{|x|^2}{8t}}\,\frac{x_1}{8t}\right)(r\vec{e}_1) \\
&= \frac{4}{(8\pi t)^{n/2}}\, e^{-\frac{r^2}{8t}}\,\frac{r}{8t} > 0,
\end{aligned}
$$

where we have used the semigroup property of $\mathscr{W}_t$, so (c) is proved. Property (d) is now a consequence of (c). □

The classical definition of equivalence of metrics and quasi-metrics in a quantitative form given by $d \sim \delta$ if for some constants $0 < c_1 \leq c_2 < \infty$ we have that $c_1 d \leq \delta \leq c_2 d$, does not apply for $d_t(x,y)$ and $|x-y|$ in $\mathbb{R}^n$. Nevertheless property (d) in Proposition 6.2 shows that the equivalence takes place in different sense. That is, the families $\mathscr{B}_{d_t}$ and $\mathscr{B}_{|\cdot|}$ of d_t-balls and Euclidean balls are the same. On the other hand, the quantitative equivalence $c_1 d \leq \delta \leq c_2 d$ provide equivalence of balls, not coincidence. So that, in some sense, the result of (d) is stronger than quantitative equivalence.

6.3. A non isotropic homogeneous case

A special case of the general diffusion equation $\frac{\partial u}{\partial t} = \nabla \cdot A\nabla u$ is provided by the homogeneous but non isotropic case with A a symmetric constant and positive definite $n \times n$ matrix. In this case the divergence and non divergence form of $\nabla \cdot A\nabla u$ coincide. Let $A = (a_{ij})$, and let $B = (b_{ij})$ be its inverse. The general heat equation in this case is explicitly given by

$$\frac{\partial u}{\partial t} = \sum_{i=1}^{n}\sum_{j=1}^{n} a_{ij}\frac{\partial^2 u}{\partial x_i \partial x_j} \text{ on } \mathbb{R}^{n+1}_{+} = \mathbb{R}^n \times \mathbb{R}^+.$$

The fundamental solution is now provided by the multivariate Gaussian distributions determined by the covariances defined by the anisotropy matrix $A = (a_{ij})$.

Let us precise the above. For fixed $x \in \mathbb{R}^n$, U_t, a constant times the function

$$V_t(x,z) = \frac{1}{(4\pi)^{n/2}t^{n/2}(\det A)^{1/2}} e^{\frac{-\left\langle z-x, A^{-1}(z-x)\right\rangle}{4t}}$$

as a function of $t > 0$ and $z \in \mathbb{R}^n$, solves the problem

$$\begin{cases} \dfrac{\partial U_t}{\partial t} = \sum\limits_{i=1}^{n}\sum\limits_{j=1}^{n} \dfrac{\partial^2}{\partial z_i \partial z_j} U_t, \quad t > 0, z \in \mathbb{R}^n; \\ U_0(x,z) = \delta_x(z). \end{cases}$$

In the definition of V_t the angular brackets $\langle\cdot,\cdot\rangle$ denote the inner scalar product in $\mathbb{R}^n$. We leave as exercises for the reader most of the computations in this section. In particular, the proof of the above claims.

Proposition 6.3. *For $t > 0$ fixed, the function*

$$d_{A,t}(x,y) = \sqrt{\int_{z\in\mathbb{R}^n} |V_t(x,z) - V_t(y,z)|^2\, dz}$$

is a metric defined on $\mathbb{R}^n \times \mathbb{R}^n$.

Proof. Follows the lines of the proof of Proposition 6.1. $\square$

On the other hand, the quadratic form induced in $\mathbb{R}^n$ by the elliptic matrix A defines the norm $\|x\|_A = \sqrt{\langle x, A^{-1}x\rangle}$ and hence the metric $d_A(x,y) = \|x-y\|_A$. We leave to the reader the task of comparing the metrics d_A and $d_{A,t}$ for $t > 0$.

6.4. A general spectral approach to diffusive metrization

In this section we aim to introduce strategy of metrization of a measure space through orthonormal bases for the space of square integrable measurable functions.

Let $(X, \mathscr{F}, \mu)$ be a σ-finite measure space. Notice that we have not a priori given any metric or topology on X. We want to introduce metric and hence topology on X based on the topology that we certainly have on the function spaces defined on X.

As usual we denote by L^p or $L^p(X)$ the Banach space of those measurable real functions on X such that $\int_X |f|^p \, d\mu < \infty$ for $1 \leq p < \infty$ and $\operatorname{ess\,sup}_X |f| < \infty$ for $p = \infty$. The norms are $\|f\|_p = \left(\int_X |f|^p \, d\mu\right)^{1/p}$ for $1 \leq p < \infty$ and $\|f\|_\infty = \operatorname{ess\,sup}_{x \in X} |f(x)|$. The special case $p = 2$ has a Hilbert space structure with the inner product $\langle f, g \rangle = \int_X f g d\mu$. The Hilbert structure of L^2 with the property of separability is a natural environment for the existence and the construction and design of orthonormal bases. A sequence $\mathcal{B} = \{\phi_n : n \geq 0\}$, which could be finite when the space X itself is finite, is said to be an orthonormal basis for $L^2(X)$, if $\|\phi_n\| = 1$ for every n, $\langle \phi_n, \phi_m \rangle = 0$ when $n \neq m$ and for every $f \in L^2(X)$ we have

$$f = \sum_{n \geq 0} \langle f, \phi_n \rangle \, \phi_n,$$

where the convergence of the series is understood in the sense of the L^2-norm

$$\left\| f - \sum_{n=0}^{N} \langle f, \phi_n \rangle \, \phi_n \right\|_{L^2} \longrightarrow 0 \quad \text{as } N \to \infty.$$

Let us say that a function $f \in L^2(X)$ is simple or that $f \in \mathcal{S}(\mathcal{B})$ if f is a linear (finite) combination of elements in $\mathcal{B}$. In other words $\mathcal{S}(\mathcal{B})$ is the linear span of $\mathcal{B}$. Let $\mathcal{S}_N(\mathcal{B})$ be the linear span of $\{\phi_0, \phi_1, \dots, \phi_N\}$.

Lemma 6.4. *The identity operator on $\mathcal{S}_N(\mathcal{B})$ is an integral operator with kernel*

$$K_N(x, y) = \sum_{n=0}^{N} \phi_n(y)\phi_n(x)$$

in the sense that for every $f \in \mathcal{S}_N(\mathcal{B})$ we have

$$f(x) = \int_X K_N(x, y) f(y) d\mu(y).$$

PROOF. Let $f = \sum_{n=0}^{N} c_n \phi_n$, with $c_n \in \mathbb{R}$, be given. Then

$$\int_X f(y)\phi_n(y)d\mu(y) = \langle f, \phi_n \rangle = c_n,$$

so that

$$\begin{aligned} f &= \sum_{n=0}^{N} \left(\int_X f(y)\phi_n(y)d\mu(y) \right) \phi_n \\ &= \int_X \left(\sum_{n=0}^{N} \phi_n(y)\phi_n \right) f(y)d\mu(y) \\ &= \int_X K_N(\cdot, y) f(y) d\mu(y). \end{aligned}$$ □

In most of the well known instances of the above, the functions ϕ_n in the basis $\mathcal{B}$ are much better than L^2-functions. In the classical Fourier case the functions ϕ_n are $\mathscr{C}^\infty$ and bounded. The wavelet cases provide bounded sequences. We shall assume that each ϕ_n is well defined for every $x \in X$. So that the kernel $K_N(x, y)$ is well defined and symmetric on the whole product measure space $X \times X$.

Of course, in such a general setting, very little can be said about the convergence of the series $\sum_{n \geq 0} \phi_n(y)\phi_n(x)$. On the other hand, we can help the convergence of the series by multiplying each tensor product $\phi_n(x)\phi_n(y)$ by the terms of a sequence $\{\alpha_n : n \geq n\}$ which tends to zero as $n \to \infty$. So the chances of convergence of $\sum_{n \geq 0} \alpha_n \phi_n(x)\phi_n(y)$ are now better. In doing so we may obtain some integrable kernels to produce the corresponding integral operators defined in $L^2(X)$. The most interesting case for our purposes is instead the search of differential type operators making possible to produce diffusions on X. This possibility is based on the good behavior of the individual members of $\mathcal{B}$. The paradigmatic and better understood case is of course the Fourier case. If we want to produce differential type operators instead of integral operators, and with the guide of the case of the Laplacian which is negative, since $\widehat{\Delta\varphi}(\xi) = -4\pi^2 |\xi|^2 \widehat{\varphi}(\xi)$, we can take a sequence λ_n of negative numbers with $|\lambda_{n+1}| > |\lambda_n|$ and $|\lambda_n| \to +\infty$ as $n \to \infty$.

In our restricted attention to $\mathcal{S}_N(\mathcal{B})$ instead of the whole space $L^2(X)$, we have no difficulty at defining such a Laplacian type operator. Let Λ denote the sequence $\{\lambda_n : n \geq 0\}$ with $\lambda_{n+1} < \lambda_n \leq 0$, $\lambda_n \to -\infty$, $n \to \infty$.

Thus, given $(X, \mathscr{F}, \mu)$ a σ-finite measure space, an orthonormal basis $\mathcal{B} = \{\phi_n : n \geq 0\}$ for $L^2(X)$, a sequence Λ as above and a positive integer N, we define the $\mathcal{B}, \Lambda, N$-Laplacian of $f \in \mathcal{S}_N(\mathcal{B})$ by

$$\Delta^N_{\mathcal{B},\Lambda} f = \sum_{n=0}^{N} \lambda_n \left\langle f, \phi_n \right\rangle \phi_n.$$

Which being N finite has also the kernel representation

$$\Delta^N_{\mathcal{B},\Lambda} f = \int_X K_{N,\Lambda}(x,y) f(y) d\mu(y),$$

with $K_{N,\Lambda}(x,y) = \sum_{n=0}^{N} \lambda_n \phi_n(x)\phi_n(y)$.

Let us now observe that in the previous sections the unit mass Dirac delta at a point $x \in \mathbb{R}^n$ can be seen as the identity operator when we are in such convolutional settings. Now that Lemma 6.4 gives us a good interpretation for the identity operator on $\mathcal{S}_N(\mathcal{B})$ in our setting, and the above definition of $\Delta^N_{\mathcal{B},\Lambda}$, we may build diffusions on X by solving the problem, for fixed $x \in X$,

$$(P_x) = \begin{cases} \dfrac{\partial u_x}{\partial t} = \Delta^N_{\mathcal{B},\Lambda} u_x, & \text{in}\, X \times \mathbb{R}^+; \\ u_x(z,0) = K_N(x,z). \end{cases}$$

Here $u_x : X \times \mathbb{R}^+_0 \to \mathbb{R}$, $u_x = u_x(z,t)$ and the operator $\Delta^N_{\mathcal{B},\Lambda}$ acts on the variable z.

THEOREM 6.5. *The function*

$$u_x(z,t) = \sum_{n=0}^{N} e^{\lambda_n t} \phi_n(x)\phi_n(z)$$

is well defined for every $t \geq 0$ as a function in $\mathcal{S}_N(\mathcal{B})$ and solves problem (P_x).

PROOF. For x fixed and $t \geq 0$ fixed, $u_x(\cdot, t)$ is a linear combination of the first $N+1$ terms of $\mathcal{B}$. On the other hand, taking term by term differentiation with respect to t of the $\mathscr{C}^\infty$ function of t defined by $u_x(z,\cdot)$ we see that

$$\begin{aligned} \frac{\partial u_x}{\partial t}(z,t) &= \sum_{n=0}^{N} \lambda_n e^{\lambda_n t} \phi_n(x)\phi_n(z) \\ &= \sum_{n=0}^{N} \lambda_n \left\langle \sum_{k=0}^{N} e^{\lambda_k t} \phi_k(x)\phi_k, \phi_n \right\rangle \phi_n(z) \\ &= \Delta^N_{\mathcal{B},\Lambda} \left(\sum_{k=0}^{N} e^{\lambda_k t} \phi_k(x)\phi_k(z) \right) \\ &= \Delta^N_{\mathcal{B},\Lambda} u_x(z,t). \end{aligned}$$

On the other hand, clearly

$$u_x(z,0) = \sum_{n=0}^{N} e^{\lambda_n \cdot 0}\phi_n(x)\phi_n(z) = K_N(x,z). \qquad \square$$

Notice that since the sequence of λ_n's is negative, the factor $e^{\lambda_n t}$ for $t > 0$ is contributing to convergence if we worry about the size of N. So the terms corresponding to large values of n become less relevant.

Now, from Theorem 6.5, we can launch two diffusions, one starting at $x \in X$ and the other starting at $y \in X$ with $x \neq y$ by solving the two problems

$$(P_x) = \begin{cases} \dfrac{\partial u_x}{\partial t} = \Delta^N_{\mathcal{B},\Lambda} u_x \\ u_x(z,0) = K_N(x,z) \end{cases}$$

$$(P_y) = \begin{cases} \dfrac{\partial u_y}{\partial t} = \Delta^N_{\mathcal{B},\Lambda} u_y \\ u_y(z,0) = K_N(y,z) \end{cases}$$

with the same lenght N. Hence the function

$$d^N_t(x,y) = \sqrt{\int_{z\in X} |u_x(z,t) - u_y(z,t)|^2 \, d\mu(z)}$$

for $t > 0$ fixed is well defined.

PROPOSITION 6.6. *The function d^N_t has an explicit formula in terms of the orthonormal basis $\mathcal{B}$ of $L^2(X)$ and of the eigenvalues Λ of the operator $\Delta_{\mathcal{B},\Lambda}$ given by*

$$d^N_t(x,y) = \sqrt{\sum_{n=0}^{N} e^{2\lambda_n t} |\phi_n(x) - \phi_n(y)|^2}.$$

PROOF. Notice that from Theorem 6.5

$$\begin{aligned}
[d^N_t(x,y)]^2 &= \int_{z\in X} |u_x(z,t) - u_y(z,t)|^2 \, d\mu(z) \\
&= \int_{z\in X} \left| \sum_{n=0}^{N} e^{\lambda_n t}[\phi_n(x)\phi_n(z) - \phi_n(y)\phi_n(z)] \right|^2 d\mu(z) \\
&= \int_{z\in X} \left| \sum_{n=0}^{N} e^{\lambda_n t}[\phi_n(x) - \phi_n(y)]\phi_n(z) \right|^2 d\mu(z).
\end{aligned}$$

The last expression for t, N, x and y fixed is the square of the norm of a function given by its Fourier series in terms of the basis $\mathcal{B}$. So that by Plancherel-Parseval we have

$$[d_t^N(x,y)]^2 = \sum_{n=0}^{N} e^{2\lambda_n t} \left|\phi_n(x) - \phi_n(y)\right|^2,$$

which is the desired inequality. □

PROPOSITION 6.7. *For each $N \in \mathbb{N}$ and each $t > 0$, the function d_t^N is a pseudometric in X. In other words, $d_t^N(x,y) \geq 0$ for every $x, y \in X$; $d_t^N(x,x) = 0$ for every $x \in X$ and $d_t^N(x,y) \leq d_t^N(x,z) + d_t^N(z,y)$ for every $x, y, z \in X$.*

PROOF. Follows readily from the definition of d_t^N and the triangle inequality for the $L^2(X)$-norm. □

Let us provide here a simple ilustration of the above. Let $X = \{1, 2, \ldots, n\}$ be a finite but large set. The space $L^2(X)$ with the counting measure on X can be identified with $\mathbb{R}^n$. Let $\mathcal{B} = \{\vec{e_1}, \ldots, \vec{e_n}\}$ denote the canonical basis of $\mathbb{R}^n$. Let $\lambda_n < \lambda_{n-1} < \cdots < \lambda_2 < \lambda_1 \leq 0$ be given, then Propositions 6.6 and 6.7 give the pseudo-metric generated by the diffusion induced by $\Delta_{\mathcal{B},\Lambda}$. Precisely, for $i, j \in X$, $d_t^2(i,j) = \sum_{k=1}^{n} e^{2\lambda_k t} \left|\vec{e_k}(i) - \vec{e_k}(j)\right|^2$, where $\vec{e_k}(i)$ is the i-th component of $\vec{e_k}$, so that

$$d_t^2(i,j) = \begin{cases} 0, & \text{if } i = j \\ e^{2\lambda_i t} + e^{2\lambda_j t}, & \text{if } i \neq j. \end{cases}$$

or

$$d_t(i,j) = \begin{cases} 0, & \text{if } i = j \\ \sqrt{e^{2\lambda_i t} + e^{2\lambda_j t}}, & \text{if } i \neq j. \end{cases}$$

Notice that when every λ_i vanishes, we have $d_t(i,j) = \sqrt{2} = \|\vec{e_i} - \vec{e_j}\|$. On the other hand, i and j become closer with respect to d_t when λ_i and λ_j are more negative. More interesting and useful cases will be considered in next sections.

6.5. The trigonometric case

Let $X = [-\pi, \pi) \sim S^1 = \{|z| = 1\}$ be equipped with the Lebesgue measure dx. Consider $\mathcal{B} = \left\{\frac{1}{\sqrt{2\pi}} e^{ikx} : k \in \mathbb{Z}\right\}$ the classical Fourier basis for $L^2([-\pi, \pi])$. For $f \in L^2([-\pi, \pi])$

the function

$$\Theta(x,t) = \sum_{k\in\mathbb{Z}} e^{-t|k|2} \left\langle f, \frac{e^{ik\cdot}}{\sqrt{2\pi}} \right\rangle \frac{e^{ikx}}{\sqrt{2\pi}}$$

solves the heat problem

$$\begin{cases} \dfrac{\partial\Theta}{\partial t} = \dfrac{\partial^2\Theta}{\partial x^2}, \\ \Theta(x,0) = f(x). \end{cases}$$

The corresponding kernel description of Θ is given by

$$\Theta(x,t) = \frac{1}{2\pi}\int_{-\pi}^{\pi} K_t(x,y)f(y)dy,$$

with

$$K_t(x,y) = \sum_{k\in\mathbb{Z}} e^{-t|k|^2} e^{ikx} e^{-iky} = \sum_{k\in\mathbb{Z}} e^{-t|k|^2} e^{ik(x-y)}.$$

PROPOSITION 6.8.

(a) $d_t(x,y) = \sqrt{\int_{-\pi}^{\pi} |K_t(x,z) - K_t(y,z)|^2\,dz}$ *is a well defined pseudo-metric on* $[-\pi,\pi]$*;*

(b) $d_t^2(x,y) = \sum_{k\in\mathbb{Z}} e^{-2t|k|^2}\left|e^{ikx} - e^{iky}\right|^2 = \sum_{k\in\mathbb{Z}} e^{-2t|k|^2}\left|1 - e^{ik(x-y)}\right|^2$*;*

(c) *on* $[-\pi,\pi)$ *each* d_t *is a metric;*

(d) *for* $|z| < \frac{\pi}{2}$*, we have* $d_t(z,0) \geq ce^{-t}|z|$*;*

(e) *for* $|z| < \frac{\pi}{2}$ *and* $|z|\log\frac{1}{|z|} < t$ *we have* $d_t(z,0) \leq c(t)|z|$*.*

PROOF.

(a) Notice that for $t > 0$, since $0 < e^{-t} < 1$, the series defining K_t is uniformly convergent. Then, the integral defining d_t is convergent. Clearly d_t is symmetric and for every x, $d_t(x,x) = 0$. On the other hand, the triangle inequality follows from Minkowski inequality for the $L^2([-\pi,\pi])$-norm.

(b) Is a particular case of Proposition 6.6.

(c) Since $d_t(x,y) = \sum_{k\in\mathbb{Z}} e^{-2t|k|^2}\left|1 - e^{ik(x-y)}\right|^2$ we have that $d_t(x,y) = 0$ if and only if $x - y = 2\pi j$ for some $j \in \mathbb{Z}$. On the interval $[-\pi,\pi)$ the equation $x - y = 2\pi j$ holds only when $j = 0$. Or when $x = y$.

(d) Let $|z| < \frac{\pi}{2}$. Then

$$\begin{aligned} d_t^2(z,0) &= \sum_{k\in\mathbb{Z}} e^{-2t|k|^2}\left|1 - e^{ikz}\right|^2 \\ &= \sum_{k\in\mathbb{Z}} e^{-2t|k|^2}[(1-\cos kz)^2 + \sin^2 kz] \end{aligned}$$

$$
\begin{aligned}
&= 2\sum_{k\in\mathbb{Z}} e^{-2t|k|^2}[1-\cos kz] \\
&= 4\sum_{k\geq 1} e^{-2t|k|2}[1-\cos kz] \\
&\geq 4e^{-2t}(1-\cos z) \\
&\geq ce^{-2t}\left|z\right|^2,
\end{aligned}
$$

which proves (d).

(e) Let $|z| < \frac{\pi}{2}$ and $|z|\log\frac{1}{|z|} < t$. Then

$$
\begin{aligned}
d_t^2(z,0) &= \sum_{1\leq k\leq \frac{1}{|z|}} e^{-2tk^2}(1-\cos kz) + \sum_{k\geq\frac{1}{|z|}} e^{-2tk^2}(1-\cos kz) \\
&\leq \left|z\right|^2 \sum_{1\leq k\leq\frac{1}{|z|}} e^{-2tk^2}k^2 + 2\sum_{k\geq\frac{1}{|z|}}(e^{-2t})^k \\
&\leq c_1(t)\left|z\right|^2 + c_2(t)e^{-2t\frac{1}{|z|}}.
\end{aligned}
$$

For $t > |z|\log\frac{1}{|z|}$ we have that $-\frac{t}{|z|} < -\log\frac{1}{|z|}$ so that

$$
d_t^2(z,0) \leq c_1(t)\left|z\right|^2 + c_2(t)e^{-\log\frac{1}{|z|^2}} = c(t)\left|z\right|2. \qquad \square
$$

The results of the above proposition show again that, as in the case of the Weierstrass kernel, the diffusion on a compact interval produce a family of metrics which are locally equivalent to the Euclidean metric of the setting. In the current case the metrics d_t are locally equivalent to the standard metric in S^1.

6.6. The diffusion metric associated to the fractional Laplacian in $\mathbb{R}^n$

The probabilistic view of the standard diffusion in $\mathbb{R}^n$ associated to the classical Laplacian Δ, is provided by Brownian Motion, mathematically described by Wiener Process. The Wiener Process belongs to a much larger family of Stochastic Processes called the Lévy Process or the Lévy Flights. The analytical counterpart of the Lévy Flights is provided by the diffusions generate by the fractional powers the Laplacian $(-\Delta)^s$. The diversity of approaches to the theory is far beyond the scope of these notes. Nevertheless, perhaps the most simple way of introducing these difussion is also the most useful for our purposes.

The solutions of initial value problems of the form

$$(P) = \begin{cases} \dfrac{\partial u}{\partial t} = (-\Delta)^s u \\ u(x,0) = f(x) \end{cases}$$

for $0 < s < 1$ can be described in terms of the Fourier Transform. In fact, in terms of the Fourier Transform $\widehat{\ }$ in the space variable for fixed time, the solution of (P) is given by

$$\widehat{u}(\xi, t) = e^{-t|\xi|^{2s}} \widehat{f}(\xi).$$

This formula for $\widehat{u}$ is very general. For example if we take as initial data $f = \delta_0$, the Dirac delta, we have that $e^{-t|\xi|^{2s}} = \widehat{u}(\xi, t)$ solves (P) with $f = \delta$. So that we also can provide, via the Fourier Analysis, solutions for

$$(P_x) = \begin{cases} \dfrac{\partial u_x}{\partial t} = (-\Delta)^s u_x \\ u_x(\cdot, 0) = \delta_x \end{cases}$$

and

$$(P_y) = \begin{cases} \dfrac{\partial u_y}{\partial t} = (-\Delta)^s u_y \\ u_y(\cdot, 0) = \delta_y \end{cases}$$

with $x \neq y$ both in $\mathbb{R}^n$. Precisely,

$$\widehat{u_x}(\xi, t) = e^{-t|\xi|^{2s}} e^{-2\pi i \xi \cdot x}, \text{ and}$$
$$\widehat{u_y}(\xi, t) = e^{-t|\xi|^{2s}} e^{-2\pi i \xi \cdot y}.$$

Since the above two functions of ξ belong to $L^2(\mathbb{R}^n)$, then

$$d_t(x, y) = \|\widehat{u_x}(\cdot, t) - \widehat{u_y}(\cdot, t)\|_2$$

is well defined.

Again, we explore the relation of $d_t(x, y)$ with the Euclidean distance, at least locally.

PROPOSITION 6.9. *For $t > 0$ we have*

(a) $d_t^2(x, y) = \int_{\xi \in \mathbb{R}^n} e^{-2t|\xi|^{2s}} \left|1 - e^{-2\pi i \xi \cdot (x-y)}\right|^2 d\xi$;

(b) *d_t is bounded above;*

(c) *d_t is translation invariant;*

(d) *d_t is radial.*

PROOF. Properties (a) and (b) are clear. Property (c) follows from (a). Let us check (d). Using spherical coordinates in $\mathbb{R}^n$ we have

$$\begin{aligned}
d_t^2(x,0) &= \int_{\xi\in\mathbb{R}^n} e^{-2t|\xi|^{2s}} \left|1-e^{-2\pi i\xi\cdot x}\right|^2 d\xi \\
&= \int_0^\infty e^{-2t\rho^{2s}} \int_{\xi'\in S^{n-1}} \left|1-e^{-2\pi i(\xi'\cdot x')\rho|x|}\right|^2 d\sigma(\xi')\rho^{n-1}d\rho \\
&= \int_0^\infty e^{-2t\rho^{2s}} \left(\int_{\xi'\in S^{n-1}} \left|1-e^{-2\pi i\xi_1'\rho|x|}\right|^2 d\sigma(\xi')\right)\rho^{n-1}d\rho.
\end{aligned}$$

In the last integral we used the rotation invariance of the surface integral, with ξ_1' the first component of the vector $\xi'\in S^{n-1}$. So that

$$d_t^2(x,0) = \int_0^\infty e^{-2t\rho^{2s}}\rho^{n-1}\varphi(\rho\,|x|)d\rho,$$

with

$$\varphi(\lambda) = \int_{S^{n-1}} \left|1-e^{-2\pi i\xi_1'\lambda}\right|^2 d\sigma(\xi').$$

Hence $d_t^2(x,0)$ depends only on $|x|$. □

Notice that (b) in Proposition 6.9 shows that there is no hope for a global equivalence between d_t and the Euclidean distance in $\mathbb{R}^n$. Nevertheless we next show that locally they are equivalent. Let us first give an estimate for the behavior of the function $\varphi(\lambda)$ introduced in the proof of Proposition 6.9, for λ small.

LEMMA 6.10. *Let* $\varphi(\lambda) = \int_{S^{n-1}}\left|1-e^{-2\pi i\xi_1\lambda}\right|^2 d\sigma(\xi)$. *Then there exist numbers* c_1, c_2 *with* $0<c_1<c_2<\infty$ *for which*

$$c_1 \leq \lambda^{-2}\varphi(\lambda) \leq c_2$$

for $0\leq\lambda\leq\frac{1}{2\pi}$.

PROOF. Let us first compute $\psi(\lambda)$

$$\begin{aligned}
\varphi(\lambda) &= \int_{S^{n-1}} \left|1-e^{-2\pi i\xi_1\lambda}\right|^2 d\sigma(\xi) \\
&= \int_{S^{n-1}} [(1-\cos 2\pi\xi_1\lambda)^2+\sin^2 2\pi\xi_1\lambda]d\sigma(\xi) \\
&= 2\int_{S^{n-1}} (1-\cos 2\pi\xi_1\lambda)d\sigma(\xi')
\end{aligned}$$

$$
\begin{aligned}
&= 2\int_{S^{n-1}}\left(\sum_{n\geq 1}(-1)^{n+1}\frac{(2\pi\xi_1\lambda)^n}{(2n)!}\right)d\sigma(\xi)\\
&= 8\pi^2\lambda^2\sum_{n\geq 1}(-1)^{n+1}\frac{(2\pi\lambda)^{2(n-1)}}{(2n)!}\left(\int_{S^{n-1}}\xi_1^{2n}d\sigma(\xi)\right)\\
&= 8\pi^2\lambda^2\left(\frac{1}{2}\int_{S^{n-1}}\xi_1^2 d\sigma(\xi)-\frac{(2\pi\lambda)^2}{24}\int_{S^{n-1}}\xi_1^4 d\sigma(\xi)+\cdots\right).
\end{aligned}
$$

For $0\leq\lambda\leq\frac{1}{2\pi}$ the series above is alternating with decreasing absolute value and we are done. □

THEOREM 6.11. *For each $t>0$ there exist three positive numbers c_1, c_2 and c_3, depending on t, such that, for $|x|\leq c_1$ we have that $c_2|x|\leq d_t(x,0)\leq c_3|x|$.*

PROOF. With the above notation we have

$$
d_t^2(x,0)=\int_0^\infty e^{-2t\rho^{2s}}\rho^{n-1}\varphi(\rho|x|)d\rho=\int_0^{\frac{1}{2\pi|x|}}+\int_{\frac{1}{2\pi|x|}}^\infty = I+II.
$$

Assume $0<|x|\leq 1$. Since I and II are both nonnegative we only have to show that for $|x|$ small, $I\simeq|x|^2$ and $II\leq c(t)|x|^2$. To prove that $I\simeq|x|^2$ let us apply Lemma 6.10. Since in I, $0\leq\rho|x|\leq\frac{1}{2\pi}$ we have that $\varphi(\rho|x|)\simeq\rho^2|x|^2$, so that

$$
I\simeq|x|^2\int_0^{\frac{1}{2\pi|x|}}e^{-2t\rho^{2s}}\rho^{n-1}\rho^2 d\rho\simeq|x|^2.
$$

Of course the equivalence constants depend on t. For the second term, since $e^{-t\rho^{2s}}\rho^{n-2s}$ is bounded above as a function of $\rho\geq 1$ with constant depending on t, we have

$$
\begin{aligned}
II &= \int_{\frac{1}{2\pi|x|}}^\infty e^{-2t\rho^{2s}}\rho^{n-1}\varphi(\rho|x|)d\rho\\
&\leq c\int_{\frac{1}{2\pi|x|}}^\infty e^{-2t\rho^{2s}}\rho^{n-1}d\rho\\
&= c\int_{\frac{1}{2\pi|x|}}^\infty e^{-t\rho^{2s}}\left(e^{-t\rho^{2s}}\rho^{n-2s}\right)\rho^{2s-1}d\rho\\
&\leq c(t)\int_{(\frac{1}{2\pi|x|})^{2s}}^\infty e^{-tr}dr\\
&= c(t)e^{-t\left(\frac{1}{2\pi|x|}\right)^{2s}}\\
&\leq c(t)|x|^2
\end{aligned}
$$

for $|x|$ small enough. $\square$

6.7. Comments, problems and further results

(1) For $m > 1$ consider the diffusion distances generated by the elliptic operator defined in $\mathbb{R}^2$ by
$$L_m u = \frac{\partial^2 u}{\partial x^2} + m\frac{\partial^2 u}{\partial y^2}.$$
How are those metrics related to the Euclidean distance in the plane $\mathbb{R}^2$?

(2) In the general approach of Section 6.4, consider the limit cases $t \to 0$ and $t \to +\infty$ for $d_t^N(x,y)$.

(3) The introduction of diffusion metrics in the analysis of data sets was first provided by [**CL06**]. See also [**BBL$^+$17**].

(4) The result in the second section is contained in [**AAGM21b**].

CHAPTER 7

The dyadic fractional diffusion metric

7.1. Introduction

This chapter is devoted to consider a problem which is analogous to the one considered in the last section of Chapter 6. The analogy concerns the fractional aspect of the differential calculus involved in $(-\triangle)^s$. In some settings there are not integer orders of differentiation, nevertheless some fractional derivatives make sense. The difference of the subject considered here and that of Chapter 6 is given by the change of trigonometric bases by wavelets in $\mathbb{R}^+$. Even when we lose the translation or rotation invariance that was crucial for the results in Chapter 6, the diffusion distance generated by the Haar system is closely related to the dyadic metric on $\mathbb{R}^+$. The results of this chapter are contained in [**AAGM21b**].

7.2. Haar basis and dyadic diffusion

Let $\mathscr{D}$ be the family of all dyadic intervals in $\mathbb{R}^+ = \{x \geq 0\}$. Precisely

$$\mathscr{D} = \left\{ I_k^j = [k2^{-j}, (k+1)2^{-j}) \colon j \in \mathbb{Z}, k \in \mathbb{N}_0 \right\}.$$

With $\mathscr{D}^j = \left\{ I_k^j \colon k \in \mathbb{N}_0 \right\}$ we have that $\mathscr{D} = \bigcup_{j \in \mathbb{Z}} \mathscr{D}^j$.

Let $\mathscr{H} = \left\{ h_k^j = 2^{j/2} h_0^0 (2^j x - k) \colon j \in \mathbb{Z}, k \in \mathbb{N}_0 \right\}$ be the Haar wavelet system in $\mathbb{R}^+$, with $h_0^0 = \mathcal{X}_{[0,\frac{1}{2})}(x) - \mathcal{X}_{[\frac{1}{2},1)}(x)$, where as usual $\mathcal{X}_E$ denotes the indicator function of the set E. The family $\mathscr{H}$ constitutes an orthonormal basis of $L^2(\mathbb{R}^+)$. Let h_I denote the Haar wavelet supported on the dyadic interval I, so for $I = I_k^j$ we have that $h_I = h_k^j$. Let $I(h)$ denote the dyadic interval that supports the wavelet $h \in \mathscr{H}$.

Definition 7.1. The dyadic distance is defined by

$$\delta(x, y) = \inf \left\{ |I| : I \text{ is a dyadic interval containing } x \text{ and } y \right\}.$$

Notice that if $x \neq y$ there exists a smallest dyadic interval containing x and y, which we will denote by $I(x, y)$. Taking $I(x, x) = \{x\}$, we have that $\delta(x, y) = |I(x, y)|$ for every $x, y \in \mathbb{R}^+$.

The metric δ on $\mathbb{R}^+$ is not translation invariant and is an upper bound for the Euclidean. In fact $|x-y| \leq \delta(x,y)$. Of course, they are not equivalent. This means that $\delta(x,y)$ is in general much larger than $|x-y|$. Hence we could expect some better integrability properties of the powers of $\delta(x,y)$, locally and/or globally. Nevertheless, the behavior of the local and global integral properties of $\delta(x,y)$ are exactly the same as those of the powers of $|x-y|$. From a general point of view these properties are consequences of the fact that $\left(\mathbb{R}^+, \delta, m\right)$ is a normal or 1-Ahlfors regular space of homogeneous type (see [**MS79**]) without atoms and with infinite total Lebesgue measure m. Then the integrals of $\delta^\alpha(x,y)$, $\alpha \in \mathbb{R}$, inside $B_\delta(x,r)$ and outside $B_\delta(x,r)$, for $r>0$, are exactly the same as the integrals of $|x-y|^\alpha$ inside and outside the corresponding Euclidean balls $(x-r, x+r)$. In particular, the local and global singularity is provided by $\delta(x,y)^{-1} = \frac{1}{\delta(x,y)}$. Hence, the natural fractional integrals or Riesz type operators of the setting are given by kernels of the form $\delta(x,y)^{-1+s} = \frac{1}{\delta(x,y)^{1-s}}$ for $s>0$. So that the natural fractional differential operators are defined by kernels of the form $\delta(x,y)^{-1-s} = \frac{1}{\delta(x,y)^{1+s}}$ for $0<s<1$. Of course, as in the Euclidean case, the strong local singularity of this kernel needs for some regularity of the functions in the domain of the operator. As proved in [**AG18b**] the indicator function of a dyadic interval belongs to the class of Lipschitz-1 functions with respect to δ. In particular, the Haar wavelets in $\mathscr{H}$ are all smooth in this sense. Actually, for f bounded and Lipschitz-σ for $0<s<\sigma\leq 1$ we have that

$$D^s_{dy} f(x) = \int_{\mathbb{R}^+} \frac{f(y)-f(x)}{\delta(x,y)^{1+s}}\, dy$$

is well defined. We call $D^s_{dy} f$ the dyadic fractional Laplacian of f in $\mathbb{R}^+$.

The initial value problem

$$\begin{cases} \dfrac{\partial u}{\partial t}(x,t) = D^s_{dy} u(x,t) \\ u(x,0) = f(x) \end{cases}$$

was considered in [**AA16**] and, like in the Euclidean case, can be solved as an integral operator, which of course lacks the convolution structure. In fact

$$u(x,t) = \int_{\mathbb{R}^+} K_s(x,y;t) f(y)\, dy,$$

where

$$K_s(x,y;t) = \sum_{h\in\mathscr{H}} e^{-t|I(h)|^{-s}} h(x)h(y).$$

7.3. Dyadic fractional diffusion metric

With the kernel K_s obtained in the above section and the ideas in Chapter 6 we may try to define a fractional dyadic diffusion distance given, for $t > 0$ and $0 < s < 1$ by

$$d_t(x,y) = \sqrt{\int_{z\in\mathbb{R}^+} |K_s(x,z;t) - K_s(y,z;t)|^2 \, dy}.$$

In the next results we shall see the good definition and the metric character of d_t, and determine its spectral representation through the Haar wavelet system.

PROPOSITION 7.1. *Let $s > 0$ and $t > 0$ be given. Then d_t is well defined, is a metric on $\mathbb{R}^+$ and can be computed as*

$$d_t(x,y) = \sqrt{\sum_{h\in\mathscr{H}} e^{-2t|I(h)|^{-s}} |h(x) - h(y)|^2}.$$

PROOF. First, notice that the diffusion kernel $K_s(x,y;t)$ is well defined and finite for every $x, y \in \mathbb{R}^+$. Indeed, as $|h_I(w)| = |I|^{-\frac{1}{2}}\mathcal{X}_I(w)$ so

$$K_s(x,y;t) = \sum_{I\supseteq I(x,y)} e^{-t|I|^{-s}} h_I(x)h_I(y)$$

whose absolute series is bounded above by

$$\sum_{I\supseteq I(x,y)} |I|^{-1} = \sum_{j\in\mathbb{N}_0} 2^{-j}|I(x,y)|^{-1} = 2\,|I(x,y)|^{-1} = 2\delta(x,y)^{-1}.$$

By definition, d_t is the norm of the difference of the diffusion kernel at time t centered at two points in consideration, so the metric properties follow trivially. As well, by Parseval's identity

$$\begin{aligned} d_t(x,y)^2 &= \|K_s(x,\cdot;t) - K_s(y,\cdot;t)\|^2 \\ &= \left\| \sum_{h\in\mathscr{H}} e^{-t|I(h)|^{-s}} \left[h(x) - h(y)\right] h \right\|^2 \\ &= \sum_{h\in\mathscr{H}} e^{-2t|I(h)|^{-s}} |h(x) - h(y)|^2 . \end{aligned}$$

The finiteness of $d_t(x,y)$ will follow from the next results. □

Let us now proceed to determine the structure of d_t and compare it with the dyadic distance $\delta(x,y)$ on $\mathbb{R}^+$.

LEMMA 7.2. *Let $s > 0$. For $t > 0$ define*

$$\psi_t(\lambda) = \sqrt{\frac{2}{\lambda}\eta_t\left(\lambda^{-s}\right)}$$

with $\eta_t(\sigma) = 2e^{-2t\sigma} + \sum_{\ell\geq 1} 2^\ell e^{-2t2^{s\ell}\sigma}$. Then, when restricted to the sequence of integer powers of 2, $\{2^j : j \in \mathbb{Z}\}$, we have

(a) *ψ_t is strictly increasing;*

(b) *$\psi_t(0^+) = 0$;*

(c) *$\psi_t(+\infty) \simeq t^{-\frac{1}{2s}}$.*

PROOF. Define, for $i \in \mathbb{Z}$,

$$\begin{aligned} f(i) &:= \frac{1}{2}\,\psi_t^2(2^i) \\ &= 2^{1-i}e^{-2t2^{-is}} + \sum_{\ell\geq 1} 2^{\ell-i}e^{-2t2^{-is}2^{\ell s}} \\ &= 2^{1-i}e^{-2t2^{-is}} + \sum_{k=\ell-i\geq 1-i} 2^k e^{-2t2^{ks}}. \end{aligned}$$

Then

$$f(i+1) = 2^{-i}e^{-2t2^{-(i+1)s}} + \sum_{k\geq -i} 2^k e^{-2t2^{ks}}$$

and so

$$\begin{aligned} f(i+1) - f(i) &= 2^{-i}e^{-2t2^{-(i+1)s}} - 2.2^{-i}e^{-2t2^{-is}} + 2^{-i}e^{-2t2^{-is}} \\ &= 2^{-i}e^{-2t2^{-is}2^{-s}} - 2^{-i}e^{-2t2^{-is}} \\ &= 2^{-i}\left[\xi^{2^{-s}} - \xi\right] > 0 \end{aligned}$$

because the function ξ^x is monotone decreasing in the variable x (since $\xi := e^{-2t2^{-is}}$ is positive and less than one) and $2^{-s} < 1$. This shows that ψ_t^2 is an increasing function and therefore so is ψ_t, on account of its positivity. Thus (a) is proved.

To check (b) notice that

$$\lim_{i\to-\infty} f(i) = \lim_{i\to-\infty} 2^{1-i}e^{-2t2^{-is}} = 2\lim_{x\to+\infty} xe^{-2tx^s} = 0$$

and so

$$\lim_{i\to-\infty} \psi_t(2^i) = 0.$$

In order to prove (c) notice first that

$$\begin{aligned}
\lim_{i\to+\infty} f(i) &= \lim_{i\to+\infty} 2^{1-i}e^{-2t2^{-is}} + \sum_{k\in\mathbb{Z}} 2^k e^{-2t2^{ks}} \\
&= \sum_{k\in\mathbb{Z}} 2^k e^{-2t2^{ks}} \\
&< \sum_{k\in\mathbb{Z}} 2 \int_{2^{k-1}}^{2^k} e^{-2tx^s}\, dx \\
&= 2\int_0^{+\infty} e^{-2tx^s}\, dx < +\infty
\end{aligned}$$

which implies that $\lim_{i\to+\infty}\psi_t(2^i) = \psi_t(+\infty) < +\infty$. On the other hand, we attain a lower bound from

$$\sum_{k\in\mathbb{Z}} 2^k e^{-2t2^{ks}} > \sum_{k\in\mathbb{Z}} \int_{2^{k-1}}^{2^k} e^{-2tx^s}\, dx = \int_0^{+\infty} e^{-2tx^s}\, dx.$$

So, since $\psi_t(+\infty) = \sqrt{2\lim_{i\to+\infty} f(i)}$, we have

$$\sqrt{2}\, c_t(s) < \psi_t(+\infty) < 2\, c_t(s)$$

for $c_t(s) = \sqrt{\int_0^{+\infty} e^{-2tx^s}\, dx} = t^{-\frac{1}{2s}}\sqrt{\int_0^{+\infty} e^{-2x^s}\, dx}$. □

At this point it is important to remark that, in contrast with property (d) in Proposition 6.2, now for $0 < t_1 < t_2$ we have that $d_{t_2}(x,y) \le d_{t_1}(x,y)$ for every x, $y \in \mathbb{R}^+$. On the other hand, there is no constant $C > 0$ such that the inequality $d_{t_1}(x,y) \le C d_{t_2}(x,y)$ holds for every x, $y \in \mathbb{R}^+$. In fact, both observations above follow from the fact that

$$\frac{d_{t_2}^2(x,y)}{d_{t_1}^2(x,y)} \le e^{-2(t_2-t_1)\delta^{-s}(x,y)}$$

for every x and y in $\mathbb{R}^+$.

From Lemma 7.2 we can deduce that the graph of ψ_t is flatter as t increases and, conversely, it reaches higher values at infinity as t approaches zero.

THEOREM 7.3. *Let d_t be the fractional dyadic diffusion metric of order $s > 0$ at $t > 0$. Let ψ_t be as in Lemma 7.2 with $\psi_t(0) := 0$. Then*

(a) *$d_t(x,y) = \psi_t(\delta(x,y))$ for $x, y \in \mathbb{R}^+$;*

(b) *the family of d_t-balls, given as usual by $B_t(x,r) = \{y \in \mathbb{R}^+ : d_t(x,y) < r\}$ for $x \in \mathbb{R}^+$ and $r > 0$, coincides with $\mathscr{D}$, the family of all dyadic intervals.*

Proof. In order to prove (a), let us use the representation formula for d_t^2 provided by Proposition 7.1. For $x \neq y$,

$$
\begin{aligned}
d_t^2(x,y) &= \sum_{h:\, x\in I(h)\vee y\in I(h)} e^{-2t|I(h)|^{-s}} |h(x)-h(y)|^2 \\
&= e^{-2t|I(x,y)|^{-s}} \left|h_{I(x,y)}(x) - h_{I(x,y)}(y)\right|^2 \\
&\qquad + \sum_{h:\, x\in I(h)\wedge y\notin I(h)} e^{-2t|I(h)|^{-s}} |h(x)|^2 \\
&\qquad + \sum_{h:\, x\notin I(h)\wedge y\in I(h)} e^{-2t|I(h)|^{-s}} |h(y)|^2 \\
&= 4|I(x,y)|^{-1} e^{-2t|I(x,y)|^{-s}} + 2\sum_{\ell\geq 1} e^{-2t\left(2^{-\ell}|I(x,y)|\right)^{-s}} \left(2^{-\ell}|I(x,y)|\right)^{-1} \\
&= \frac{2}{|I(x,y)|}\left[2e^{-2t|I(x,y)|^{-s}} + \sum_{\ell\geq 1} 2^{\ell} e^{-2t|I(x,y)|^{-s}2^{\ell s}}\right] \\
&= \frac{2}{|I(x,y)|}\, \eta_t\left(|I(x,y)|^{-s}\right) \\
&= \frac{2}{\delta(x,y)}\, \eta_t\left(\frac{1}{\delta(x,y)^s}\right) \\
&= \psi_t^2\big(\delta(x,y)\big).
\end{aligned}
$$

Item (b) follows readily from the fact that for $0 < r < \psi_t(+\infty)$ we have

$$
B_t(x,r) = \left\{y \in \mathbb{R}^+ \colon \psi_t(\delta(x,y)) < r\right\} = I,
$$

where I is the largest dyadic interval containing x for which $\psi_t(|I|)$ is less than r. $\square$

7.4. Comments, problems and further results

(1) Let $f(x) = \mathcal{X}_{[0,1)}(x)$. Compute the Haar series for f and the series for the dyadic derivative of order $s \in (0,1)$ of f. What happens when $s \to 0^+$ and $s \to 1^-$?

(2) Prove that $\delta(x,y)$ is an ultra-metric in $\mathbb{R}^+$. That is, $\delta(x,y) = 0$ if and only if $x = y$, $\delta(x,y) = \delta(y,x)$ and $\delta(x,z) \leq \max\{\delta(x,y), \delta(y,z)\}$ for every x, y and z in $\mathbb{R}^+$.

(3) With the notation in Theorem 7.3 and $t > 0$, show that the d_t-balls are the dyadic intervals.

(4) The results in this chapter are contained in [**AAGM21b**].

CHAPTER 8

Divergence and Laplacian. A general approach to diffusion and diffusion metrics

8.1. Introduction

Taking as starting point for the basic operator defining diffusion the form div grad, we consider in this chapter a general form of a divergence operator that can be applied in several settings. In particular, in the discrete and useful case of weighted undirected graphs. We start by stating the definition of the Kirchhoff divergence in a very general setting containing all the further realizations of the basic theory. Then, we consider the derived metrization problem both in the general setting and in the special cases which are relevant in the applications. We also illustrate some particular instances of interest.

8.2. The generalized divergence

In this section we follow the lines of [**AG20**]. Let X be a set. Let $\mathscr{S}_1$ be a topological algebra of real valued functions defined on X. Let $\mathscr{S}_2$ be a topological algebra of functions defined on $X \times X$ taking also real values. Set $\mathscr{S}_1 \otimes \mathscr{S}_1$ to denote the set

$$\mathscr{S}_1 \otimes \mathscr{S}_1 = \{(\varphi \otimes \eta)(x,y) = \varphi(x)\eta(y) : \varphi \in \mathscr{S}_1 \text{ and } \eta \in \mathscr{S}_1\},$$

and $\sigma(\mathscr{S}_1 \otimes \mathscr{S}_1)$ to denote the linear span of $\mathscr{S}_1 \otimes \mathscr{S}_1$. A basic assumption relating $\mathscr{S}_1$ and $\mathscr{S}_2$ is in order. We assume, and we shall profusely illustrate it, that $\mathscr{S}_1 \otimes \mathscr{S}_1$ is continuously contained in $\mathscr{S}_2$ and that $\sigma(\mathscr{S}_1 \otimes \mathscr{S}_1)$ is dense in $\mathscr{S}_2$.

We shall denote with $\mathscr{S}_i'$, $i = 1, 2$, the dual spaces (topological), with single brackets $\langle\ ,\ \rangle$ the duality $\mathscr{S}_1$-$\mathscr{S}_1'$ and with double brackets $\langle\langle\ ,\ \rangle\rangle$ the duality $\mathscr{S}_2$-$\mathscr{S}_2'$.

Let us illustrate the above situation in a well known Euclidean case. Let $X = \mathbb{R}^n$ so $X \times X \simeq \mathbb{R}^{2n}$, and $\mathscr{S}_1 = \mathscr{S}(\mathbb{R}^n)$ the class of Schwartz functions on $\mathbb{R}^n$. The dual $\mathscr{S}_1' = \mathscr{S}'(\mathbb{R}^n)$ is the space of Schwartz tempered distributions. The action of $T \in \mathscr{S}_1'$ on $\varphi \in \mathscr{S}_1$ is denoted by $\langle T, \varphi\rangle \in \mathbb{R}$. On the other hand, $\mathscr{S}_2 = \mathscr{S}(\mathbb{R}^{2n})$ is the Schwartz class of smooth functions in $\mathbb{R}^{2n}$, and $\mathscr{S}_2' = \mathscr{S}'(\mathbb{R}^{2n})$ are the tempered distributions on $\mathbb{R}^{2n}$. Now, the action of $S \in \mathscr{S}_2'$ on a function $\Phi \in \mathscr{S}_2$ is denoted by $\langle\!\langle S, \Phi \rangle\!\rangle$. This notation of capital greek characters for the functions in $\mathscr{S}_2$ will be preserved in the sequel.

Let us start by showing how a given "distribution" $S \in \mathscr{S}_2'$ and a given "test function" $\Phi \in \mathscr{S}_2$ defines naturally a "distribution" $T \in \mathscr{S}_1'$.

LEMMA 8.1. *Let $S \in \mathscr{S}_2'$ and $\Phi \in \mathscr{S}_2$ be given and fixed. Then, the functional $\Sigma = \Sigma_{S,\Phi}$ defined for $\varphi \in \mathscr{S}_1$ by*

$$\langle \Sigma, \varphi \rangle = \langle\!\langle S, \varphi\Phi \rangle\!\rangle$$

is well defined and belongs to $\mathscr{S}_1'$.

PROOF. Let $\varphi \in \mathscr{S}_1$ be a test function on X. It is easy to deduce from the relation between $\mathscr{S}_1$ and $\mathscr{S}_2$ stated before, that the function $\varphi\Phi$ defined by $(\varphi\Phi)(x,y) = \varphi(x)\Phi(x,y)$ for $(x,y) \in X \times X$ also belongs to $\mathscr{S}_2$. Hence, since $S \in \mathscr{S}_2'$ we have that $\langle\!\langle S, \varphi\Phi \rangle\!\rangle$ is a well defined real number. Hence we have a well defined function from $\mathscr{S}_1$ to $\mathbb{R}$, by

$$\varphi \xrightarrow{\Sigma} \langle\!\langle S, \varphi\Phi \rangle\!\rangle \, .$$

The linearity of Σ is clear;

$$\langle \Sigma, \alpha\varphi_1 + \beta\varphi_2 \rangle = \langle\!\langle S, \alpha\varphi_1\Phi + \beta\varphi_2\Phi \rangle\!\rangle = \alpha \langle\!\langle S, \varphi_1\Phi \rangle\!\rangle + \beta \langle\!\langle S, \varphi_2\Phi \rangle\!\rangle = \alpha \langle \Sigma, \varphi_1 \rangle + \beta \langle \Sigma, \varphi_2 \rangle \, .$$

On the other hand, since $\mathscr{S}_1 \times \mathscr{S}_1$ is continuously contained in $\mathscr{S}_2$, we have, for $\varphi_n \to 0$ in $\mathscr{S}_1$ that $\varphi_n\Phi \to 0$ in $\mathscr{S}_2$ and, since S is continuous in $\mathscr{S}_2$, we have $\langle \Sigma, \varphi_n \rangle \to 0$ in $\mathbb{R}$. $\square$

Now we are in position to define the divergence or Kirchhoff divergence operator. But let us first give some heuristic idea underlying the precise definition. The objects S and T are structural to the model that we are considering. For example, S could be the matrix of weights of the edges $\mathcal{E} = \mathcal{V} \times \mathcal{V}$ of a graph and T the vector of weights of the vertices $\mathcal{V} = X$ of the graph. Given a function Φ on the edges (a vector field) we would like to find its divergence ψ, a function on the vertices (a scalar field) associated to the structure provided by S and T on the graph $(\mathcal{V}, \mathcal{E})$. Since we are looking for an operator that, in its more classical instances, is a differential operator, to wit the divergence, it is natural to expect that our definition should involve some frequencies forbidden operation of division of the distribution S by the distribution T. Nevertheless these two distributions belong to quite different settings $\mathscr{S}_2'$ and $\mathscr{S}_1'$. Lemma 8.1 helps us to transport S from $\mathscr{S}_2'$ to Σ in $\mathscr{S}_1'$. So that we shall look for a correct sense for the object

$$\operatorname{Kir}_{T,S}\Phi = \frac{\Sigma_{S,\Phi}}{T}.$$

Actually we shall be very demanding the object $\operatorname{Kir}_{T,S}\Phi$ since in all the important instances it becames a function in $\mathscr{S}_1$ with the same "regularity" of $\Phi \in \mathscr{S}_2$.

Definition 8.1 (Kirchhoff divergence of $\Phi \in \mathscr{S}_2$ with respect to $T \in \mathscr{S}_1'$ and $S \in \mathscr{S}_2'$). A function $\psi : X \to \mathbb{R}$ is said to be a Kirchhoff divergence of Φ with respect to T and S if

(a) $\varphi\psi \in \mathscr{S}_1$ for every $\varphi \in \mathscr{S}_1$;
(b) $\psi T = \Sigma_{S,\Phi}$.

Remark 8.1. Condition (b) above explicitly means that

$$\langle T, \varphi\psi\rangle = \langle\!\langle S, \varphi\Phi\rangle\!\rangle$$

for every $\varphi \in \mathscr{S}_1$.

Not always, but sometimes we have that for $f \in \mathscr{S}_1$ the function

$$\nabla f(x,y) = f(y) - f(x),$$

which we call the gradient of f, belongs to $\mathscr{S}_2$. Following the classical pattern for the Laplace operator as the iteration $\Delta = \operatorname{div}\operatorname{grad} = \nabla\cdot\nabla = \nabla^2$, we say that

$$\Delta_{S,T} f = \operatorname{Kir}_{S,T}(\nabla f),$$

when it exists, is a Laplacian for f with respect to S and T.

8.3. The classical Laplacian seen from the Kirchhoff divergence

In this section we aim to provide distributions $T \in \mathscr{D}'(\mathbb{R}^n)$ and $S \in \mathscr{D}'(\mathbb{R}^{2n})$ such that for a given smooth f we have that

$$\Delta f(x) = \operatorname{Kir}_{T,S}(f(y) - f(x)),$$

where Δ is the classical Laplacian in $\mathbb{R}^n$, i.e.

$$\Delta f(x) = \sum_{i=1}^{n} \frac{\partial^2 f}{\partial x_i^2}(x).$$

Let us start by the construction of the distribution $S \in \mathscr{D}'(\mathbb{R}^{2n})$. Let π be the Lebesgue n-dimensional measure on the diagonal of $\mathbb{R}^{2n}$. Precisely, for E a Borel set in $\mathbb{R}^{2n}$

define $\pi(E) = |\{x \in \mathbb{R}^n : (x, x) \in E\}|$, where the vertical bars denote the n-dimensional Lebesgue volume.

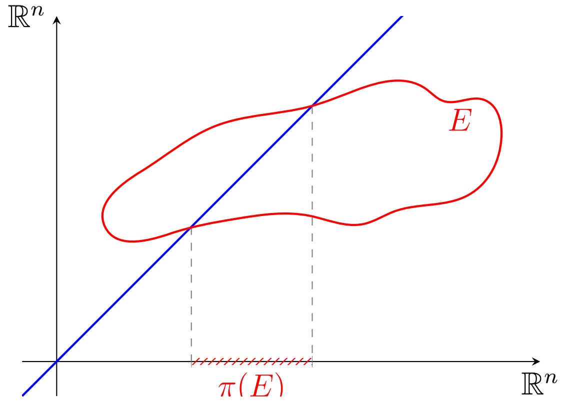


FIGURE 14. The action of π on a Borel set E of $\mathbb{R}^{2n}$.

Since π is a locally finite measure it defines a distribution in $\mathscr{D}'(\mathbb{R}^{2n})$; in fact, for a given $\Phi \in \mathscr{D}(\mathbb{R}^{2n}) = \mathscr{C}_c^\infty(\mathbb{R}^{2n})$,

$$\langle\!\langle \pi, \Phi \rangle\!\rangle = \iint_{\mathbb{R}^{2n}} \Phi(x, y) d\pi(x, y) = \int_{\mathbb{R}^n} \Phi(x, x) dx.$$

The support of π coincides with the diagonal of $\mathbb{R}^{2n}$. If we denote by (x, y) the points in $\mathbb{R}^{2n}$ and explicitly in terms of its coordinates $(x, y) = (x_1, \ldots, x_n; y_1, \ldots, y_n)$ any distribution in $\mathscr{D}'(\mathbb{R}^n)$ can be differentiated up to any order with respect to any to the variables $x_1, x_2, \ldots, x_n; y_1, y_2, \ldots, y_n$. In particular we may take all the pure second derivatives with respect to the variables y_j and add them in order to produce a new distribution in $\mathscr{D}'(\mathbb{R}^{2n})$. Let us proceed in this way with the distribution induced by π in $\mathbb{R}^{2n}$. Set

$$S = \sum_{j=1}^{n} \frac{\partial^2 \pi}{\partial y_j^2} \in \mathscr{D}'(\mathbb{R}^n).$$

PROPOSITION 8.2. *Let T be the Lebesgue measure Λ on $\mathbb{R}^n$, i.e. $\langle T, \varphi \rangle = \int_{\mathbb{R}^n} \varphi dx$. Let S as above. Then*

$$\Delta f(x) = \operatorname{Kir}_{\Lambda, S}(f(y) - f(x)).$$

PROOF. Let us first compute $\operatorname{Kir}_{\Lambda,S} \Phi$ for $\Phi \in \mathscr{D}(\mathbb{R}^{2n})$. Take $\varphi \in \mathscr{D}(\mathbb{R}^n)$, then

$$\begin{aligned}
\langle\!\langle S, \varphi\Phi \rangle\!\rangle &= \sum_{j=1}^{n} \left\langle\!\!\left\langle \frac{\partial^2 \pi}{\partial y_j^2}, \varphi\Phi \right\rangle\!\!\right\rangle \\
&= \sum_{j=1}^{n} \left\langle\!\!\left\langle \pi, \frac{\partial^2}{\partial y_j^2} \varphi\Phi \right\rangle\!\!\right\rangle
\end{aligned}$$

$$
\begin{aligned}
&= \sum_{j=1}^{n} \left\langle\!\left\langle \pi, \varphi(x) \frac{\partial^2 \Phi}{\partial y_j^2} \right\rangle\!\right\rangle \\
&= \sum_{j=1}^{n} \int_{\mathbb{R}^n} \varphi(x) \frac{\partial^2 \Phi}{\partial y_j^2}(x,x) dx \\
&= \int_{\mathbb{R}^n} \varphi(x) \left(\sum_{j=1}^{n} \frac{\partial^2 \Phi}{\partial y_j^2}(x,x) \right) d\Lambda(x) \\
&= \langle T, \varphi \Delta_y \Phi \rangle \\
&= \langle T, \varphi \psi \rangle ,
\end{aligned}
$$

so that $\psi(x) = (\Delta_y \Phi)(x,x)$ is a Kirchhoff divergence of Φ associated to T and S. Taking $\Phi(x,y) = f(y) - f(x)$, we have $(\Delta_y \Phi)(x,y) = \Delta f(y)$. So that

$$
\psi(x) = (\Delta_y \Phi)(x,x) = \Delta f(x),
$$

as desired. □

8.4. Fractional Kirchhoff divergence and fractional Laplacian

In Section 6.6 of Chapter 6 we introduced the fractional powers $(-\Delta)^s$ of the Laplacian, in terms of the Fourier Transform,

$$
((-\Delta)^s f)\widehat{\ }(\xi) = (2\pi)^{2s} |\xi|^{2s} \widehat{f}(\xi).
$$

Which recovers the Laplacian when $s = 1$. The kernel approach to the operator $(-\Delta)^s$ for $0 < s < 1$ with $|x-y|^{-(n+2s)}$ becomes more singular as s increases. For $0 < s < \frac{1}{2}$ the kernel is less singular and is well defined on Hölder-Lipschitz classes. This fact allows the extension of the case $0 < s < \frac{1}{2}$ to metric spaces. For $\frac{1}{2} \leq s < 1$, instead, more regularity is required and the integrals have to be taken as principal values. The formal aspect of the kernel approach to $(-\Delta)^s$ is given by

$$
(-\Delta)^s f(x) = \int_{\mathbb{R}^n} \frac{f(y) - f(x)}{|x-y|^{n+2s}} dy.
$$

In this section we aim to write $(-\Delta)^s$ in the factorized div grad form as we did in the previous section for the case $s = 1$. The integral expression above shows clearly the basic order zero gradient $f(y) - f(x)$ of f. So that we have to find a Kirchhoff divergence operator allowing us to write $(-\Delta)^s$ in the frame of Section 8.2 above. Let us consider the case $0 < s < \frac{1}{2}$.

LEMMA 8.3. *Let* $0 < s < \frac{1}{2}$. *Then*

(a) *the function* $g(x,y) = \frac{\Phi(x,y)-\Phi(x,x)}{|x-y|^{n+2s}}$ *belongs to* $L^1(\mathbb{R}^{2n})$ *for every* $\Phi \in \mathscr{D}(\mathbb{R}^{2n})$*;*

(b) *the linear functional* $S : \mathscr{D}(\mathbb{R}^{2n}) \to \mathbb{R}$ *given by*

$$\langle\langle S, \Phi \rangle\rangle = \iint_{\mathbb{R}^{2n}} \frac{\Phi(x,y)-\Phi(x,x)}{|x-y|^{n+2s}} dxdy$$

defines a distribution in $\mathscr{D}'(\mathbb{R}^{2n})$.

PROOF. Let K be a compact set in $\mathbb{R}^n$ containing the projection in the variables x of the support of Φ, i.e. $\operatorname{supp}\Phi \subset K \times \mathbb{R}^n$. Set ω_{n-1} to denote the surface area of the unit sphere of $\mathbb{R}^n$. Then

$$\begin{aligned}
&\iint_{\mathbb{R}^{2n}} \frac{\Phi(x,y)-\Phi(x,x)}{|x-y|^{n+2s}} dxdy \\
&= \int_K \int_{\mathbb{R}^n} \frac{\Phi(x,y)-\Phi(x,x)}{|x-y|^{n+2s}} dydx \\
&\le \int_K \left\{ \int_{|x-y|<1} \frac{\Phi(x,y)-\Phi(x,x)}{|x-y|^{n+2s}} dy + 2\left\|\Phi\right\|_\infty \int_{|x-y|\ge 1} \frac{dy}{|x-y|^{n+2s}} dy \right\} dx \\
&\le \int_K \left\{ \int_{|x-y|<1} \frac{\left\|\nabla_y \Phi\right\|_\infty |x-y|}{|x-y|^{n+2s}} dy + \frac{\omega_{n-1}\left\|\Phi\right\|_\infty}{s} \right\} dx \\
&= \omega_{n-1} |K| \left(\frac{\left\|\nabla_y \Phi\right\|_\infty}{1-2s} + \frac{\left\|\Phi\right\|_\infty}{s} \right).
\end{aligned}$$

This proves (a). The linearity of S is clear. In order to prove the continuity of the functional

$$\langle\langle S, \Phi \rangle\rangle = \iint_{\mathbb{R}^{2n}} \frac{\Phi(x,y)-\Phi(x,x)}{|x-y|^{n+2s}} dxdy$$

defined for $\Phi \in \mathscr{D}(\mathbb{R}^{2n})$, take a sequence $\{\Phi_k : k \ge 1\} \subset \mathscr{D}(\mathbb{R}^{2n})$ that tends to zero in the inductive limit topology of $\mathscr{D}(\mathbb{R}^{2n})$. This means that there exists a compact set $\mathbb{K}$ in $\mathbb{R}^{2n}$ containing the supports of the Φ_k's, i.e. $\mathbb{K} \supset \cup_{k\ge 1} \operatorname{supp}\Phi_k$, and all the derivatives of Φ_k converge uniformly to zero in $\mathbb{R}^{2n}$. Let K be the projection of $\mathbb{K}$ in the $x = (x_1, \dots, x_n)$ variables of $\mathbb{R}^{2n}$. Now, from the estimate above we have that

$$\begin{aligned}
|\langle\langle S, \Phi_k \rangle\rangle| &\le \int_K \int_{\mathbb{R}^n} \frac{\Phi_k(x,y)-\Phi_k(x,x)}{|x-y|^{n+2s}} dxdy \\
&\le \omega_{n-1} |K| \left(\frac{\left\|\nabla_y \Phi_k\right\|_\infty}{1-2s} + \frac{\left\|\Phi_k\right\|_\infty}{s} \right),
\end{aligned}$$

which tends to zero when k tends to infinity. □

The distribution S built in Lemma 8.3 and the distribution T provided by the Lebesgue measure on $\mathbb{R}^n$ give the basic ingredients, through Lemma 8.1, to obtain a Kirchhoff divergence operator $\operatorname{Kir}_{T,S}\Phi$ defined for $\Phi \in \mathscr{D}(\mathbb{R}^{2n})$.

LEMMA 8.4. *Let $0 < s < \frac{1}{2}$. For each function $\Phi \in \mathscr{D}(\mathbb{R}^{2n})$ the function ψ defined on $\mathbb{R}^n$ by*

$$\psi(x) = \int_{\mathbb{R}^n} \frac{\Phi(x,y) - \Phi(x,x)}{|x-y|^{n+2s}} dy$$

belongs to $\mathscr{D}(\mathbb{R}^n)$ and

$$\|\psi\|_\infty \leq \omega_{n-1} \left(\frac{\|\nabla_y \Phi\|_\infty}{1-2s} + \frac{\|\Phi\|_\infty}{s} \right).$$

PROOF. For x outside the first projection of the support of Φ we have, clearly, that $\psi(x) = 0$. Notice that, changing variables,

$$\psi(x) = \int_{\mathbb{R}^n} \frac{\Phi(x, x-y) - \Phi(x,x)}{|y|^{n+2s}} dy.$$

So that the differentiability of ψ follows from that of Φ. Finally, as we proved in the previous lemma

$$|\psi(x)| \leq \omega_{n-1} \left(\frac{\|\nabla_y \Phi\|_\infty}{1-2s} + \frac{\|\Phi\|_\infty}{s} \right)$$

for every x, and we are done. □

PROPOSITION 8.5. *Let $0 < s < \frac{1}{2}$ be given. Let S be the distribution defined in Lemma 8.3. Take T as the Lebesgue measure on $\mathbb{R}^n$. Then, the function ψ provided by Lemma 8.4 is a Kirchhoff divergence of $\Phi \in \mathscr{D}(\mathbb{R}^{2n})$ with respect to T and S. In other words*

$$\psi(x) = \operatorname{Kir}_{T,S}\Phi(x) = \int_{y\in\mathbb{R}^n} \frac{\Phi(x,y) - \Phi(x,x)}{|x-y|^{n+2s}} dy.$$

PROOF. We only have to check (b) in Definition 8.1, that is

$$\langle T, \varphi\psi \rangle = \langle\!\langle S, \varphi\Phi \rangle\!\rangle$$

for every $\varphi \in \mathscr{D}(\mathbb{R}^n)$. Take $\varphi \in \mathscr{D}(\mathbb{R}^n)$. Then

$$\begin{aligned}
\langle\!\langle S, \varphi\Phi \rangle\!\rangle &= \iint_{\mathbb{R}^{2n}} \frac{\varphi(x)\Phi(x,y) - \varphi(x)\Phi(x,x)}{|x-y|^{n+2s}} dxdy \\
&= \int_{\mathbb{R}^n} \varphi(x) \left(\int_{\mathbb{R}^n} \frac{\Phi(x,y) - \Phi(x,x)}{|x-y|^{n+2s}} dy \right) dx
\end{aligned}$$

$$
\begin{aligned}
&= \int_{\mathbb{R}^n} \varphi(x)\psi(x)dx \\
&= \langle T, \varphi\psi \rangle ,
\end{aligned}
$$

as desired. □

We are in position to state the main result of this section.

THEOREM 8.6. *Let* $0 < s < \frac{1}{2}$. *Let* T *be the Lebesgue measure on* $\mathbb{R}^n$ *and* S *the distribution in* $\mathscr{D}'(\mathbb{R}^{2n})$ *provided by Lemma 8.3, i.e.*

$$
\langle\langle S, \Phi \rangle\rangle = \iint_{\mathbb{R}^{2n}} \frac{\Phi(x,y) - \Phi(x,x)}{|x-y|^{n+2s}} dxdy.
$$

Then, for f *bounded with bounded gradient we have*

$$
(-\Delta)^s f(x) = \mathrm{Kir}_{T,S}(f(y) - f(x)).
$$

PROOF. The estimate for ψ given in Lemma 8.4 shows that $\mathrm{Kir}_{T,S}$ is well defined for $\Phi(x,y) = f(y) - f(x)$ with f and its gradient in $L^\infty(\mathbb{R}^n)$. Now

$$
\begin{aligned}
\mathrm{Kir}_{T,S}(f(y) - f(x)) &= \int_{y \in \mathbb{R}^n} \frac{(f(y) - f(x)) - (f(x) - f(x))}{|x-y|^{n+2s}} dy \\
&= \int_{y \in \mathbb{R}^n} \frac{f(y) - f(x)}{|x-y|^{n+2s}} dy \\
&= (-\Delta)^{\frac{s}{2}} f(x).
\end{aligned}
$$

□

8.5. The fractional Laplacian as a $\mathrm{Kir}_{T,S}$ grad operator for the case $\frac{1}{2} \le s < 1$

When $\frac{1}{2} \le s < 1$ and $\Phi \in \mathscr{D}(\mathbb{R}^{2n})$ the function $\frac{\Phi(x,y)-\Phi(x,x)}{|x-y|^{n+2s}}$ is generally not absolutely integrable in $\mathbb{R}^{2n}$ and the distribution S used in Section 8.4 is no longer valid. Nevertheless, the distribution can be defined correctly as a principal value.

LEMMA 8.7. *Let* $\frac{1}{2} \le s < 1$. *For* $\varepsilon > 0$ *let us denote with* B_ε *the* ε*-band about the diagonal of* $\mathbb{R}^n \times \mathbb{R}^n$, *i.e.* $B_\varepsilon = \{(x,y) \in \mathbb{R}^n \times \mathbb{R}^n : |x-y| < \varepsilon\}$. *Set* B_ε^c *to denote the complement,* $\mathbb{R}^n \times \mathbb{R}^n \setminus B_\varepsilon$, *of* B_ε. *Then*

(a) *for* $\Phi \in \mathscr{D}(\mathbb{R}^{2n})$, *the*

$$
\lim_{\varepsilon \to 0} \iint_{B_\varepsilon^c} \frac{\Phi(x,y) - \Phi(x,x)}{|x-y|^{n+2s}} dxdy
$$

exists and is finite;

(b) *the application* $S : \mathbb{R}^{2n} \to \mathbb{R}$ *given by*

$$\Phi \xrightarrow{S} \lim_{\varepsilon\to 0} \iint_{B_\varepsilon^c} \frac{\Phi(x,y)-\Phi(x,x)}{|x-y|^{n+2s}} dxdy$$

defines a distribution in $\mathscr{D}'(\mathbb{R}^{2n})$.

Proof. With $\nabla_y \Phi$ we denote the gradient operator of $\Phi(x,\cdot)$ as a function of the second variables $y = (y_1,\dots,y_n)$, for x fixed in $\mathbb{R}^n$. That is

$$\nabla_y \Phi(x,y) = \sum_{i=1}^n \frac{\partial \Phi}{\partial y_i}(x,y) e_i,$$

where $\{e_i : i = 1,\dots,n\}$ is the canonical basis of $\mathbb{R}^n$. It is clear that the fact that s is now large, $s \geq \frac{1}{2}$, improves the integrability of $\frac{\Phi(x,y)-\Phi(x,x)}{|x-y|^{n+2s}}$ at infinity. Let us see this by estimating precisely the integrals

$$\iint_{B_\varepsilon^c} \frac{\Phi(x,y)-\Phi(x,x)}{|x-y|^{n+2s}} dxdy,$$

for $\varepsilon > 0$. Let $\Phi \in \mathscr{D}(\mathbb{R}^{2n})$ be given, and let K be a compact set in $\mathbb{R}^n$ such that $\operatorname{supp}\Phi \subset K \times \mathbb{R}^n$. Then

$$\begin{aligned}\iint_{B_\varepsilon^c} \frac{\Phi(x,y)-\Phi(x,x)}{|x-y|^{n+2s}} dxdy &= \int_{x\in K} \left(\int_{|x-y|>\varepsilon} \frac{\Phi(x,y)-\Phi(x,x)}{|x-y|^{n+2s}} dy \right) dx \\ &\leq C_{n,s} \|\Phi\|_\infty |K| \varepsilon^{-2s}.\end{aligned}$$

Notice now that for $0 < \varepsilon < 1$,

$$\begin{aligned}\int_{\varepsilon\leq|x-y|<1} \frac{\nabla_y\Phi(x,x)\cdot(x-y)}{|x-y|^{n+2s}} dy &= \sum_{j=1}^n \frac{\partial\Phi}{\partial y_j}(x,x) \int_{\varepsilon\leq|x-y|<1} \frac{x_j-y_j}{|x-y|^{n+2s}} dy \\ &= \sum_{j=1}^n \frac{\partial\Phi}{\partial y_j}(x,x) \int_{\varepsilon\leq|y|<1} \frac{y_j}{|y|^{n+2s}} dy = 0,\end{aligned}$$

since each $\frac{y_j}{|y|^{n+2s}}$ is bounded and odd in the symmetric annulus $\{y : \varepsilon \leq |y| < 1\}$. So that we may write

$$\begin{aligned}I_\varepsilon &= \iint_{B_\varepsilon^c} \frac{\Phi(x,y)-\Phi(x,x)}{|x-y|^{n+2s}} dxdy \\ &= \int_{x\in K} \left(\int_{\varepsilon\leq|x-y|<1} \frac{\Phi(x,y)-\Phi(x,x)-\nabla_y\Phi(x,x)\cdot(y-x)}{|x-y|^{n+2s}} dy \right. \\ &\qquad\qquad \left. + \int_{|x-y|\geq 1} \frac{\Phi(x,y)-\Phi(x,x)}{|x-y|^{n+2s}} dy \right) dx.\end{aligned}$$

In order to prove the convergence of I_ε as $\varepsilon \to 0$, let us check the Cauchy character of $\{I_\varepsilon : 0 < \varepsilon < 1\}$. Take $0 < \delta < \varepsilon < 1$. Then from the formula for I_ε we get

$$\begin{aligned} |I_\delta - I_\varepsilon| &= \left| \int_{x\in K} \left(\int_{\delta \le |x-y| < \varepsilon} \frac{\Phi(x,y) - \Phi(x,x) - \nabla_y \Phi(x,x)\cdot(y-x)}{|x-y|^{n+2s}} dy \right) dx \right| \\ &\le \int_{x\in K} \int_{\delta\le|x-y|<\varepsilon} \sup_{\alpha=2} \left\| \partial_y^\alpha \Phi \right\|_\infty \frac{|x-y|^2}{|x-y|^{n+2s}} dy dx \\ &= C_{n,s} |K| \sup_{\alpha=2} \left\| \partial_y^\alpha \Phi \right\|_\infty (\varepsilon^{2(1-s)} - \delta^{2(1-s)}), \end{aligned}$$

which tends to zero for $\varepsilon \to 0$.

It is easy to check that the application $S : \mathscr{D}(\mathbb{R}^{2n}) \to \mathbb{R}$ defined by

$$\langle\langle S, \Phi \rangle\rangle = \lim_{\varepsilon\to 0} \iint_{B_\varepsilon^c} \frac{\Phi(x,y) - \Phi(x,x)}{|x-y|^{n+2s}} dx dy$$

is linear.

To prove that $S \in \mathscr{D}'(\mathbb{R}^{2n})$, we only need to check its continuity. Consider a sequence $\{\Phi_k : k \ge 1\} \subset \mathscr{D}(\mathbb{R}^{2n})$ such that $\Phi_k \to 0$ in $\mathscr{D}(\mathbb{R}^{2n})$ as $k \to \infty$. Then, there exists a compact set $\mathbb{K}$ in $\mathbb{R}^{2n}$ with $\mathbb{K} \supset \cup_{k\ge 1} \operatorname{supp} \Phi_k$ and $\partial^\alpha \Phi_k \rightrightarrows 0$ uniformly for every multi-index $\alpha \in (\mathbb{N}\cup\{0\})^{2n}$. Let K be a compact set in $\mathbb{R}^n$ such that $K \times \mathbb{R}^n \supseteq \mathbb{K}$, then

$$\begin{aligned} |\langle\langle S, \Phi_k \rangle\rangle| &= \lim_{\varepsilon\to 0} \left| \int_{x\in K} \left(\int_{\varepsilon\le|x-y|<1} \frac{\Phi_k(x,y) - \Phi_k(x,x) - \nabla_y \Phi_k(x,x)\cdot(y-x)}{|x-y|^{n+2s}} dy \right.\right. \\ &\qquad \left.\left. + \int_{|x-y|\ge 1} \frac{\Phi_k(x,y) - \Phi_k(x,x)}{|x-y|^{n+2s}} dy \right) dx \right| \\ &\le \limsup_{\varepsilon\to 0} \int_{x\in K} \int_{\varepsilon\le|x-y|<1} \frac{|\Phi_k(x,y) - \Phi_k(x,x) - \nabla_y \Phi_k(x,x)\cdot(y-x)|}{|x-y|^{n+2s}} dy dx \\ &\qquad + c_{n,s} \|\Phi_k\|_\infty |K| \\ &\le c_{n,s} |K| \left(\sup_{|\alpha|=2} \|\partial^\alpha \Phi_k\|_\infty + \|\Phi_k\|_\infty \right), \end{aligned}$$

which tends to zero for $k \to \infty$. $\square$

LEMMA 8.8. *For $\Phi \in \mathscr{D}(\mathbb{R}^{2n})$ we have*

$$\psi(x) = \lim_{\varepsilon\to 0} \int_{|x-y|>\varepsilon} \frac{\Phi(x,y) - \Phi(x,x)}{|x-y|^{n+2s}} dy$$

is a well defined continuous function with compact support in $\mathbb{R}^n$.

PROOF. Set

$$\psi_\varepsilon(x) = \int_{\{y:|x-y|>\varepsilon\}} \frac{\Phi(x,y)-\Phi(x,x)}{|x-y|^{n+2s}}dy.$$

The above arguments allows proving that $\{\psi_\varepsilon : \varepsilon > 0\}$ is of Cauchy type in the uniform norm on the compact K with $K \times \mathbb{R}^n \supset \operatorname{supp}\Phi$. □

THEOREM 8.9. *Let T be the distribution in $\mathbb{R}^n$ induced by the Lebesgue measure. Let S be the distribution provided by Lemma 8.7. Then*

(a) *for $\Phi \in \mathscr{D}(\mathbb{R}^{2n})$*

$$\operatorname{Kir}_{T,S}\Phi(x) = \lim_{\varepsilon\to 0^+}\int_{|x-y|\geq\varepsilon} \frac{\Phi(x,y)-\Phi(x,x)}{|x-y|^{n+2s}}dy;$$

(b) *for $\varphi \in \mathscr{D}(\mathbb{R}^n)$*

$$(-\Delta)^s\varphi(x) = \operatorname{Kir}_{T,S}(\varphi(s)-\varphi(x)).$$

PROOF. We have only to check (a). Take $\Phi \in \mathscr{D}(\mathbb{R}^{2n})$ and φ any test function in $\mathscr{D}(\mathbb{R}^n)$. Then

$$\begin{aligned}
\langle\!\langle S, \varphi\Phi\rangle\!\rangle &= \lim_{\varepsilon\to 0^+}\iint_{B_\varepsilon^c} \frac{\varphi(x)\Phi(x,y)-\varphi(x)\Phi(x,x)}{|x-y|^{n+2s}}dxdy\\
&= \lim_{\varepsilon\to 0^+}\int_{\mathbb{R}^n}\varphi(x)\left(\int_{|x-y|\geq\varepsilon}\frac{\Phi(x,y)-\Phi(x,x)}{|x-y|^{n+2s}}dy\right)dx.
\end{aligned}$$

Hence, from Lemma 8.8 and the Lebesgue dominated convergence theorem, we have

$$\begin{aligned}
\langle\!\langle S, \varphi\Phi\rangle\!\rangle &= \int_{\mathbb{R}^n}\varphi(x)\left(\lim_{\varepsilon\to 0^+}\int_{|x-y|\geq\varepsilon}\frac{\Phi(x,y)-\Phi(x,x)}{|x-y|^{n+2s}}dy\right)dx\\
&= \int_{\mathbb{R}^n}\varphi(x)\psi(x)dx\\
&= \langle T, \varphi\psi\rangle\,,
\end{aligned}$$

for every $\varphi \in \mathscr{D}(\mathbb{R}^n)$. Therefore ψ is a Kirchhoff divergence of Φ with respect to T and S. □

8.6. The case of S and T given by locally finite measures

Let $X = (X,\tau)$ be a locally compact topological space. With our abstract approach in the search of Kirchhoff divergences, take $\mathscr{S}_1 = \mathscr{C}_c(X)$, the space of compactly supported continuous functions with real values defined on X. Let $\mathscr{S}_2 = \mathscr{C}_c(X\times X)$ the space of compactly supported continuous functions with real values defined on $X\times X$. Borel measures which are finite on compact sets of X and $X \times X$ provide the distributions in $\mathscr{S}_1'$ and $\mathscr{S}_2'$ respectively. Given a measure μ on the Borel sets of X that is finite on compact sets of X, it defines the distribution

$$\langle T_\mu, \varphi\rangle = \int_X \varphi d\mu,$$

with $\varphi \in \mathscr{S}_1$. That is, T_μ is linear and continuous on $\mathscr{S}_1$. On the other hand, given a Borel measure π on $X \times X$ that is finite on the compact subsets of $X \times X$, it defines the distribution

$$\langle\langle S_\pi, \Phi\rangle\rangle = \iint_{X\times X} \Phi d\pi,$$

with $\Phi \in \mathscr{S}_2$.

Lemma 8.10. *Let X, $\mathscr{S}_1$, $\mathscr{S}_2$, $\mathscr{S}_1'$, $\mathscr{S}_2'$, μ and π be as before. Then, ψ is a Kirchhoff divergence of $\Phi \in \mathscr{S}_2$ if and only if ψ satisfies*

$$\int_X \varphi\psi d\mu = \iint_{X\times X} \varphi\Phi d\pi \tag{8.1}$$

for every $\varphi \in \mathscr{S}_1$.

Proof. Just write the equation

$$\langle T_\mu, \varphi\psi\rangle = \langle\langle S_\pi, \varphi\Phi\rangle\rangle$$

by the definitions of T_μ and S_π. $\square$

In this case we write $\mathrm{Kir}_{\mu,\pi}\Phi$ instead of $\mathrm{Kir}_{T_\mu,S_\pi}\Phi$ to denote the function ψ. It is worthy realizing that equation (8.1) may have no solution or more than one solution.

Example 1. Let $X = [0,1]$ with its usual topology. Take $\mu = \delta_0$ the Dirac delta and $d\pi = dxdy$, the area probability measure on $X \times X = [0,1]^2$. Then for a continuous function ψ and every $\varphi \in \mathscr{C}([0,1])$ equation (8.1) reads

$$\varphi(0)\psi(0) = \int_{[0,1]} \varphi\psi d\delta_0 = \iint_{[0,1]^2} \varphi(x)\Phi(x,y)dxdy.$$

Thus, if we take $\Phi \equiv 1$ on $[0,1]^2$, we have $\varphi(0)\psi(0) = \int_{[0,1]} \varphi(x)dx$, for every $\varphi \in \mathscr{C}([0,1])$. For $\varphi \in \mathscr{C}([0,1])$ with $\varphi(0) = 0$ and $\int_{[0,1]} \varphi = 1$ we have $0\cdot\psi(0) = 1$, which has no solution in $\mathscr{C}([0,1])$.

Example 2. Let X, $\mathscr{S}_1$, $\mathscr{S}_2$ be as in Example 1. Take again two probability measures $\mu = \delta_0$ in $[0,1]$ and $\pi = \delta_0 \times \delta_0$ in $[0,1]^2$. Again, when considering $\Phi \equiv 1$

equation (8.1) gives $\varphi(0)\psi(0) = \varphi(0)\Phi(0,0) = \varphi(0)$. So that any $\psi \in \mathscr{C}([0,1])$ such that $\psi(0) = 1$ is a solution of (8.1).

The situation becomes more interesting when, in some sense, π is a "coupling" for μ. Let us precise this fact in two cases which reflect independence and determinism.

THEOREM 8.11. *Let X, $\mathscr{S}_1$, $\mathscr{S}_2$ be as before. Let μ be a positive Borel measure on X which is finite on compact subsets of X. Assume that $\pi = \pi_1 \times \pi_2$ with π_1 absolutely continuous with respect to μ and π_2 a Borel measure on X which is finite on the compact subsets of X. Then, if $\frac{d\pi_1}{d\mu}$ denotes the Radon-Nikodym derivative of π_1 with respect to μ and $\Phi \in \mathscr{S}_2$, we have that*

$$\operatorname{Kir}_{\mu,\pi} \Phi(x) = \frac{d\pi_1}{d\mu}(x) \int_{y\in X} \Phi(x,y) d\pi_2(y)$$

is a Kirchhoff divergence for Φ with respect to μ and π. Also, when $\pi_2(X) < \infty$ and f is continuous and bounded, we have a μ,π-Laplacian of f given by

$$\Delta_{\mu,\pi} f(x) = \frac{d\pi_1}{d\mu}(x) \left(\int_{y\in X} f(y) d\pi_2(y) - f(x)\pi_2(X) \right).$$

In particular f is μ,π-harmonic if and only if f is constant,

$$f(x) = \frac{1}{\pi_2(X)} \int_{y\in X} f(y) d\pi_2(y).$$

PROOF. For $\varphi \in \mathscr{S}_1$ and $\Phi \in \mathscr{S}_2$ we have

$$\begin{aligned}
\iint_{X\times X} \varphi\Phi d\pi &= \int_{x\in X} \varphi(x) \left(\int_{y\in X} \Phi(x,y) d\pi_2(y) \right) d\pi_1(x) \\
&= \int_{x\in X} \varphi(x) \left[\frac{d\pi_1}{d\mu}(x) \int_{y\in X} \Phi(x,y) d\pi_2(y) \right] d\mu(x) \\
&= \int_{x\in X} \varphi(x)\psi(x) d\mu(x).
\end{aligned}$$

□

For deterministic coupling we have the following result.

THEOREM 8.12. *Let (X,τ) be a locally compact topological space. Let μ be a Borel measure on X such that $\mu(K) < \infty$ for every compact set K of X. Let F be a given continuous function from X to X.*

Let $G : X \to X \times X$ be given by

$$G(x) = (x, F(x)).$$

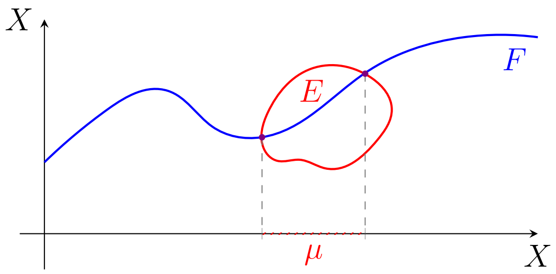


FIGURE 15. Deterministic coupling.

Let π be the measure defined on the Borel subsets of $X \times X$ by

$$\pi = \mu \circ G^{-1}.$$

Precisely, for E a Borel subset of $X \times X$,

$$\pi(E) = \mu(G^{-1}(E)) = \mu(\{x \in X : (x, F(x)) \in E\}).$$

Then, for $\Phi \in \mathscr{S}_2 = \mathscr{C}_c(X \times X)$ we have that the function

$$\mathrm{Kir}_{\mu,\pi}\, \Phi(x) = \Phi(x, F(x))$$

is a Kirchhoff divergence of Φ with respect to μ and π. Moreover, for $f : X \to \mathbb{R}$ continuous we have a well defined Laplacian of f with respect to μ and π and is explicitly given by

$$\Delta_{\mu,\pi} f = f \circ F - f.$$

PROOF. Let us start by proving a basic formula which allows us computing integrals with respect to π in terms of integrals with respect to μ. Notice that for E a Borel subset of $X \times X$, if we denote by $\mathcal{X}_E = \mathcal{X}_E(x, y)$ the indicator function of E, the definition of π in terms of μ gives

$$\begin{aligned}\iint_{X\times X} \mathcal{X}_E(x, y) d\pi(x, y) = \pi(E) = \mu(G^{-1}(E))&\\ = \int_X \mathcal{X}_{G^{-1}(E)}(x) d\mu(x)&\\ = \int_X \mathcal{X}_E(x, F(x)) d\mu(x).&\end{aligned}$$

Now, with standard arguments in measure theory, the last formula

$$\iint_{X\times X} \mathcal{X}_E d\pi = \int_X \mathcal{X}_E(x, F(x)) d\mu(x)$$

extends to functions $\Theta \in \mathscr{S}_2$ to provide

$$\iint_{X\times X} \Theta d\pi = \int_X \Theta(x, F(x))d\mu(x).$$

Let us apply the last formula to $\Theta(x,y) = \varphi(x)\Phi(x,y)$ with any $\varphi \in \mathscr{S}_1$ and $\Phi \in \mathscr{S}_2$. Then

$$\int_{X\times X} \varphi(x)\Phi(x,y)d\pi(x,y) = \int_X \varphi(x)\Phi(x,F(x))d\mu(x)$$

for every $\varphi \in \mathscr{S}_1$. Which is equation (8.1) from Lemma 8.10 for every $\varphi \in \mathscr{S}_1$. Hence $\Phi(x,F(x))$ works as a divergence for Φ with respect to μ and π. Now the formula for the Laplace type operator follows readily by taking $\Phi(x,y) = f(y) - f(x)$,

$$\begin{aligned}\Delta_{\mu,\pi} f(x) &= \mathrm{Kir}_{\mu,\pi}(f(y) - f(x)) \\ &= f(F(x)) - f(x) \\ &= (f \circ F - f)(x).\end{aligned}$$

□

8.7. Problems, comments and further results

(1) With the notation given in Lemma 8.1, compute $\Sigma_{S,\Phi}$ when S is the distribution in $\mathscr{S}'(\mathbb{R}^{2n})$ defined by the function $f \equiv 1$, and $\Phi(\bar{x},\bar{y}) = e^{-(|\bar{x}|^2+|\bar{y}|^2)}$. Compute also $\mathrm{Kir}_{T,S}\,\Phi$ with S and Φ as above and T given by the function $e^{-|\bar{x}|^2}$ in $\mathbb{R}^n$.

(2) With the notation of Theorem 8.12, take $(X,\tau) = [0,1]$ with its usual topology. Let μ be Lebesgue measure on $[0,1]$. Characterize the harmonic measure associated to the μ,π-Laplacian $\Delta_{\mu,\pi}$ if $F(x) = -x$.

(3) The results of this chapter are contained in [**AG22**]. See also [**AG20**].

CHAPTER 9

Divergence and Laplacian on discrete structures

9.1. Introduction

Most of the results of this chapter are interesting particular cases of the general setting discussed in the previous chapter. Perhaps the most useful application of these discrete versions is the metrization of graph structures through the diffusion technique. Also, some theoretical approximation results of continuous settings by natural and standard discretization are in order.

9.2. Divergence and Laplacian defined by Dirac deltas and affinities on the Euclidean space

Take $X = \mathbb{R}^n$ in our general setting of the previous chapter. Take $\mathscr{S}_1 = \mathscr{D}(\mathbb{R}^n)$ and $\mathscr{S}_2 = \mathscr{D}(\mathbb{R}^{2n})$ the usual test function spaces for general distributions on $\mathbb{R}^n$. Set δ_x to denote the measure (distribution) defined by the Dirac delta at $x \in \mathbb{R}^n$. In other words, $\langle \delta_x, \varphi \rangle = \varphi(x)$, $\varphi \in \mathscr{S}_1$ as a distribution. Or $\delta_x(E) = 1$ if $x \in E$, and $\delta_x(E) = 0$ if $x \notin E$, as a measure. Let $\{x_k : k \geq 1\}$ be a given sequence of points in $\mathbb{R}^n$ and let $\{a_k : k \geq 1\}$ be a sequence of positive real numbers which is locally finite with respect to $\{x_k : k \geq 1\}$. That is, for every bounded set B in $\mathbb{R}^n$, $\sum_{\{k : x_k \in B\}} a_k < \infty$. Then, the measure μ defined by

$$\mu(E) = \sum_{k \geq 1} a_k \delta_{x_k}(E) = \sum_{\{k : x_k \in E\}} a_k$$

is of Borel type and is finite on compact sets of $\mathbb{R}^n$. In a similar way, take a sequence of nonnegative real numbers $\{w_{ij} : i, j \geq 1\}$ which is locally finite with respect to the sequence of points of $\mathbb{R}^n \times \mathbb{R}^n$ given by $\{(x_i, x_j) : i, j \geq 1\}$. In other words, for every bounded subset B of $\mathbb{R}^n \times \mathbb{R}^n$ we have

$$\sum_{\{(i,j) : (x_i, x_j) \in B\}} w_{ij} < \infty.$$

Set, for A a Borel subset of $\mathbb{R}^n \times \mathbb{R}^n$,

$$\pi(A) = \sum_{i \geq 1} \sum_{j \geq 1} w_{ij} \delta_{(x_i, x_j)}(A) = \sum_{\{(i,j) : (x_i, x_j) \in A\}} w_{ij},$$

which defines a Borel measure on $\mathbb{R}^n \times \mathbb{R}^n$ that is finite on compact subsets of $\mathbb{R}^n \times \mathbb{R}^n$.

Now, in the search for a Kirchhoff divergence of $\Phi \in \mathscr{S}_2$ and a corresponding Laplacian operator associated to the couple of measures μ on $\mathbb{R}^n$ and π on $\mathbb{R}^n \times \mathbb{R}^n$, we may apply the result in Lemma 8.10 of the previous chapter and look for a solution ψ of

$$\int_{\mathbb{R}^n} \varphi\psi d\mu = \iint_{\mathbb{R}^n\times\mathbb{R}^n} \varphi\Phi d\pi$$

for every $\varphi \in \mathscr{S}_1 = \mathscr{D}(\mathbb{R}^n)$.

Let us state and prove the main result of this section. Recall that given a measure ν on a product space which is finite, we have well defined marginals ν^1 and ν^2. If ν is a finite measure on $X \times X$ and E is a Borel subset of X, the first marginal ν^1 is defined on E by $\nu^1(E) = \iint_{E\times X} d\nu = \nu(E \times X)$.

THEOREM 9.1. *Let μ and π be as before and Φ a given function in $\mathscr{S}_2$. Then,*

(a) $\pi_\Phi(A) = \iint_A \Phi d\pi$ *for A a Borel subset of $\mathbb{R}^n \times \mathbb{R}^n$ is a finite measure on $\mathbb{R}^n \times \mathbb{R}^n$ and the first marginal π^1_Φ of π_Φ is absolutely continuous with respect to μ;*

(b) *the Radon-Nikodym derivative of π^1_Φ with respect to μ is a Kirchhoff divergence of Φ with respect to π and μ. In other words,*

$$\operatorname{Kir}_{\mu,\pi} \Phi = \frac{dS_\Phi}{d\mu};$$

(c) *explicitly, for every $k \geq 1$*

$$\operatorname{Kir}_{\mu,\pi} \Phi(x_k) = \frac{1}{a_k} \sum_{j\geq 1} w_{kj}\Phi(x_k, x_j);$$

(d) *if the measure π is finite, i.e. $\sum_{i\geq 1}\sum_{j\geq 1} w_{ij} < \infty$, then, for $f \in \mathscr{S}_1$, we can take $\Phi(x,y) = f(y) - f(x)$ and*

$$\Delta_{\mu,\pi} f(x_k) = \frac{1}{a_k} \sum_{j\geq 1} w_{jk}(f(x_j) - f(x_k));$$

(e) *if π is finite, f is μ,π-harmonic if and only if*

$$f(x_k) = \frac{1}{\sum_{j\geq 1} w_{jk}} \sum_{j\geq 1} w_{jk} f(x_j).$$

PROOF. Notice that

$$\pi^1_\Phi(E) = \pi_\Phi(E \times \mathbb{R}^n) = \iint_{E\times\mathbb{R}^n} \Phi d\pi = \sum_{\{k: x_k\in E\}} \sum_{j\geq 1} w_{kj}\Phi(x_k, x_j).$$

If E is a Borel subset of $\mathbb{R}^n$ such that $\mu(E) = 0$, then, since all the a_k are positive we have that $E \cap \{x_k : k \geq 1\} = \emptyset$. Hence $\pi^1_\Phi(E) = 0$ and (a) is proved.

Let us check (b). We have

$$\begin{aligned}\iint_{\mathbb{R}^n\times\mathbb{R}^n} \varphi\Phi d\pi &= \sum_{k\geq 1}\sum_{j\geq 1} w_{kj}\varphi(x_k)\Phi(x_k, x_j)\\ &= \sum_{k\geq 1}\varphi(x_k)\left(\sum_{j\geq 1} w_{kj}\Phi(x_k, x_j)\right)\\ &= \int_{\mathbb{R}^n}\varphi(x)dS^1_\Phi(x)\\ &= \int_{\mathbb{R}^n}\varphi(x)\frac{dS^1_\Phi}{d\mu}d\mu(x)\\ &= \int_{\mathbb{R}^n}\varphi(x)\psi(x)d\mu(x),\end{aligned}$$

for every $\varphi \in \mathscr{S}_1$ with $\psi = \frac{dS^1_\Phi}{d\mu}$. Notice that

$$\pi^1_\Phi(\{x_k\}) = \sum_{j\geq 1} w_{kj}\Phi(x_k, x_j)$$

and $\mu(\{x_k\}) = a_k$. So that $\frac{d\pi^1_\Phi}{d\mu}(x_k) = \frac{1}{a_k}\sum_{j\geq 1} w_{kj}\Phi(x_k, x_j)$.

Items (d) and (e) follow readily from (c). □

Note that equation in (e) for harmonic functions, i.e. $\Delta_{\mu,\pi} f \equiv 0$, is a mean value formula.

A particular case of the above, closely related with the classical harmonic functions is provided by the particular case of the finite difference scheme for the numerical approximation of solutions of partial differential equations. Let us state the result precisely.

THEOREM 9.2. *Let $h > 0$ be given and fixed. For $\vec{k} = (k_1, \ldots, k_n) \in \mathbb{Z}^n$, set $x_{\vec{k}} = h\vec{k}$. With the notation in Theorem 9.1, let us weight each $x_{\vec{k}}$ taking $a_{\vec{k}} = h^n$, the volume of the n-cube of side h, for every $\vec{k} \in \mathbb{Z}^n$. Take $\mu_h = \sum_{\vec{k}\in\mathbb{Z}^n} h^n\delta_{x_{\vec{k}}}$. Now define the weight $w_{\vec{k}\vec{j}}$ in the following way,*

$$w_{\vec{j}\vec{k}} = \begin{cases} 0 & \text{if } \vec{j} = \vec{k} \text{ or } \left|\vec{j} - \vec{k}\right| > 1,\\ h^{n-2} & \text{if } \left|\vec{j} - \vec{k}\right| = 1.\end{cases}$$

Set

$$\pi_h = \sum_{\vec{j}\in\mathbb{Z}^n}\sum_{\vec{k}\in\mathbb{Z}^n} w_{\vec{j}\vec{k}}\delta_{(x_{\vec{j}},x_{\vec{k}})}.$$

Then

$$\mathrm{Kir}_{\mu_h,\pi_h}\Phi(h\vec{k}) = \frac{1}{h^2}\sum_{m=1}^{n}\left[\Phi(h\vec{k},h(\vec{k}+\vec{e}_m)) + \Phi(h\vec{k},h(\vec{k}-\vec{e}_m))\right]$$

where $\vec{e}_m$ is the m-th vector of the canonical basis of $\mathbb{R}^n$. For $f\in\mathscr{S}_1$ we have

$$\Delta_h f(h\vec{k}) = \Delta_{\mu_h,\pi_h} f(h\vec{k}) = \sum_{m=1}^{n}\frac{f(h(\vec{k}+\vec{e}_m)) - 2f(h\vec{k}) + f(h(\vec{k}-\vec{e}_m))}{h^2}.$$

Moreover, the μ_h,π_h-harmonic functions for which

$$f(h\vec{k}) = \frac{1}{2n}\sum_{m=1}^{n}\left[f(h(\vec{k}+\vec{e}_m)) + f(h(\vec{k}-\vec{e}_m))\right].$$

Proof. The result is just a corollary of Theorem 9.1 taking into account that

$$\left\{\vec{j}\in\mathbb{Z}^n : \left|\vec{k}-\vec{j}\right| = 1\right\} = \left\{\vec{k}+\vec{e}_m : m=1,\dots,n\right\}\cup\left\{\vec{k}-\vec{e}_m : m=1,\dots,n\right\}. \qquad \square$$

We also have a discretization for fractional divergences and fractional Laplacians.

Theorem 9.3. *Let h, $\{x_{\vec{k}} : \vec{k}\in\mathbb{Z}^n\}$ and μ_h be as in Theorem 9.2. As the sequence of weights take, instead, for $\alpha>0$*

$$w_{\vec{j}\vec{k}} = \begin{cases} 0 & \text{if } \vec{j}=\vec{k},\\ h^{n-\alpha}\frac{1}{\left|\vec{j}-\vec{k}\right|^{n+\alpha}} & \text{if } \vec{j}\neq\vec{k}.\end{cases}$$

Let $\pi_h^\alpha = \sum_{\vec{k}}\sum_{\vec{j}} w^\alpha_{\vec{j}\vec{k}}\delta_{(h\vec{k},h\vec{j})}$. Then, for $\Phi\in\mathscr{S}_2$ we have

$$\mathrm{Kir}_{\mu_h,\pi_h^\alpha}\Phi(h\vec{k}) = \frac{1}{h^\alpha}\sum_{\vec{j}\neq\vec{k}}\frac{\Phi(h\vec{k},h\vec{j})}{\left|\vec{k}-\vec{j}\right|^{n+\alpha}}.$$

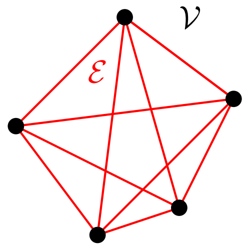
For $f\in\mathscr{S}_1$,

$$\Delta_h^\alpha f(h\vec{k}) = \frac{1}{h^\alpha}\sum_{\vec{j}\neq\vec{k}}\frac{f(h\vec{j})-f(h\vec{k})}{\left|\vec{k}-\vec{j}\right|^{n+\alpha}}.$$

Moreover, f is α,h-harmonic if

$$f(h\vec{k}) = \frac{1}{c(\alpha)}\sum_{\vec{j}\neq\vec{k}}\frac{f(h\vec{j})}{\left|\vec{k}-\vec{j}\right|^{n+\alpha}}, \qquad \text{with } c(\alpha) = \sum_{\vec{j}\neq\vec{0}}\left|\vec{j}\right|^{-n-\alpha}.$$

9.3. The case of finite graphs



Let $(\mathcal{V}, \mathcal{E}) = \mathcal{G}$ be an undirected graph. Assume that $\mathcal{V} = \{1, 2, \ldots, n\}$ and that

$$\mathcal{E} = \{\{i, j\} : i, j \in \mathcal{V}; i \neq j\}$$

is the set of all edges joining every pair of vertices in $\mathcal{V}$.

In the abstract framework above we have that $X = \mathcal{V}$ and, except for the diagonal, $X \times X = \mathcal{E}$. Assume that each vertex has assigned an intensity measure by a positive number $i \to a_i > 0$. Assume also that the edge joining nodes i and j is a measure of affinity $w_{ij} \geq 0$ between those nodes. When $w_{ij} = 0$ there is not affinity between nodes i and j in $\mathcal{V}$ and we can remove from $\mathcal{E}$ the edge $\{i, j\}$. The sequence of a_i's defines a positive measure μ on $\mathcal{V}$ and the sequence of the w_{ij}'s defines a nonnegative measure π on $\mathcal{E}$. In fact, for A a subset of $\mathcal{V}$ the measure μ is given by $\mu(A) = \sum_{i \in A} a_i$. For $E \subset \mathcal{E}$, we have $\pi(E) = \sum_{\{i,j\} \in E} w_{ij}$. We assume that $w_{ii} = 0$ since we have no loops in the graph.

Proposition 9.4. *Let $\mathcal{G} = (\mathcal{V}, \mathcal{E})$, μ and π be as before. Then, for any function $\Phi = \Phi(i, j)$ defined on $\mathcal{E}$, the function $\psi : \mathcal{V} \to \mathbb{R}$ given by*

$$\psi(i) = \frac{1}{a_i} \sum_{j=1}^{n} w_{ij} \Phi(i, j)$$

is a Kirchhoff divergence of Φ with respect to μ and π. Moreover, for $f : \mathcal{V} \to \mathbb{R}$ we have a well defined Laplacian by

$$\Delta_{\mu,\pi} f(i) = \frac{1}{a_i} \sum_{j=1}^{n} w_{ij} (f(j) - f(i)).$$

Proof. We have to check that $\int_{\mathcal{V}} \varphi \psi d\mu = \iint_{\mathcal{E}} \varphi \Phi d\pi$, for every $\varphi : \mathcal{V} \to \mathbb{R}$. In fact,

$$\begin{aligned}
\iint_{\mathcal{E}} \varphi \Phi d\pi &= \sum_{i=1}^{n} \sum_{j=1}^{n} \varphi(i) \Phi(i, j) w_{ij} \\
&= \sum_{i=1}^{n} \varphi(i) \left(\frac{1}{a_i} \sum_{j=1}^{n} \Phi(i, j) w_{ij} \right) a_i \\
&= \sum_{i=1}^{n} \varphi(i) \psi(i) a_i \\
&= \int_{\mathcal{V}} \varphi \psi d\mu,
\end{aligned}$$

as desired. The formula for the Laplacian follows directly from the formula for the Kirchhoff divergence. □

The result in Proposition 9.4 brings a matrix description and computation of the Laplacian $\Delta f = \Delta_{\mu,\pi} f$. In doing so, the computational tools for matrix analysis are providing the spectral theory that we need to pose the problem in the general setting for metrization described above.

PROPOSITION 9.5. *Let*

$$A = \begin{pmatrix} a_1 & \cdots & 0 \\ & \ddots & \\ 0 & \cdots & a_n \end{pmatrix}$$

with $a_i > 0$ for every $i = 1, \ldots, n$. Let

$$W = \begin{pmatrix} 0 & w_{12} & w_{13} & \cdots & w_{1n} \\ w_{12} & 0 & w_{23} & \cdots & w_{2n} \\ \vdots & \vdots & \vdots & \ddots & \vdots \\ w_{1n} & w_{2n} & w_{3n} & \cdots & 0 \end{pmatrix} = (w_{ij} : i, j = 1, \ldots, n)$$

with $w_{ii} = 0$ for each $i = 1, \ldots, n$ and $w_{ij} = w_{ji}$.

Let $f : \mathcal{V} \to \mathbb{R}$ which can be given by the n-vector of its values $f = (f_1, f_2, \ldots, f_n)$. Let

$$D = \begin{pmatrix} \sum_j w_{1j} & 0 & \cdots & 0 \\ 0 & \sum_j w_{2j} & \cdots & 0 \\ \vdots & \vdots & \ddots & \vdots \\ 0 & 0 & \cdots & \sum_j w_{nj} \end{pmatrix}$$

be the diagonal matrix with diagonal $(\sum_j w_{ij} : i = 1, \ldots, n)$ (the usually called degree matrix). Then, the μ, π-Laplacian of f can be computed in matrix form as the n-vector Δf given by

$$\Delta f = A^{-1}(W - D) f.$$

Or, avoiding the test function f, the μ, π-Laplacian is the matrix

$$\Delta = A^{-1}(W - D).$$

PROOF. Notice that $(\Delta f)_i$ is the i-th component of the product $A^{-1}(W-D)f$ which is given by

$$\begin{aligned}
\frac{1}{a_i}\sum_{j=1}^{n}(w_{ij}-D_{ij})f_j &= \frac{1}{a_i}\sum_{j=1}^{n}(w_{ij}f_j - D_{ij}f_j) \\
&= \frac{1}{a_i}\left(\sum_{j=1}^{n} w_{ij}f_j - \sum_{j=1}^{n} D_{ij}f_j\right) \\
&= \frac{1}{a_i}\left(\sum_{j=1}^{n} w_{ij}f_j - D_{ii}f_i\right) \\
&= \frac{1}{a_i}\left(\sum_{j=1}^{n} w_{ij}f_j - \left(\sum_{j=1}^{n} w_{ij}\right) f_i\right) \\
&= \frac{1}{a_i}\left(\sum_{j=1}^{n} w_{ij}(f_j - f_i)\right) \\
&= \Delta_{\mu,\pi} f(i),
\end{aligned}$$

according to Proposition 9.4. □

Even when on finite settings the function spaces are all of them the same and the norms are equivalent, the Hilbert structure is still important and no so invariant. Recall that the basic space in our general setting is $L^2(X,\mu)$ which in the current case is the space of all real functions defined on $\mathcal{V}$. Nevertheless the underlying norm and scalar product are important when orthogonality matters. Since μ is defined by the sequence $\{a_i : i = 1,\dots,n\}$ then $\|f\|_2^2 = \sum_{i=1}^{n}(f_i)^2 a_i$, so that the inner or scalar product is

$$\langle f, g\rangle_A = \int_{\mathcal{V}} fg\,d\mu = \sum_{i=1}^{n} f_i g_i a_i.$$

This scalar product is important for the analysis of the duality associated to our Laplacian.

PROPOSITION 9.6. *The operator Δ in Proposition 9.5 above is self-adjoint with respect to the inner product $\langle f, g\rangle_A$ in $L^2(X,\mu)$.*

PROOF. Let f and g in $L^2(X,\mu)$ (two vectors in $\mathbb{R}^n$). Then

$$\langle \Delta f, g\rangle_A = \left\langle A^{-1}(W-D)f, g\right\rangle_A$$

$$
\begin{aligned}
&= \sum_{i=1}^{n} (\Delta f)_i g_i a_i \\
&= \sum_{i=1}^{n} \left(\frac{1}{a_i} \sum_{j=1}^{n} (w_{ij} - D_{ij}) f_j \right) g_i a_i \\
&= \sum_{i=1}^{n} \sum_{j=1}^{n} (w_{ij} - D_{ij}) f_j g_i \\
&= \sum_{j=1}^{n} \sum_{i=1}^{n} (w_{ij} - D_{ij}) f_j g_i \\
&= \sum_{j=1}^{n} \left(\frac{1}{a_j} \sum_{i=1}^{n} (w_{ji} - D_{ji}) g_i \right) f_j a_j \\
&= \langle f, \Delta g \rangle_A .
\end{aligned}
$$

□

PROPOSITION 9.7. *For Δ as before we have that $-\Delta$ is positive definite in the sense that*

$$\langle -\Delta f, f \rangle_A \geq 0$$

for every f.

PROOF. As before

$$
\begin{aligned}
\langle -\Delta f, f \rangle_A &= \sum_{i=1}^{n} (-\Delta f)_i f_i a_i \\
&= \sum_{i=1}^{n} \sum_{j=1}^{n} (D_{ij} - w_{ij}) f_j f_i \\
&= n \sum_{j=1}^{n} D_{ij} f_j f_i - \sum_{i=1}^{n} \sum_{j=1}^{n} w_{ij} f_i f_j \\
&= \sum_{i=1}^{n} D_{ii} f_i^2 - \sum_{i=1}^{n} \sum_{j=1}^{n} w_{ij} f_i f_j \\
&= \sum_{i=1}^{n} \sum_{j=1}^{n} w_{ij} f_i^2 - \sum_{i=1}^{n} \sum_{j=1}^{n} w_{ij} f_i f_j \\
&= \sum_{i=1}^{n} \sum_{j=1}^{n} w_{ij} (f_i^2 - f_i f_j) \\
&= \frac{1}{2} \left(\sum_{i=1}^{n} \sum_{j=1}^{n} w_{ij} (f_i^2 - f_i f_j) + \sum_{i=1}^{n} \sum_{j=1}^{n} w_{ij} (f_j^2 - f_i f_j) \right)
\end{aligned}
$$

$$= \frac{1}{2} \sum_{i=1}^{n} \sum_{j=1}^{n} w_{ij} (f_i^2 + f_j^2 - 2 f_i f_j)$$

$$= \frac{1}{2} \sum_{i=1}^{n} \sum_{j=1}^{n} w_{ij} (f_i - f_j)^2 \geq 0. \qquad \square$$

COROLLARY 9.8. *The operator Δ is diagonalizable. Moreover, there exists a sequence of nonpositive numbers λ and a sequence of n-orthonormal vectors with respect to the inner product $\langle f, g \rangle_A$ such that the eigenvalues can be arranged as*

$$\lambda_{n-1} \leq \lambda_{n-2} \leq \ldots \leq \lambda_1 \leq \lambda_0 = 0$$

and

$$\Delta \phi_j = \lambda_j \phi_j, \quad j = 0, 1, \ldots, n-1$$

with $\langle \phi_j, \phi_i \rangle_A = \delta_{ij}$.

PROOF. Follows from Propositions 9.6 and 9.7 and basic results of linear algebra. $\square$

So far, given a weighted graph $\mathcal{G}$, we have been able to provide an orthonormal sequence $\{\phi_j\}$ for $L^2(\mathcal{V}, d\mu)$ and the corresponding sequence $\{\lambda_j\}$ of eigenvalues, and we are in position to apply our general approach to metrization.

9.4. Problems, comments and further results

(1) With the notation in Section 9.2, let $x_{\vec{j}} = \vec{j} = (j_1, \ldots, j_n) \in \mathbb{Z}^n$; $a_{\vec{j}} = 1$ for every $\vec{j}$; $w_{\vec{i}\vec{j}} = \left|\vec{i} - \vec{j}\right|^{-(n+1)}$ if $\vec{i} \neq \vec{j}$ and $w_{\vec{i}\vec{i}} = 0$. Write the Laplacian of a function f defined on $\mathbb{Z}^n$. Give conditions on f for the existence of the Laplacian.

(2) With the notation of Theorem 9.2 provide conditions on f in such a way that $\Delta_h f$ tends to the classical Laplacian of f in some sense (weak).

(3) The results of Chapter 9 are contained in [**AG22**].

CHAPTER 10

An application to the metrization of AMBA based on public transport

10.1. Introduction

This chapter contains a special case of the results in [AAGM21a] as an application of the general results of the last section in the previous chapter.

The acronym AMBA is used to name the 41 cities that concentrate one third of the total population of Argentina and is spatially concentrated around Buenos Aires City. The following map depicts their distribution.

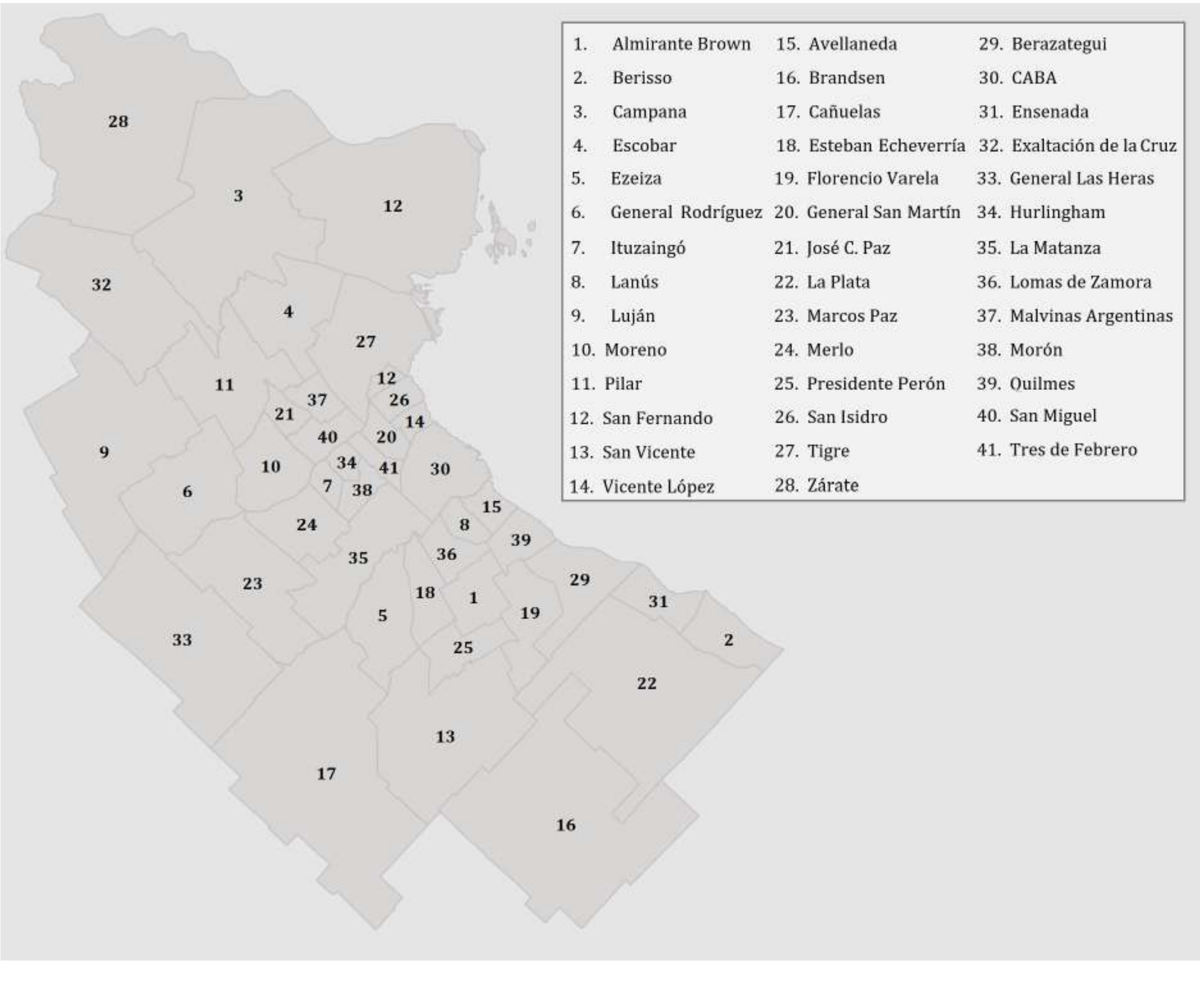


FIGURE 16. The cities of AMBA.

Aside from the geographical distance between locations i and j in the map there is a valuable information given by the public transport system in AMBA. The system SUBE keeps a great amount of information that allows to have another geometry provided by a connectivity distance built on this big data source.

With the notation used in Chapter 9 we have here the sets $\mathcal{V} = \{1, 2, 3, \dots, 41\}$ and $\mathcal{E} = \{\{i, j\} : i, j = 1, \dots, 41 \text{ and } i \neq j\}$. In what follows we shall take on $\mathcal{V}$ the counting measure normalized to a probability. That is $a_i = \frac{1}{41}$ for every $i = 1, \dots, 41$. For the matrix $W = (w_{ij} : i, j = 1, \dots, 41)$ we shall take the much more subtle construction of a probability matrix, i.e. $\sum_{i,j} w_{ij} = 1$, starting from profuse data of the system SUBE which collects all the public transport system of AMBA.

Once the matrix W is given, the results in Chapter 9 provide the Laplace operator of the setting

$$\Delta = A^{-1}(W - D),$$

with

$$A^{-1} = \begin{pmatrix} 41 & 0 & \dots & 0 \\ 0 & 41 & \dots & 0 \\ \vdots & \vdots & \ddots & \vdots \\ 0 & 0 & \dots & 41 \end{pmatrix} \quad \text{and} \quad D = \begin{pmatrix} \sum_j w_{1j} & 0 & \dots & 0 \\ 0 & \sum_j w_{2j} & \dots & 0 \\ \vdots & \vdots & \ddots & \vdots \\ 0 & 0 & \dots & \sum_j w_{41j} \end{pmatrix}.$$

Using `Python` we can compute the eigenvalues and eigenvectors of Δ and we have a natural associated diffusive metric

$$d_t^2(i, j) = \sum_{l \geq 0} e^{2t\lambda_l} \left| \phi_l(i) - \phi_l(j) \right|^2,$$

where λ_l are the nonpositive eigenvalues of Δ and ϕ_l are the corresponding eigenvectors. Here t is fixed but small. Hence, we can plot the balls with some center and different radii provided by such d_t. These balls will provide an idea of proximity which is different from the Euclidean one and could be of help when considering the propagation of COVID-19 and other diseases through the public transport system.

10.2. The matrix W and the metrics d_t

The unnormalized matrix weighting, through data provided by SUBE, the degree of connection of any two of the 41 cities in AMBA is given by

0	7	0	19	808	10	16	6223	5	54	24	45	1843	417	3745	55	53	4183	3551	135	22	482	12	60	5915	184	81	2	612	34539	4	0	1	30	1048	20782	32	206	8355	35	163
7	0	0	0	3	0	0	7	0	2	1	0	1	2	11	2	0	5	31	0	0	7105	0	1	0	0	0	1	40	258	352	0	0	0	6	12	2	1	48	0	0
0	0	0	846	0	24	1	2	31	31	227	17	0	27	1	0	1	1	1	12	30	4	5	3	0	37	211	1103	1	433	0	120	0	3	12	5	60	4	1	13	1
19	0	846	0	8	103	23	15	29	618	5626	529	1	1635	15	0	0	22	14	252	1435	14	3	62	3	2047	5772	122	3	4235	0	90	0	67	90	100	2631	72	16	982	102
808	3	0	6	0	2	14	1021	1	39	8	16	178	76	498	1	1003	7551	222	36	12	44	4	46	298	54	22	2	64	7537	5	0	0	9	958	2685	11	49	214	12	71
10	0	24	103	2	0	150	12	991	4470	1316	37	0	123	18	0	1	13	4	98	427	4	23	544	0	115	111	7	10	2198	0	26	2	130	220	31	66	267	4	203	146
16	0	1	23	14	150	0	31	20	2938	64	28	3	142	22	0	2	45	11	140	104	11	81	4467	4	199	65	0	5	6070	0	0	1	885	1482	78	65	6420	18	429	484
6223	7	2	15	1021	12	31	0	2	74	30	35	515	321	10406	14	60	2292	1898	146	37	264	9	142	720	165	86	1	486	39521	7	3	0	23	971	19166	40	99	4146	39	226
5	0	31	29	1	991	20	2	0	609	266	4	0	16	8	0	0	4	1	20	108	5	3	126	0	18	18	8	1	949	0	104	1	53	38	6	15	55	6	41	10
54	2	31	618	39	4470	2938	74	609	0	3242	620	4	1727	115	0	9	63	28	1578	5041	40	195	7911	7	1666	2172	3	32	22871	2	35	27	885	2727	214	1309	5152	52	7601	2064
24	1	227	5626	8	1316	64	30	266	3242	0	309	4	2188	44	0	1	25	29	430	3588	24	10	277	1	1719	2481	20	10	7229	1	493	0	227	197	77	4031	247	32	1676	430
45	0	17	529	16	37	28	35	4	620	309	0	2	2223	48	0	0	36	43	271	424	20	5	74	5	7362	9170	5	21	5958	1	1	0	34	197	124	622	63	45	529	98
1843	1	0	1	178	0	3	515	0	4	4	2	0	28	236	368	12	321	65	8	2	54	0	6	936	9	7	0	39	2679	2	0	0	4	73	966	1	7	104	0	18
417	2	27	1635	76	123	142	321	16	1727	2188	2223	28	0	249	0	10	313	284	6142	1843	85	22	647	68	10087	4845	13	129	44844	5	10	3	217	1738	1071	5817	265	327	1407	1061
3745	11	1	15	498	18	22	10406	8	115	44	48	236	249	0	7	24	988	2515	129	51	670	4	155	364	144	66	3	1994	36923	11	0	0	31	527	3538	49	106	10313	45	144
55	2	0	0	1	0	0	14	0	0	0	0	368	0	7	0	0	9	15	0	0	103	0	1	30	0	0	0	6	57	0	0	0	0	2	35	1	0	1	0	2
53	0	1	0	1003	1	2	60	0	9	1	0	12	10	24	0	0	307	10	2	0	10	35	11	18	3	2	0	5	549	0	0	0	1	954	161	0	13	23	0	19
4183	5	1	22	7551	13	45	2292	4	63	25	36	321	313	988	9	307	0	460	158	25	146	8	130	299	188	84	2	218	16876	1	0	0	82	3783	11399	26	295	572	23	181
3551	31	1	14	222	4	11	1898	1	28	29	43	65	284	2515	15	10	460	0	92	19	2509	1	26	72	179	60	1	6772	21292	46	0	0	23	403	1960	27	87	11126	26	119
135	0	12	252	36	98	140	146	20	1578	430	271	8	6142	129	0	2	158	92	0	1295	50	24	615	30	6059	1615	12	50	26014	1	0	0	947	1512	553	822	1010	103	1430	12210
22	0	30	1435	12	427	104	37	108	5041	3588	424	2	1843	51	0	0	25	19	1295	0	17	9	163	0	1314	3286	12	6	10500	0	25	0	685	284	86	4783	712	26	11265	1595
482	7105	4	14	44	4	11	264	5	40	24	20	54	85	670	103	10	146	2509	50	17	0	2	50	58	55	47	2	3040	8465	4337	0	2	17	199	455	46	88	2410	21	43
12	0	5	3	4	23	81	9	3	195	10	5	0	22	4	0	35	8	1	24	9	2	0	2196	1	17	10	0	3	1101	0	0	123	41	646	13	3	257	1	15	92
60	1	3	62	46	544	4467	142	126	7911	277	74	6	647	155	1	11	130	26	615	163	50	2196	0	11	436	235	0	32	26468	0	4	139	671	8217	293	308	12490	63	311	1672
5915	0	0	3	298	0	4	720	0	7	1	5	936	68	364	30	18	299	72	30	0	58	1	11	0	39	20	0	39	5330	1	0	0	0	94	1273	5	18	136	7	35
184	0	37	2047	54	115	199	165	18	1666	1719	7362	9	10087	144	0	3	188	179	6059	1314	55	17	436	39	0	7521	6	74	17645	1	6	0	539	1017	506	3462	531	156	1060	859
81	0	211	5772	22	111	65	86	18	2172	2481	9170	7	4845	66	0	2	84	60	1615	3286	47	10	235	20	7521	0	59	31	12837	1	18	0	310	519	394	6661	299	75	3068	441
2	1	1103	122	2	7	0	1	8	3	20	5	0	13	3	0	0	2	1	12	12	2	0	0	0	6	59	0	2	465	0	10	0	0	5	6	10	2	1	4	6
612	40	1	3	64	10	5	486	1	32	10	21	39	129	1994	6	5	218	6772	50	6	3040	3	32	39	74	31	2	0	14064	46	0	0	8	198	549	27	69	11521	10	65
34539	258	433	4235	7537	2198	6070	39521	949	22871	7229	5958	2679	44844	36923	57	549	16876	21292	26014	10500	8465	1101	26468	5330	17645	12837	465	14064	0	132	98	47	7238	88321	45769	8749	21285	28156	13912	32648
4	352	0	0	5	0	0	7	0	2	1	1	2	5	11	0	0	1	46	1	0	4337	0	0	1	1	1	0	46	132	0	0	0	0	4	9	1	0	46	0	0
0	0	120	90	0	26	0	3	104	35	493	1	0	10	0	0	0	0	0	0	25	0	0	4	0	6	18	10	0	98	0	0	0	2	1	1	10	4	1	16	4
1	0	0	0	0	2	1	0	1	27	0	0	0	3	0	0	0	0	0	0	0	2	123	139	0	0	0	0	0	47	0	0	0	3	11	0	0	17	1	0	3
30	0	3	67	9	130	885	23	53	885	227	34	4	217	31	0	1	82	23	947	685	17	41	671	0	539	310	0	8	7238	0	2	3	0	1090	75	237	5857	14	2567	1604
1048	6	12	90	958	220	1482	971	38	2727	197	197	73	1738	527	2	954	3783	403	1512	284	199	646	8217	94	1017	519	5	198	88321	4	1	11	1090	0	3635	176	18829	476	473	8905
20782	12	5	100	2685	31	78	19166	6	214	77	124	966	1071	3538	35	161	11399	1960	553	86	455	13	293	1273	506	394	6	549	45769	9	1	0	75	3635	0	123	351	5449	96	1019
32	2	60	2631	11	66	65	40	15	1309	4031	622	1	5817	49	1	0	26	27	822	4783	46	3	308	5	3462	6661	10	27	8749	1	10	0	237	176	123	0	291	25	7029	414
206	1	4	72	49	267	6420	99	55	5152	247	63	7	265	106	0	13	295	87	1010	712	88	257	12490	18	531	299	2	69	21285	0	4	17	5857	18829	351	291	0	108	1696	4405
8355	48	1	16	214	4	18	4146	6	52	32	45	104	327	10313	1	23	572	11126	103	26	2410	1	63	136	156	75	1	11521	28156	46	1	1	14	476	5449	25	108	0	31	129
35	0	13	982	12	203	429	39	41	7601	1676	529	0	1407	45	0	0	23	26	1430	11265	21	15	311	7	1060	3068	4	10	13912	0	16	0	2567	473	96	7029	1696	31	0	2408
163	0	1	102	71	146	484	226	10	2064	430	98	18	1061	144	2	19	181	119	12210	1595	43	92	1672	35	859	441	6	65	32648	0	4	3	1604	8905	1019	414	4405	129	2408	0

FIGURE 17. SUBE unnormalized matrix.

Once the above matrix is normalized to probability and introduced in the general algorithm with the sequence $a_i = \frac{1}{41}$ and $t = \frac{1}{10} = 0.10$, that computes the eigenvalues of $\Delta = A^{-1}(W - D)$ its eigenfunctions and $d^2_{\frac{1}{10}}(i,j) = \sum_{l\geq 0} e^{\frac{\lambda_l}{5}} \left|\phi_l(i) - \phi_l(j)\right|^2$, implemented here in `Python`. The matrix $d_{\frac{1}{10}}(i,j)$ is

	1	2	3	4	5	6	7	8	9	10	11	12	13	14	15	16	17	18	19	20	21	22	23	24	25	26	27	28	29	30	31	32	33	34	35	36	37	38	39	40	41
1	0	9.9	14.3	8.43	8.22	9.75	8.76	6.63	11	8.55	8.79	8.21	10.2	7.5	6.15	12.9	11.8	7.6	7.93	6.75	8.24	9.72	9.21	8.49	7.78	7.23	7.95	11.7	7.6	5.36	9.56	14.6	8.59	7.83	7.01	6.58	8.38	7.43	6.68	7.6	6.6
2	9.9	0	15.9	11	10.8	12	11.2	9.68	13	11.1	11.2	10.8	12.4	10.3	9.34	14.7	13.7	10.4	10.6	9.73	10.8	11.7	11.6	11	10.5	10.1	10.6	13.6	10.3	8.88	11.8	16.2	11.1	10.5	9.93	9.74	10.9	10.2	9.73	10.3	9.63
3	14.3	15.9	0	15	14.9	15.8	15.2	14.1	16.6	15.1	15.2	14.9	16.1	14.6	13.9	17.9	17.2	14.6	14.8	14.2	14.9	15.8	15.5	15.1	14.7	14.4	14.8	17	14.6	13.6	15.7	19.2	15.1	14.7	14.3	14.2	15	14.5	14.2	14.6	14.1
4	8.43	11	15	0	9.47	10.8	9.94	8.17	11.9	9.73	9.83	9.44	11.2	8.82	7.75	13.7	12.7	8.97	9.26	8.22	9.45	10.8	10.3	9.71	9.14	8.59	9.12	12.6	8.94	7.18	10.7	15.3	9.78	9.13	8.45	8.23	9.54	8.75	8.22	8.91	8.1
5	8.22	10.8	14.9	9.47	0	10.7	9.77	7.95	11.8	9.58	9.8	9.28	11.1	8.66	7.53	13.6	12.5	8.67	9.07	8.02	9.31	10.7	10.2	9.53	8.95	8.43	9.05	12.4	8.76	6.94	10.5	15.2	9.61	8.95	8.24	8	9.43	8.6	8.02	8.75	7.89
6	9.75	12	15.8	10.8	10.7	0	11.1	9.53	12.9	10.8	11.1	10.7	12.3	10.1	9.18	14.6	13.6	10.2	10.5	9.58	10.7	11.9	11.4	10.9	10.4	9.92	10.5	13.5	10.2	8.7	11.7	16.1	10.9	10.4	9.77	9.59	10.8	10.1	9.58	10.2	9.47
7	8.76	11.2	15.2	9.94	9.77	11.1	0	8.51	12.2	9.95	10.2	9.76	11.5	9.17	8.11	13.9	12.9	9.29	9.56	8.56	9.78	11.1	10.6	9.87	9.45	8.94	9.54	12.8	9.26	7.56	10.9	15.5	10.1	9.42	8.76	8.57	9.9	8.99	8.57	9.24	8.44
8	6.63	9.68	14.1	8.17	7.95	9.53	8.51	0	10.8	8.29	8.55	7.94	9.99	7.21	5.76	12.7	11.6	7.34	7.69	6.42	7.98	9.51	8.98	8.24	7.56	6.93	7.68	11.5	7.32	4.95	9.34	14.5	8.33	7.55	6.7	6.3	8.12	7.14	6.4	7.31	6.27
9	11	13	16.6	11.9	11.8	12.9	12.2	10.8	0	12	12.2	11.8	13.3	11.3	10.5	15.4	14.5	11.4	11.6	10.8	11.8	12.9	12.5	12	11.5	11.1	11.6	14.3	11.4	10.1	12.8	16.9	12.1	11.5	11	10.8	11.9	11.3	10.8	11.4	10.7
10	8.55	11.1	15.1	9.73	9.58	10.8	9.95	8.29	12	0	9.97	9.55	11.3	8.92	7.88	13.8	12.8	9.09	9.37	8.32	9.45	10.9	10.4	9.55	9.25	8.71	9.29	12.7	9.06	7.23	10.8	15.4	9.69	9.22	8.5	8.35	9.67	8.75	8.35	8.88	8.2
11	8.79	11.2	15.2	9.83	9.8	11.1	10.2	8.55	12.2	9.97	0	9.78	11.5	9.16	8.15	13.9	13	9.32	9.6	8.59	9.72	11.1	10.6	9.8	9.48	8.95	9.51	12.9	9.29	7.53	10.9	15.5	10.1	9.47	8.82	8.61	9.93	9.14	8.6	9.24	8.48
12	8.21	10.8	14.9	9.44	9.28	10.7	9.76	7.94	11.8	9.55	9.78	0	11.1	8.61	7.52	13.6	12.6	8.77	9.06	8	9.29	10.6	10.2	9.52	8.94	8.31	8.86	12.4	8.74	6.92	10.5	15.2	9.6	8.93	8.24	8.01	9.4	8.59	8	8.72	7.88
13	10.2	12.4	16.1	11.2	11.1	12.3	11.5	9.99	13.3	11.3	11.5	11.1	0	10.6	9.66	14.9	14	10.7	10.9	10	11.1	12.2	11.8	11.3	10.8	10.4	10.9	13.8	10.6	9.28	12.1	16.4	11.4	10.8	10.2	10	11.3	10.5	10	10.6	9.95
14	7.5	10.3	14.6	8.82	8.66	10.1	9.17	7.21	11.3	8.92	9.16	8.61	10.6	0	6.74	13.2	12.1	8.11	8.42	7.21	8.64	10.1	9.6	8.9	8.3	7.59	8.32	12	8.08	5.94	9.94	14.9	9.01	8.29	7.5	7.27	8.7	7.91	7.27	8.05	7.13
15	6.15	9.34	13.9	7.75	7.53	9.18	8.11	5.76	10.5	7.88	8.15	7.52	9.66	6.74	0	12.5	11.3	6.89	7.25	5.89	7.55	9.15	8.6	7.83	7.11	6.43	7.23	11.2	6.84	4.27	8.97	14.2	7.92	7.1	6.2	5.88	7.7	6.66	5.84	6.84	5.72
16	12.9	14.7	17.9	13.7	13.6	14.6	13.9	12.7	15.4	13.8	13.9	13.6	14.9	13.2	12.5	0	16	13.2	13.4	12.8	13.6	14.5	14.2	13.8	13.4	13	13.4	15.9	13.2	12.1	14.4	18.2	13.8	13.4	12.9	12.8	13.7	13.1	12.8	13.2	12.7
17	11.8	13.7	17.2	12.7	12.5	13.6	12.9	11.6	14.5	12.8	13	12.6	14	12.1	11.3	16	0	12.2	12.4	11.7	12.6	13.6	13.2	12.8	12.3	11.9	12.4	15.1	12.2	10.9	13.5	17.4	12.8	12.3	11.8	11.7	12.7	12.1	11.7	12.2	11.6
18	7.6	10.4	14.6	8.97	8.67	10.2	9.29	7.34	11.4	9.09	9.32	8.77	10.7	8.11	6.89	13.2	12.2	0	8.55	7.42	8.8	10.2	9.72	9.04	8.42	7.86	8.53	12.1	8.21	6.21	10	14.9	9.12	8.42	7.63	7.32	8.93	8.05	7.42	8.2	7.29
19	7.93	10.6	14.8	9.26	9.07	10.5	9.56	7.69	11.6	9.37	9.6	9.06	10.9	8.42	7.25	13.4	12.4	8.55	0	7.77	9.09	10.4	9.98	9.32	8.73	8.19	8.83	12.3	8.42	6.59	10.3	15.1	9.41	8.72	8	7.75	9.22	8.37	7.64	8.51	7.64
20	6.75	9.73	14.2	8.22	8.02	9.58	8.56	6.42	10.8	8.32	8.59	8	10	7.21	5.89	12.8	11.7	7.42	7.77	0	8.02	9.56	9.03	8.25	7.62	6.94	7.72	11.5	7.39	5.07	9.39	14.5	8.39	7.6	6.77	6.5	8.17	7.19	6.5	7.36	6.27
21	8.24	10.8	14.9	9.45	9.31	10.7	9.78	7.98	11.8	9.45	9.72	9.29	11.1	8.64	7.55	13.6	12.6	8.8	9.09	8.02	0	10.7	10.2	9.54	8.97	8.42	9	12.5	8.77	6.94	10.5	15.2	9.63	8.95	8.27	8.05	9.34	8.6	8.04	8.56	7.89
22	9.72	11.7	15.8	10.8	10.7	11.9	11.1	9.51	12.9	10.9	11.1	10.6	12.2	10.1	9.15	14.5	13.6	10.2	10.4	9.56	10.7	0	11.4	10.9	10.4	9.9	10.4	13.5	10.2	8.65	11.6	16.1	10.9	10.4	9.75	9.56	10.8	10.1	9.52	10.2	9.45
23	9.21	11.6	15.5	10.3	10.2	11.4	10.6	8.98	12.5	10.4	10.6	10.2	11.8	9.6	8.6	14.2	13.2	9.72	9.98	9.03	10.2	11.4	0	10.3	9.87	9.39	9.96	13.1	9.69	8.1	11.3	15.8	10.5	9.86	9.23	9.04	10.3	9.54	9.03	9.68	8.91
24	8.49	11	15.1	9.71	9.53	10.9	9.87	8.24	12	9.55	9.8	9.52	11.3	8.9	7.83	13.8	12.8	9.04	9.32	8.25	9.54	10.9	10.3	0	9.21	8.68	9.29	12.6	9.01	7.16	10.7	15.4	9.84	9.18	8.35	8.3	9.66	8.8	8.3	8.99	8.15
25	7.78	10.5	14.7	9.14	8.95	10.4	9.45	7.56	11.5	9.25	9.48	8.94	10.8	8.3	7.11	13.4	12.3	8.42	8.73	7.62	8.97	10.4	9.87	9.21	0	8.05	8.7	12.2	8.4	6.49	10.2	15	9.29	8.6	7.87	7.62	9.1	8.24	7.62	8.39	7.49
26	7.23	10.1	14.4	8.59	8.43	9.92	8.94	6.93	11.1	8.71	8.95	8.31	10.4	7.59	6.43	13	11.9	7.86	8.19	6.94	8.42	9.9	9.39	8.68	8.05	0	8.05	11.6	7.83	5.7	9.74	14.7	8.78	8.04	7.25	7	8.52	7.65	7	7.8	6.84
27	7.95	10.6	14.8	9.12	9.05	10.5	9.54	7.68	11.6	9.29	9.51	8.86	10.9	8.32	7.23	13.4	12.4	8.53	8.83	7.72	9	10.4	9.96	9.29	8.7	8.05	0	12.3	8.5	6.59	10.3	15.1	9.38	8.69	7.97	7.74	9.05	8.33	7.74	8.43	7.6
28	11.7	13.6	17	12.6	12.4	13.5	12.8	11.5	14.3	12.7	12.9	12.4	13.8	12	11.2	15.9	15.1	12.1	12.3	11.5	12.5	13.5	13.1	12.6	12.2	11.6	12.3	0	12	10.8	13.4	17.3	12.7	12.2	11.7	11.5	12.5	11.9	11.5	12	11.4
29	7.6	10.3	14.6	8.94	8.76	10.2	9.26	7.32	11.4	9.06	9.29	8.74	10.6	8.08	6.84	13.2	12.2	8.21	8.42	7.39	8.77	10.1	9.69	9.01	8.4	7.83	8.5	12	0	6.18	10	14.9	9.09	8.39	7.64	7.39	8.9	8.02	7.39	8.17	7.25
30	5.36	8.88	13.6	7.18	6.94	8.7	7.56	4.95	10.1	7.23	7.53	6.92	9.28	5.94	4.27	12.1	10.9	6.21	6.59	5.07	6.94	8.65	8.1	7.16	6.49	5.7	6.59	10.8	6.18	0	8.5	13.9	7.38	6.47	5.21	5.03	7.11	5.99	5.07	6.16	4.86
31	9.56	11.8	15.7	10.7	10.5	11.7	10.9	9.34	12.8	10.8	10.9	10.5	12.1	9.94	8.97	14.4	13.5	10	10.3	9.39	10.5	11.6	11.3	10.7	10.2	9.74	10.3	13.4	10	8.5	0	16	10.8	10.2	9.59	9.4	10.6	9.8	9.39	10	9.28
32	14.6	16.2	19.2	15.3	15.2	16.1	15.5	14.5	16.9	15.4	15.5	15.2	16.4	14.9	14.2	18.2	17.4	14.9	15.1	14.5	15.2	16.1	15.8	15.4	15	14.7	15.1	17.3	14.9	13.9	16	0	15.4	15	14.6	14.5	15.3	14.8	14.5	14.9	14.4
33	8.59	11.1	15.1	9.78	9.61	10.9	10.1	8.33	12.1	9.69	10.1	9.6	11.4	9.01	7.92	13.8	12.8	9.12	9.41	8.39	9.63	10.9	10.5	9.84	9.29	8.78	9.38	12.7	9.09	7.38	10.8	15.4	0	9.28	8.62	8.4	9.75	8.95	8.39	9.08	8.27
34	7.83	10.5	14.7	9.13	8.95	10.4	9.42	7.55	11.5	9.22	9.47	8.93	10.8	8.29	7.1	13.4	12.3	8.42	8.72	7.6	8.95	10.4	9.86	9.18	8.6	8.04	8.69	12.2	8.39	6.47	10.2	15	9.28	0	7.85	7.63	9.09	8.14	7.62	8.34	7.47
35	7.01	9.93	14.3	8.45	8.24	9.77	8.76	6.7	11	8.5	8.82	8.24	10.2	7.5	6.2	12.9	11.8	7.63	8	6.77	8.27	9.75	9.23	8.35	7.87	7.25	7.97	11.7	7.64	5.21	9.59	14.6	8.62	7.85	0	6.75	8.41	7.21	6.78	7.62	6.56
36	6.58	9.74	14.2	8.23	8	9.59	8.57	6.3	10.8	8.35	8.61	8.01	10	7.27	5.88	12.8	11.7	7.32	7.75	6.5	8.05	9.56	9.04	8.3	7.62	7	7.74	11.5	7.39	5.03	9.4	14.5	8.4	7.63	6.75	0	8.19	7.21	6.47	7.38	6.35
37	8.38	10.9	15	9.54	9.43	10.8	9.9	8.12	11.9	9.67	9.93	9.4	11.3	8.7	7.7	13.7	12.7	8.93	9.22	8.17	9.34	10.8	10.3	9.66	9.1	8.52	9.05	12.5	8.9	7.11	10.6	15.3	9.75	9.09	8.41	8.19	0	8.75	8.18	8.76	8.05
38	7.43	10.2	14.5	8.75	8.6	10.1	8.99	7.14	11.3	8.75	9.14	8.59	10.5	7.91	6.66	13.1	12.1	8.05	8.37	7.19	8.6	10.1	9.54	8.8	8.24	7.65	8.33	11.9	8.02	5.99	9.8	14.8	8.95	8.14	7.21	7.21	8.75	0	7.21	7.98	7.02
39	6.68	9.73	14.2	8.22	8.02	9.58	8.57	6.4	10.8	8.35	8.6	8	10	7.27	5.84	12.8	11.7	7.42	7.64	6.5	8.04	9.52	9.03	8.3	7.62	7	7.74	11.5	7.39	5.07	9.39	14.5	8.39	7.62	6.78	6.47	8.18	7.21	0	7.38	6.34
40	7.6	10.3	14.6	8.91	8.75	10.2	9.24	7.31	11.4	8.88	9.24	8.72	10.6	8.05	6.84	13.2	12.2	8.2	8.51	7.36	8.56	10.2	9.68	8.99	8.39	7.8	8.43	12	8.17	6.16	10	14.9	9.08	8.34	7.62	7.38	8.76	7.98	7.38	0	7.22
41	6.6	9.63	14.1	8.1	7.89	9.47	8.44	6.27	10.7	8.2	8.48	7.88	9.95	7.13	5.72	12.7	11.6	7.29	7.64	6.27	7.89	9.45	8.91	8.15	7.49	6.84	7.6	11.4	7.25	4.86	9.28	14.4	8.27	7.47	6.56	6.35	8.05	7.02	6.34	7.22	0

FIGURE 18. The diffusion metric matrix in AMBA for $t = \frac{1}{10}$.

Aside from the uniform distribution $a_i = \frac{1}{41}$ at the nodes we use also a normalization to probability of the COVID disease at each location.

Let us only illustrate some d_t-balls for $t = 0.10$ with two different weights $\vec{a}$: the uniform $\vec{a}_u = \left(\frac{1}{41}, \ldots, \frac{1}{41}\right)$ and

$\vec{a}_d$ =(0.0023, 0.0009, 0.0004, 0.0014, 0.0015, 0.0009, 0.0012, 0.0030, 0.0007, 0.0009, 0.0011, 0.0015, 0.0008, 0.0016, 0.0049, 0.0005, 0.0006, 0.0018, 0.0015, 0.0031, 0.0013, 0.0008, 0.0012, 0.0010, 0.0019, 0.0022, 0.0014, 0.0006, 0.0019, 0.0095, 0.0011, 0.0004, 0.0015, 0.0018, 0.0018, 0.0026, 0.0013, 0.0018, 0.0029, 0.0018, 0.0034)

which is a normalization of the density of the disease in each location (total number of active infections over population) by July 2020. The algorithms are implemented in `Python`.

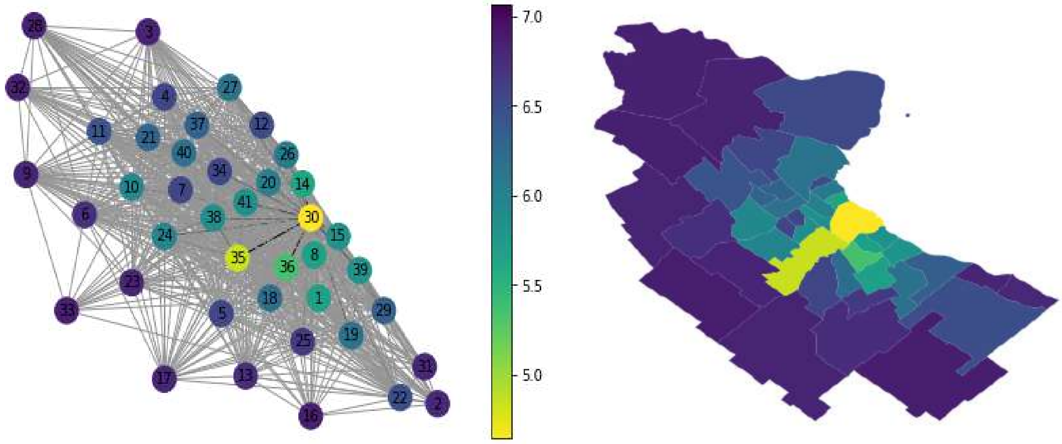


FIGURE 19. Weight $\vec{a}_u$; $t = 0.10$

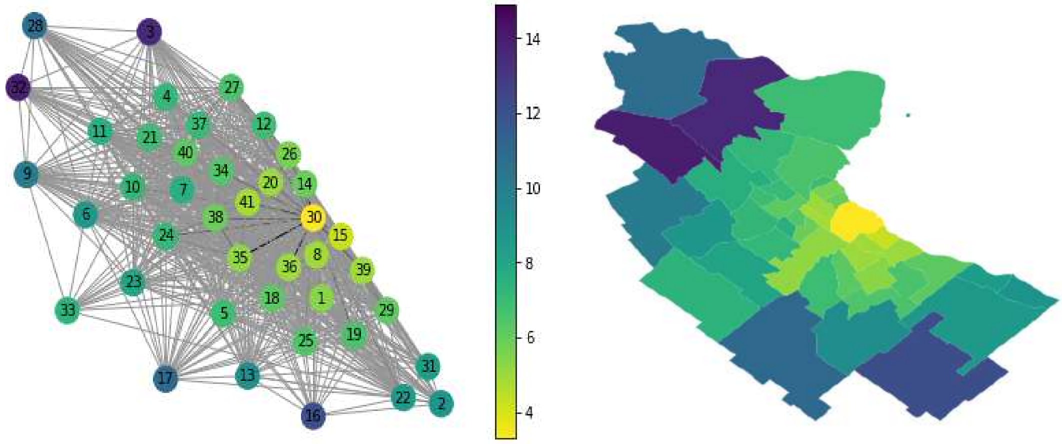


FIGURE 20. Weight $\vec{a}_d$; $t = 0.10$

10.3. Comments and further results

The results of these chapter are contained in the Technical Report [**AAC+21**]. See also [**AAGM21a**].

CHAPTER 11

Energy and the Laplacian on graphs

11.1. Introduction

One may, or should, ask why the spectral analysis based metrics d_t of the previous chapters have some real world, say physical, meaning. The energy considerations can provide a point of view that is more robust from this point of view. Recall that in a domain Ω of $\mathbb{R}^n$, the energy of a real function defined in Ω is given by the regularity part of the Sobolev norm of u

$$E(u) = \int_\Omega |\nabla u|^2 \, dx = \int_\Omega \nabla u \cdot \nabla u \, dx.$$

Here we are assuming that the "texture" of Ω is homogeneous and isotropic. Otherwise we would have

$$E(u) = \int_\Omega \nabla u \cdot A \nabla u \, dx$$

where the matrix A collects the anisotropies and heterogeneities of the media in Ω. Actually $E(u)$ is the value on the diagonal of the bilinear form

$$B(u, v) = \int_\Omega \nabla u \cdot \nabla v \, dx,$$

i.e. $E(u) = B(u, u)$. On the other hand, the Laplacian can be obtained as the Euler-Lagrange operator associated to E. Moreover, if $\Omega = \mathbb{R}^n$ and $u \in \mathscr{S}(\mathbb{R}^n)$ then

$$\begin{aligned} E(u) &= \int_{\mathbb{R}^n} |\nabla u|^2 \, dx = \sum_{j=1}^n \int_{\mathbb{R}^n} \left(\frac{\partial u}{\partial x_j} \right)^2 dx \\ &= \sum_{j=1}^n \int_{\mathbb{R}^n} \left(\widehat{\frac{\partial u}{\partial x_j}} \right)^2 d\xi \\ &= \sum_{j=1}^n \int_{\mathbb{R}^n} 4\pi^2 \xi_j^2 \, |\widehat{u}(\xi)|^2 \, d\xi \\ &= \int_{\mathbb{R}^n} 4\pi^2 \, |\xi|^2 \, |\widehat{u}(\xi)|^2 \, d\xi. \end{aligned}$$

In other words, the spectrum of the Laplacian $4\pi^2 |\xi|^2$ is defined and determining the energy on the Fourier side of the theory.

11.2. Energy of weighted undirected graphs and the variational Euler-Lagrange approach

Let $\mathcal{G} = (\mathcal{V}, \mathcal{E}, A, W)$ be a weighted undirected graph with $\#(\mathcal{V}) = n$, $A = I$ the density matrix and W a symmetric $n \times n$ matrix with nonnegative entries. Given any real valued function f on $\mathcal{V}$ and using vector notation $f(i) = f_i$ we define the energy of f with respect to $\mathcal{G}$ by

$$E(f) = \sum_{i=1}^{n} \sum_{j=1}^{n} w_{ij}(f_i - f_j)^2.$$

This notion of energy is the restriction to the diagonal $g = f$ of the bilinear form

$$B(f, g) = \sum_{i=1}^{n} \sum_{j=1}^{n} w_{ij}(f_i - f_j)(g_i - g_j).$$

By taking the Gâteaux derivative of E at f in every "direction" g, in the next result we obtain the Laplacian on $\mathcal{G}$ as the Euler-Lagrange equation associated to E.

THEOREM 11.1. *Let $\mathcal{G} = (\mathcal{V}, \mathcal{E}, A, W)$ be as before. If $f : \mathcal{V} \to \mathbb{R}$ is a minimizer of the energy E, then f is harmonic with respect to the Laplacian associated to the graph $\mathcal{G}$.*

PROOF. Set $\delta E(f, g)$ to denote the first Gâteaux variation of the Energy at "the point" f with "the direction" g. In other words

$$\delta E(f, g) = \lim_{t \to 0} \frac{1}{t}(E(f + g) - E(f)).$$

The particular form of E allows us to get an explicit formula for $\delta E(f, g)$. In fact,

$$\begin{aligned}
\frac{1}{t}(E(f+g) - E(f)) &= \frac{1}{t}\left[\sum_{i=1}^{n}\sum_{j=1}^{n} w_{ij}(f_i + tg_i - f_j - tg_j)^2 - \sum_{i=1}^{n}\sum_{j=1}^{n} w_{ij}(f_i - f_j)^2\right] \\
&= \frac{1}{t}\sum_{i=1}^{n}\sum_{j=1}^{n}\left[((f_i - f_j) + t(g_i - g_j))^2 - (f_i - f_j)^2\right] w_{ij} \\
&= \frac{1}{t}\sum_{i=1}^{n}\sum_{j=1}^{n} w_{ij}\left[2t(f_i - f_j)(g_i - g_j) + t^2(g_i - g_j)^2\right] \\
&= 2\sum_{i=1}^{n}\sum_{j=1}^{n}(f_i - f_j)w_{ij}(g_i - g_j) + t\sum_{i=1}^{n}\sum_{j=1}^{n}(g_i - g_j)^2.
\end{aligned}$$

Hence $\delta E(f,g) = 2\sum_{i=1}^n \sum_{j=1}^n (f_i - f_j) w_{ij}(g_i - g_j)$. Since we are assuming that f is a local minimizer of the energy E, we must have that $\delta E(f,g) = 0$ for every g. This equation translates into

$$\sum_{i=1}^n \sum_{j=1}^n (f_i - f_j) w_{ij}(g_i - g_j) = 0$$

for every $g : \mathcal{V} \to \mathbb{R}$. Then

$$\begin{aligned}
0 &= \sum_{i=1}^n \sum_{j=1}^n w_{ij}(f_i - f_j) g_i - \sum_{i=1}^n \sum_{j=1}^n w_{ij}(f_i - f_j) g_j \\
&= \sum_{i=1}^n \sum_{j=1}^n w_{ij}(f_i - f_j) g_i + \sum_{i=1}^n \sum_{j=1}^n w_{ij}(f_j - f_i) g_j \\
&= \sum_{i=1}^n \sum_{j=1}^n w_{ij}(f_i - f_j) g_i + \sum_{i=1}^n \sum_{j=1}^n w_{ji}(f_i - f_j) g_i \\
&= 2\sum_{i=1}^n \sum_{j=1}^n w_{ij}(f_i - f_j) g_i,
\end{aligned}$$

for every g. In the last equation above we used $w_{ij} = w_{ji}$. So that

$$\sum_{i=1}^n \sum_{j=1}^n w_{ij}(f_i - f_j) g_i = 0$$

for every g. Taking $g : \mathcal{V} \to \mathbb{R}$ to be $g(i) = 1$, $g(l) = 0$ for $l \neq i$, we get

$$\sum_{j=1}^n w_{ij}(f_i - f_j) = 0$$

for every i, which is equivalent to $\Delta_{\mathcal{G}} f(i) = 0$ for every i, with $\Delta_{\mathcal{G}}$ given in Proposition 9.5. This fact means that f is harmonic with respect to the Laplacian $\Delta_{\mathcal{G}}$ defined by the graph $\mathcal{G}$. $\square$

Let us now consider the variational form of the Laplacian type operator when we have different weights at each vertex of the graph.

Theorem 11.2. *Let $\mathcal{G} = (\mathcal{V}, \mathcal{E}, A, W)$ with $\mathcal{V}$, $\mathcal{E}$ and W as before. Assume now that each vertex $i \in \mathcal{V}$ has a positive weight a_i, hence $A = \begin{pmatrix} a_1 & & & 0 \\ & a_2 & & \\ & & \ddots & \\ 0 & & & a_n \end{pmatrix}$. If the energy $\mathscr{E}$ associated to the bilinear form*

$$\mathscr{B}(f,g) = \sum_{i=1}^n \sum_{j=1}^n w_{ij}(f_i - f_j)(g_i - g_j) a_i a_j$$

given by

$$\mathscr{E}(f) = \mathscr{B}(f,f) = \sum_{i=1}^{n}\sum_{j=1}^{n} w_{ij}(f_i - f_j)^2 a_i a_j,$$

assumes its minimum at f, then f solves

$$\sum_{j=1}^{n} w_{ij}(f_i - f_j)a_j = 0$$

for every $i \in \mathcal{V}$.

PROOF. Let, as before, compute

$$\delta\mathscr{E}(f,g) = \lim_{t\to 0}(\mathscr{E}(f+g) - \mathscr{E}(f)).$$

Now, we have $\mathscr{E}(f+g) - \mathscr{E}(f) = \sum_{i=1}^{n}\sum_{j=1}^{n} w_{ij}a_i a_j\,[2t(f_i - f_j)(g_i - g_j) + t^2(g_i - g_j)^2]$. Hence $\delta\mathscr{E}(f,g) = 2\sum_{i=1}^{n}\sum_{j=1}^{n} w_{ij}(f_i - f_j)(g_i - g_j)a_i a_j$. Since we are assuming that f is a minimum for $\mathscr{E}$, then we have the equation

$$0 = \sum_{i=1}^{n}\sum_{j=1}^{n} w_{ij}a_i a_j(f_i - f_j)(g_i - g_j)$$

for every $g : \mathcal{V} \to \mathbb{R}$. Since the matrix $(w_{ij}a_i a_j : i,j)$ is symmetric, we have that

$$\sum_{i=0}^{n} a_i\left[\sum_{j=1}^{n} w_{ij}(f_i - f_j)a_j\right] g_i = 0$$

for every g. Then

$$\sum_{j=1}^{n} w_{ij}(f_i - f_j)a_j = 0$$

for every $i \in \mathcal{V}$. □

Notice that when the distribution of weights on the vertices is not homogeneous we have, for the variational approach, a different form for the operator of Laplace type than the one obtained in the previous chapter. In fact, the non-variational form provides a nondivergence type operator

$$\frac{1}{a_i}\sum_{j=1}^{n} w_{ij}(f_i - f_j)$$

and the variational form provides a divergence form operator,

$$\sum_{j=1}^{n} w_{ij}a_i(f_i - f_j),$$

which, except for a multiplicative constant coincide when all the a_i's are the same.

The above results allow us considering the spectral analysis of the Laplacian operator of each setting as a quantification of the main direction of energy. This point of view gives us an intuition of the reasons why the diffusive metrics are providing an adequate results for applications.

11.3. Problems, comments and further results

(1) Show that the smooth functions minimizing the energy

$$E(u) = \int_{\Omega} |\nabla u|^2 \, dx$$

are harmonic.

(2) Provide conditions on a graph in such a way that the variational and non-variational Laplacians coincide.

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