

ISSN 2451-7100

IMAL preprints

<http://www.imal.santafe-conicet.gov.ar/publicaciones/preprints/index.php>

ON FRINK'S TYPE METRIZATION OF WEIGHTED GRAPHS

By

María Florencia Acosta - Hugo Aimar - Ivana Gómez

IMAL PREPRINT # 2020-0045

Publication date: August 2, 2020

Editorial: Instituto de Matemática Aplicada del Litoral
IMAL (CCT CONICET Santa Fe – UNL)
<http://www.imal.santafe-conicet.gov.ar>

Director de Publicaciones: Dr. Oscar Salinas
E-mail: salinas@santafe-conicet.gov.ar

I M A L



ON FRINK'S TYPE METRIZATION OF WEIGHTED GRAPHS

MARÍA FLORENCIA ACOSTA, HUGO AIMAR, AND IVANA GÓMEZ

ABSTRACT. Using the technique of the metrization theorem of uniformities with countable bases, in this note we provide, test and compare an explicit algorithm to produce a metric $d(x, y)$ between the vertices x and y of an affinity weighted undirected graph.

Keywords. Metrization; uniform spaces; weighted graphs.

MSC codes. 90C35, 54E15, 54E35.

Affiliation. INSTITUTO DE MATEMÁTICA APLICADA DEL LITORAL, CONICET, UNL.

Address. IMAL, CCT CONICET Santa Fe, Predio “Alberto Cassano”, Colectora Ruta Nac. 168 km 0, Paraje El Pozo, S3007ABA Santa Fe, Argentina.

E-mail. mfacosta@santafe-conicet.gov.ar; haimar@santafe-conicet.gov.ar; ivanagomez@santafe-conicet.gov.ar (corresponding author).

1. INTRODUCTION

The construction of metrics in data sets is a problem of current interest in data analysis. Of course the metrics built on a given data set should reflect, in a quantitative form, the affinity of the different data points. There are many reasons for the search of such metric structures on data sets. In particular adequate metrics provide notions of neighborhood of a given point which are not provided a priori directly by the affinity. But more important is the fact that in metric spaces many of the properties of Euclidean spaces still hold and covering and partitions can be done with a metric control which is natural for each setting.

Perhaps the best known metrization method is that of diffusive metrics due to Coifman and Laffon [4]. Once a Laplace type operator is built from the affinity matrix between data, the spectral analysis of this operator provides a diffusion kernel which gives a family of metrics on the data set at different times. The size of the eigenvalues allows the detection of the main features of and hence the approximation of a high dimensional space by another space with small dimension. In pure mathematics the problem of metrization of general topological spaces is old and well known. In particular, the metrization of the topology induced on a set X by a uniformity on $X \times X$ was considered and solved in [5], see also [3] and [6] when the uniform structure has a countable basis. The result is that a topology induced by a uniform structure is metrizable if and only if the uniformity has a countable basis. Even when so stated the results seems to have a qualitative character

its proof entails a quantitative lemma due to Frink that allows to obtain a metric from the affinity going through the uniform structure induced by the affinity between the data points.

The first use of this quantitative lemma is due to Macias and Segovia ([7]) in order to show that quasi-distances are equivalent to powers of metrics. In [1] sufficient conditions on a general affinity kernel K on an abstract set X are given in order to obtain a Newton type potential form for K in terms of a natural metric on X . Loosely speaking [1] shows that, with a quantitative transitivity hypothesis, we have that $K(x, y) = \varphi(d(x, y))$ for some “metric” d and some quasi-convex decreasing function φ defined on the positive real numbers.

In this note we aim to provide, test and compare an explicit algorithm in order to obtain a metric type function $d(x, y)$ between the vertices x and y associated to an affinity weighted graph. The algorithm gives actually a uniform family of metrics that provide together a profuse enough family of balls.

The second section of this note is devoted to state and prove the main result as a consequence of Frink’s Lemma as stated and proved in [6]. Section 3 describes the algorithm for the case of finite X . In Section 4 we test and compare the algorithm in some special weighted graphs

2. PSEUDOMETRIZATION OF AFFINITY KERNELS AND WEIGHTED UNDIRECTED GRAPHS THROUGH FRINK’S LEMMA

Even when the problem is motivated by the finite setting provided by weighted graphs, the basic theory does not need any assumption regarding cardinality. Hence, in this section, we assume that X is a set and $K : X \times X \rightarrow [0, \infty)$ is a nonnegative function such that for x and y in X , $K(x, y)$ is a measure of affinity between x and y .

A pseudo-metric on the set X is a function $d : X \times X \rightarrow [0, \infty)$ such that

- (p-m.1) $d(x, x) = 0$ for every $x \in X$;
- (p-m.2) $d(x, y) = d(y, x)$, $x, y \in X$;
- (p-m.3) $d(x, z) \leq d(x, y) + d(y, z)$ for every $x, y, z \in X$.

A pseudo-metric is a metric if $d(x, y) = 0$ only when $x = y$.

Let us now proceed to state Frink’s Lemma as given in Chapter 6 of Kelley’s book [6]. Some notation to simplify further statements is in order. With Δ we denote the diagonal of $X \times X$. In other words $\Delta = \{(x, x) : x \in X\}$. Given a subset U of $X \times X$ we write U^{-1} to denote the set $\{(x, y) \in X \times X : (y, x) \in U\}$. We say that U is symmetric if $U = U^{-1}$. Given two subsets U and V of $X \times X$, the composition is defined by $V \circ U = \{(x, z) \in X \times X : \text{there exist } y \in X \text{ with } (x, y) \in U \text{ and } (y, z) \in V\}$.

Lemma 1. *Let X be a set and let $\{U_m : m = 0, 1, 2, \dots\}$ be a sequence of subsets of $X \times X$ satisfying the following properties*

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

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

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

The above control of the given sequence $\{U_n : n = 0, 1, 2, \dots\}$ by the level sets of the pseudo-metric d seems to be of qualitative character. Nevertheless, when the sequence U_n is itself given by level sets of some function K on $X \times X$, this control becomes quantitative and allows to find a natural notion of distance provided by K .

In the sequel, for a given subset V of $X \times X$ we shall use $V^{(n)}$ to denote the composition $V \circ V \circ V \dots \circ V$ n times.

Let us now prove that under some mild conditions in K it is possible to construct increasing sequences $\{\lambda(k) : k = 0, 1, 2, \dots\}$ such that $U_{k+1} \circ U_{k+1} \circ U_{k+1} \subseteq U_k$ whenever $U_k = \{K > \lambda(k)\}$.

Lemma 2. *Let X be a set and let K be a nonnegative symmetric real function defined on $X \times X$ satisfying*

- a) $K(x, x) = \sup_{y \in X} K(x, y)$ for every $x \in X$;*
- b) $0 < \Lambda_\infty = \sup\{\alpha > 0 : \{K > \alpha\}^{(m)} = X \times X \text{ for some integer } m\} \leq \infty$.*

Then, for every Λ with $0 < \Lambda < \Lambda_\infty$ there exists a finite sequence $0 = \lambda(0) < \lambda(1) < \dots < \lambda(k) = \Lambda$ such that $\{K > \lambda(i)\}^{(3)} \subseteq \{K > \lambda(i-1)\}$ for every $i = 1, 2, \dots, k$. Moreover, $\Delta \subset \{K > \lambda(i)\}$ for every $i = 0, 1, 2, \dots, k$.

Proof. Let us first notice that the set $A = \{\alpha > 0 : \{K > \alpha\}^{(m)} = X \times X \text{ for some integer } m\}$ is an interval or the whole half line \mathbb{R}^+ . This fact follows from the monotonicity of the level sets of K . In other words if $\alpha \in A$ and $0 < \beta < \alpha$ then $\{K > \beta\} \supset \{K > \alpha\}$, so that $\{K > \beta\}^{(m)} \supset \{K > \alpha\}^{(m)} = X \times X$ and $\beta \in A$. On the other hand, for each $\alpha \in A$ we have that $\Delta \subset \{K > \alpha\}$. This follows from property *a)* of the kernel K . In fact, if for some $x_0 \in X$ we have $K(x_0, x_0) \leq \alpha$, then $\sup_{y \in X} K(x_0, y) \leq \alpha$ and for no $m \in \mathbb{N}$ the point (x_0, x_0) would belong to $\{K > \alpha\}$. But since $\alpha \in A$, for some m , $\{K > \alpha\}^{(m)} = X \times X \supset \{(x_0, x_0)\}$.

Let us pick $0 < \Lambda < \Lambda_\infty$. From the above remarks, we have that $\Lambda \in A$ and $\Delta \subset \{K > \Lambda\}$. Set $m_\Lambda = \min\{m \in \mathbb{N} : \{K > \Lambda\}^{(m)} = X \times X\}$. In other words, $\{K > \Lambda\}^{(m_\Lambda)} = X \times X$ but $\{K > \Lambda\}^{(m_\Lambda-1)} \not\subseteq X \times X$. We may assume that $m_\Lambda \geq 3$. Now, consider the set $A_1 = \{\alpha > 0 : \{K > \Lambda\}^{(3)} \subseteq \{K > \alpha\}\}$. If $A_1 = \emptyset$, the sequence

that we are looking for has only two elements $\lambda(0) = 0$ and $\lambda(1) = \Lambda$. And the desired inclusion $\{K > \lambda(1)\}^{(3)} \subseteq X \times X = \{K > \lambda(0)\}$ holds trivially. If $A_1 \neq \emptyset$ take $\Lambda_1 \in A_1$ with $\Lambda_1 > \sup A_1 - \varepsilon$ for some fixed as small as desired and positive ε . Set now $A_2 = \{\alpha > 0 : \{K > \Lambda_1\}^{(3)} \subseteq \{K > \alpha\}\}$. If $A_2 = \emptyset$, then we are done with $\lambda(0) = 0$, $\lambda(1) = \Lambda_1$ and $\lambda(2) = \Lambda$. So may keep iterating this selection process by choosing $\lambda_i \in A_i = \{\alpha > 0 : \{K > \Lambda_{i-1}\}^{(3)} \subseteq \{K > \alpha\}\}$ with $\Lambda_i > \sup A_i - \varepsilon$. Since for $\{K > \Lambda\}^{(m_\Lambda)} = X \times X$, after at most the integer part of $m_\Lambda/3$ plus one iterations the process stops providing a finite sequence of levels $\Lambda_0 := \Lambda > \Lambda_1 > \Lambda_2 > \dots > \Lambda_k$. Taking $\lambda(i) = \Lambda_{k-i}$ for $i = 0, 1, \dots, k$ we get the desired result. \square

Let us point out that for discrete settings or for continuous kernels K the choice of the sequence Λ_i in the argument above can be accomplished by taking the maximum of each A_i . Hence the ε -approximation argument is not necessary. From the above two lemmas we are in position to state and prove the main results of this section.

Theorem 3. *Let X be a set. Let K be a nonnegative symmetric function defined on $X \times X$ satisfying a) and b) in Lemma 2. Then for every sequence $\lambda = \{\lambda(i) : i = 0, 1, \dots, k = k(\lambda)\}$ as in Lemma 2, there exists a pseudo-metric d_λ defined on X such that*

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

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

with λ^{-1} the inverse of any increasing extension of $\lambda(i)$ to the whole interval $[0, k(\lambda)]$, is equivalent to the pseudo-metric d_λ with constants that are uniform in λ . Precisely,

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

Proof. From Lemma 2 the sequence $U_i = \{K > \lambda(i)\}$ satisfies i) to iv) of Lemma 1. Hence there exists a pseudo-metric d_λ defined on X such that 1) holds. In order to prove 2) take $(x, y) \in X \times X$ such that $d_\lambda(x, y) > 0$. Hence for some $i = 0, 1, \dots, k(\lambda)$ we have

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

The inequality $d_\lambda(x, y) < 2^{-i}$ and the second inclusion in 1) shows that $K(x, y) > \lambda(i-1)$. The inequality $2^{-(i+1)} \leq d_\lambda(x, y)$ and the first inclusion in 1) shows that $K(x, y) \leq \lambda(i+1)$. If λ is any strictly increasing extension of the sequence $\lambda(i)$ for $i = 0, \dots, k$ to the interval $[0, k]$ and λ^{-1} denote its inverse function, we have that $2^{-(i+1)} \leq d_\lambda(x, y) < 2^{-i}$, and

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

From this inequalities it readily follows that $\delta_\lambda = 2^{-\lambda^{-1} \circ K}$ is equivalent to d_λ . In fact,

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

□

Let us point out that the function δ_λ in the above result satisfies a triangle type inequality with triangular constant equal to 8 no matter what the kernel K or the sequence λ , satisfying Lemma 2, are. In fact,

$$\delta_\lambda(x, z) \leq 4d_\lambda(x, z) \leq 4(d_\lambda(x, y) + d_\lambda(y, z)) \leq 8(\delta_\lambda(x, y) + \delta_\lambda(y, z))$$

for every x, y and $z \in X$.

Regarding the extension of λ in order to produce the function λ^{-1} needed to explicitly give the quasi-metric δ_λ , let us observe that two extremal cases can be explicitly given. In fact, let $\bar{\lambda}^{-1} : [0, \lambda(k)] \rightarrow [0, k]$ with $\bar{\lambda}^{-1}(t) = i$ for $\bar{\lambda}(i-1) < t \leq \bar{\lambda}(i)$ and $i = 1, \dots, k$. Also $\bar{\lambda}^{-1}(0) = 0$. Another possible λ^{-1} is a lower case $\underline{\lambda}^{-1} : [0, \lambda(k)] \rightarrow [0, k-1]$ given by $\underline{\lambda}^{-1}(t) = i-1$ for $\underline{\lambda}(i-1) < t \leq \underline{\lambda}(i)$ for $i = 1, \dots, k$.

It is also worth noticing that Frink's metric and hence also δ_λ , do not reflect the scaling factor associated to the choice of Λ in Lemma 2. This is due to the fact that Frink's metric d_λ takes only values between zero and one. So that, being δ_λ equivalent to d_λ , also our quasi-metric δ_λ is bounded.

The sequence $\lambda(i)$ contains also the information of a family of δ_λ balls defined directly as level sets of the affinity kernel K .

Proposition 4. *For $0 < r < 1$ we have that the open δ_λ ball centered at $x \in X$ with radius r , is given by*

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

Proof. The inequality $K(x, y) > \lambda(\log_2 \frac{1}{r})$ is equivalent to $\delta_\lambda(x, y) < r$ which defines $B_{\delta_\lambda}(x, r)$. □

Let us point out that the actual construction of the sequence $\lambda(i)$ will depend only on K itself. Hence the δ_λ balls are strictly provided only by K .

3. THE ALGORITHM FOR THE EXPLICIT COMPUTATION OF THE SEQUENCES λ . THE FINITE CASE

In this section we consider the case of $X = \{1, 2, \dots, n\}$ for some large integer n . The kernel K defined on $X \times X$ can be regarded as an $n \times n$ symmetric matrix with positive entries K_{ij} . Since each K_{ij} is positive the hypothesis *b*) in Lemma 2 holds trivially since $\Lambda_\infty \geq \min K_{ij} > 0$. Instead hypothesis *a*) in Lemma 2 holds if $K_{ii} = \sup_j K_{ij}$.

In order to construct sequences λ , and then δ_λ , associated to this matrix K we shall need to deal in the algorithm with the composition of neighborhoods of the diagonal.

Let U and V be two subsets of $\{1, 2, \dots, n\}^2 = X \times X$. Then, as before $V \circ U = \{(i, k) : (i, j) \in U \text{ and } (j, k) \in V \text{ for some } j = 1, 2, \dots, n\}$.

Proposition 5. For a given $U \subseteq \{1, 2, \dots, n\}^n$ set $A_U = (a_{ij}(U))$ to denote the $n \times n$ rest matrix defined by $a_{ij}(U) = 1$ if $(i, j) \in U$ and $a_{ij}(U) = 0$ otherwise. Then the set $V \circ U$ is given by the non vanishing entries of the product matrix $A_U A_V$. Precisely

$$V \circ U = \left\{ (i, j) \in \{1, \dots, n\}^2 : \sum_{k=1}^n a_{ik}(U) a_{kj}(V) \geq 1 \right\}.$$

Proof. Notice that $\sum_{k=1}^n a_{ik}(U) a_{kj}(V) \geq 1$ if and only there exists $k \in \{1, \dots, n\}$ such that $a_{ik}(U) = 1$ and $a_{kj}(V) = 1$. In other words, if and only if $(i, k) \in U$ and $(k, j) \in V$, as desired. \square

The next result is important at showing when the iterated composition of a neighborhood of the diagonal finally covers the whole space $\{1, 2, \dots, n\}^2$.

Lemma 6. Let U be a set in $\{1, 2, \dots, n\}^2$ such that U contains the three main diagonals of $\{1, 2, \dots, n\}^2$. Precisely, $(i, i-1)$, (i, i) and $(i, i+1)$ belong to U for every $i = 1, 2, \dots, n$. Then there exists m such that $U^{(m)} = \{1, 2, \dots, n\}^2$.

Proof. From the representation of U in terms of the matrix A_U and the current hypothesis in U we have that the matrix A_U has ones at least in the three main diagonals. In other words, $a_{i,j} \geq 0$, $a_{i,i} = a_{i-1,i} = a_{i,i+1} = 1$. Then A_U^2 has positive values at least in the entries of the five diagonals $\Delta = \{(i, i) : i = 1, \dots, n\}$, $\Delta_1^+ = \{(i, i+1) : i = 1, \dots, n-1\}$, $\Delta_1^- = \{(i-1, i) : i = 2, \dots, n\}$, $\Delta_2^+ = \{(i, i+2) : i = 1, \dots, n-2\}$ and $\Delta_2^- = \{(i-2, i) : i = 3, \dots, n\}$. Iteration of the above argument shows that the composition of U becomes wider around the diagonal and after a finite number of compositions the set $\{1, \dots, n\}^2$ is completely covered. \square

We are now in position to describe the basic steps of an algorithm to find a sequence $\lambda(i)$ associate to the kernel K .

Algorithm. Let $K = (K_{ij})$ be a $n \times n$ symmetric matrix with positive entries.

Step 1. Compute the minimum of the values of K on the three main diagonals $\Lambda_0 = \min\{K_{i-1,i}; K_{i,i}; K_{i,i+1} : i = 1, \dots, n\}$,

Step 2. Build the matrix $A_0 = A_{\{(i,j):K_{ij} \geq \Lambda_0\}}$ as in Proposition 5;

Step 3. Compute A_0^3 ;

Step 4. Define U_0 as the subset of those (i, j) in $\{1, \dots, n\}^2$ such that the entry in (i, j) of A_0^3 is positive;

Step 5. Find $\Lambda_1 = \max\{\alpha : \{K \geq \alpha\} \supseteq U_0\}$;

Step 6. Build the matrix $A_1 = A_{\{(i,j):K_{ij} \geq \Lambda_1\}}$ as in Proposition 5;

Step 7. Compute A_1^3 ;

Step 8. Define $U_1 = \{(i, j) : \text{the entry } (i, j) \text{ of } A_1^3 \text{ is positive}\}$;

Step 9. Find $\Lambda_2 = \max\{\alpha : \{K \geq \alpha\} \supseteq U_1\}$;

...

The iteration stops after a finite number of steps so we get the sequence $\Lambda_0, \Lambda_1, \dots, \Lambda_k$. It is clear that $\Lambda_k < \Lambda_{k-1} < \dots < \Lambda_2 < \Lambda_1$. Without any extra condition on K it could happen that $\Lambda_0 \leq \Lambda_1$. But if Λ_0 is larger than all the entries of K outside the three main diagonals we have

$$\Lambda_k < \Lambda_{k-1} < \dots < \Lambda_2 < \Lambda_1 < \Lambda_0$$

Step $k + 1$. Set $\lambda(i) = \Lambda_{k-i}; i = 0, \dots, k$;

Step $k + 2$. Compute a version of λ^{-1} ;

Step $k + 3$. Define $\delta_\lambda(i, j) = 2^{-\lambda^{-1}(K_{ij})}$;

Step $k + 4$. Plot δ_λ balls $B_{\delta_\lambda}(i, r) = \{j : K_{ij} > \lambda(\log_2 \frac{1}{r})\}$ for i fixed and $0 < r < 1$.

The script in Python for this algorithm is the following.

```

1 import matplotlib.pyplot as plt
2 import networkx as nx
3
4 ## Value of n
5 n=n
6 ## Compute minimum of K
7 Kmin=np.amin(K)
8 ## Compute Lambda_0
9 lambda_0=0
10
11 aux=np.zeros((n))
12 for i in range(n-1):
13     ## Compare inner values main diagonals
14     aux[i]=min(K[i,i],K[i,i+1])
15 ## Compare the remaining values in the main diagonals
16 aux[n-1]=K[n-1,n-1]
17 lambda_0=min(aux)
18
19 ## Define matrix A
20 A=np.zeros((n,n))
21
22 for i in range(n):
23     for j in range(n):
24         if K[i,j]>=lambda_0:
25             A[i,j]=1
26
27 ## Compute B=A^3
28 B=(A.dot(A)).dot(A)
29
30 ## Compute Bpos

```

```

31 Bpos=np.zeros((n,n))
32 for i in range(n):
33     for j in range(n):
34         if B[i,j]>=1:
35             Bpos[i,j]=1
36
37 ## Compute C
38 C=K*Bpos
39
40 ## Compute minimum of the positive values of C
41 auxC=np.max(K)
42 for i in range(n):
43     for j in range(n):
44         if C[i,j]>0:
45             auxC=min(auxC,C[i,j])
46 lambda_1=auxC
47
48 ## Iterate
49 ## Variables
50
51 lambda_i=np.zeros((n))
52 lambda_i[0]=lambda_0
53 lambda_i[1]=lambda_1
54
55 A_i=np.zeros((n,n,n))
56 A_i[0,:,:]=A
57
58 B_i=np.zeros((n,n,n))
59 B_i[0,:,:]=B
60
61 Bpos_i=np.zeros((n,n,n))
62 Bpos_i[0,:,:]=Bpos
63
64 C_i=np.zeros((n,n,n))
65 C_i[0,:,:]=C
66
67 ## While
68 h=1
69 while lambda_i[h]>Kmin:
70     ## Define matrix A
71     for i in range(n):
72         for j in range(n):
73             if K[i,j]>=lambda_i[h]:
74                 A_i[h,i,j]=1
75
76     ## Compute B=A^3
77     B_i[h,:,:]=(A_i[h,:,:].dot(A_i[h,:,:])).dot(A_i[h,:,:])
78
79     ## Bpos
80     for i in range(n):
81         for j in range(n):
82             if B_i[h,i,j]>=1:
83                 Bpos_i[h,i,j]=1

```

```

84
85     ## Compute C
86     C_i[h,:,:]=K*Bpos_i[h,:,:]
87
88     ## Compute minimum of the positive values of C
89     auxC=np.max(K)
90     for i in range(n):
91         for j in range(n):
92             if C_i[h,i,j]>0:
93                 auxC=min(auxC,C_i[h,i,j])
94     lambda_i[h+1]=auxC
95     h+=1
96
97 ## End while
98
99 ## Rearranging Lambda
100 lambda_i=lambda_i[0:h+1]
101 lambda_i=lambda_i[::-1]
102
103 ## Inverse function of Lambda
104 def lambda_funct_inv(t,lambd):
105     if t<0:
106         print ('t must be larger or equal to the minimum value of
lambda')
107     if 0<=t<lambd[0]:
108         inv=0
109     for kk in range(len(lambd)-1):
110         if lambd[kk]<=t<lambd[kk+1]:
111             inv=kk+1
112     if t>=lambd[len(lambd)-1]:
113         inv=len(lambd)
114     return inv
115
116 ## Compute the matrix
117 def dist_frink_inv(nodo1,nodo2):
118     distFinv=2**(-lambda_funct_inv(K[nodo1,nodo2],lambda_i))
119     return distFinv
120
121 dist_array_Finv=np.zeros((n, n))
122 for v in range(n):
123     for w in range(n):
124         dist_array_Finv[v,w]=dist_frink_inv(v,w)
125
126 ## Construct the graph starting from K
127 G = nx.Graph()
128 G = nx.from_numpy_matrix(np.matrix(K))
129
130 ## Plot the graph
131 layout = nx.spring_layout(G)
132
133 plt.figure()
134 plt.title('Graph')
135 node_color=np.ones(n)

```

```

136 nx.draw(G, layout, node_color=node_color,with_labels=False)
137 nx.draw_networkx_labels(G, layout, font_size=12, font_family='sans-
    serif')
138 plt.show()
139
140 ## Drawing balls centered at i
141 for k in range(n):
142     for v in range(h+1):
143         if dist_array_F[i][k] > lambda_i[v]:
144             node_color[k]=h-v
145
146 node_color[i]=h+1
    
```

LISTING 1. Algorithm in Python

4. TEST AND COMPARISON WITH THE DIFFUSIVE METRIC FOR NEWTONIAN TYPE AFFINITIES

The results in [1] suggest testing the algorithm on affinities defined as discretizations of Newtonian type potentials of the form

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

for α positive. Once a discretization of K_α is given we may run our algorithm and also the well known diffusion metric introduced in [4]. See also [2]. Let us recall that the diffusive metric at time $t > 0$ is given by

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

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

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 radio, when we consider the discretization

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

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

It is worthy pointing out at 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 1 labels with the integers $0, 1, \dots, 59$ the 60 vertices of our graph.

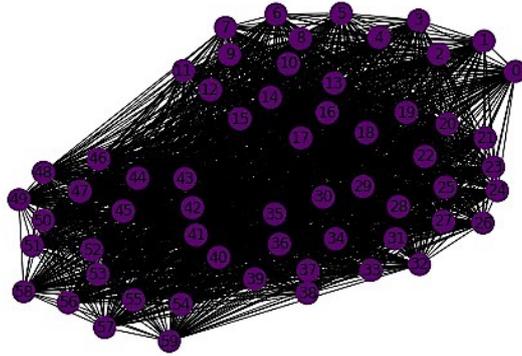
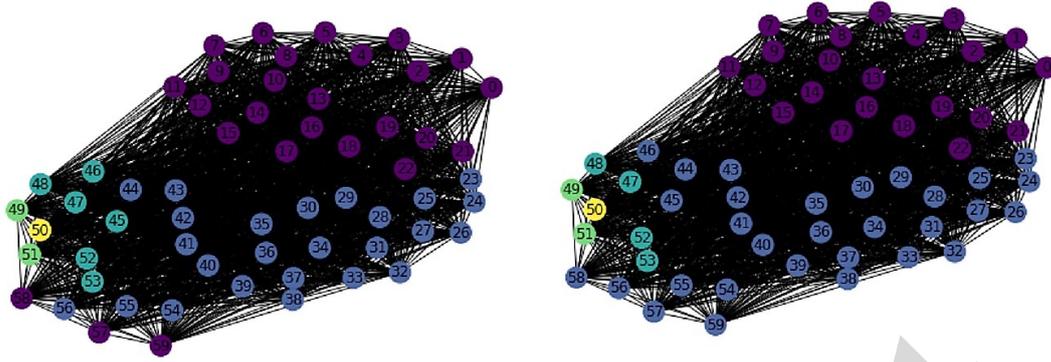


FIGURE 1. Graph

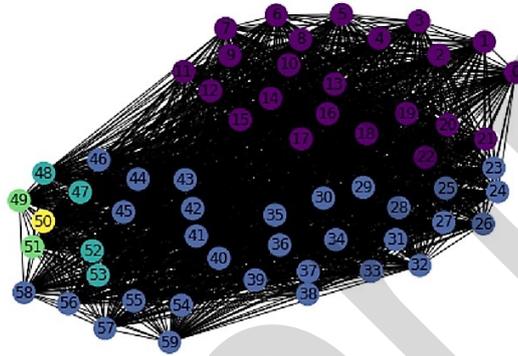
We shall now plot some balls centered at two different vertices, 25 and 50, each for the three metrics, the Euclidean metric (E), the Diffusive metric (D) with $t = 0.005$ and Frink's metric (F). The comparison of both, (D) and (F) with the Euclidean (E) is essential because K itself is built in terms 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 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 the Figure 2 and Figure 3 we use capital letters, Y, G, T, L and P for 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 $\lambda(i)$. Another somehow arbitrary step of the algorithm is the use of the main three diagonal of our affinity matrix K . Starting with the main five diagonals will produce another family of F-balls and annuli.



(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 2. Center at 50

DECLARATIONS

Funding. This work was supported by the Ministerio de Ciencia, Tecnología e Innovación-MINCYT in Argentina: Consejo Nacional de Investigaciones Científicas y Técnicas-CONICET and Agencia Nacional de Promoción Científica y Técnica-ANPCyT, (Grant PICT 2015-3631).

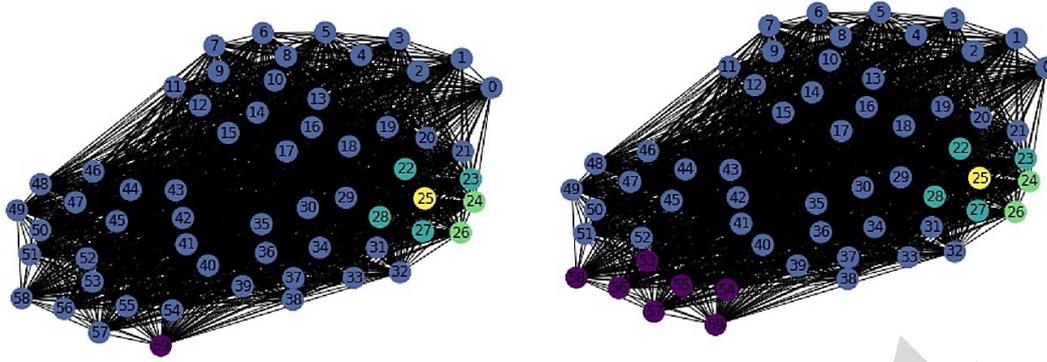
Conflicts of interest/Competing interests. The authors have no conflicts of interest to declare that are relevant to the content of this article.

Availability of data and material. Not applicable.

Code availability. We use Python, free software.

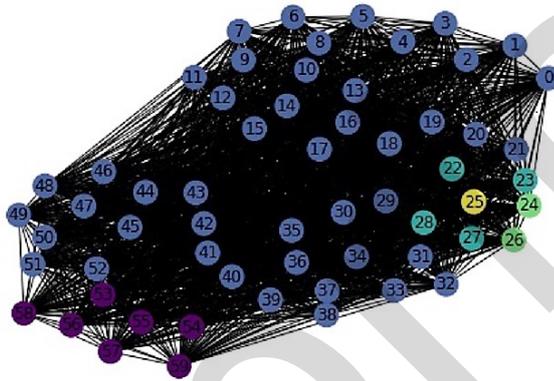
REFERENCES

[1] Hugo Aimar and Ivana Gómez, *Affinity and distance. On the Newtonian structure of some data kernels*, *Anal. Geom. Metr. Spaces* **6** (2018), 89–95. MR 3816950
 [2] M. M. Bronstein, J. Bruna, Y. LeCun, A. Szlam, and P. Vandergheynst, *Geometric deep learning: going beyond euclidean data*, *IEEE Signal Processing Magazine* **34** (2017), no. 4, 18–42.



(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 3. Center at 25

- [3] E. W. Chittenden, *On the metrization problem and related problems in the theory of abstract sets*, Bull. Amer. Math. Soc. **33** (1927), 13–34.
- [4] Ronald R. Coifman and Stéphane Lafon, *Diffusion maps*, Appl. Comput. Harmon. Anal. **21** (2006), 5–30.
- [5] A. H. Frink, *Distance functions and the metrization problem*, Bull. Amer. Math. Soc. **43** (1937), no. 2, 133–142. MR 1563501
- [6] John L. Kelley, *General topology*, Springer-Verlag, New York-Berlin, 1975, Reprint of the 1955 edition [Van Nostrand, Toronto, Ont.], Graduate Texts in Mathematics, No. 27. MR 0370454
- [7] Roberto A. Macías and Carlos Segovia, *Lipschitz functions on spaces of homogeneous type*, Adv. in Math. **33** (1979), no. 3, 257–270. MR 546295