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Supplementary Materials: Distance Closures on Complex Networks

Tiago Simas¹ and Luis M. Rocha^{1,2,3}

¹Cognitive Science Program, Indiana University, Bloomington, IN 47406, USA
²Center for Complex Networks and Systems, School of Informatics & Computing, Indiana University, Bloomington, IN 47406, USA
³Instituto Gulbenkian de Ciencia, Oeiras, Portugal

A Mathematical Background

In this appendix we present definitions that will be useful for the understanding of the paper.

A.1 A brief overview on Fuzzy Sets Theory

First we introduce the definition of T-Norms and T-Conorms first introduced by Menger et al. in (Menger, 1942; Schweizer and Sklar, 1983).

Definition 1 (T-Norm)

2

A *triangular norm* (*T*-Norm for short) is a binary operation \land on the unit interval [0, 1], i.e., a function $\land : [0,1]^2 \rightarrow [0,1]$, such that for all $x, y, z \in [0,1]$ the following four axioms are satisfied:

(T1) $x \land y = y \land x$. (T2) $x \land (y \land z) = (x \land y) \land z$. (T3) $x \land y \le x \land z$ wherever $y \le z$. (T4) $x \land 1 = x$.

A *T-Norm* is a generalisation of intersection in set theory and conjunction in logic. It was first defined in the context of probabilistic metric spaces (Schweizer and Sklar, 1983).

Definition 2 (T-Conorm)

A triangular conorm (*T*-Conorm for short) is a binary operation \lor on the unit interval [0, 1], i.e., a function $\lor : [0, 1]^2 \to [0, 1]$, such that for all $x, y, z \in [0, 1]$, satisfies (T1)-(T3) and (S4) $x \lor 0 = x$.

A T-Conorm is a generalisation of union in set theory and disjunction in logic.

There is an innumerable number of T-Norms and T-Conorms. In the following examples (Klement et al., 2000) we present the four basic T-Norms and T-Conorms.

The following are the four basic T-Norms $\wedge_M, \wedge_P, \wedge_L$ and \wedge_D given by, respectively:

Example 1 (Basic T-Norms) (1) $x \wedge_M y = min(x, y)$ (minimum),

(2)
$$x \wedge_P y = x \cdot y$$
 (product),

(3) $x \wedge_L y = max(x+y-1,0)$ (Lukasiewicz T-Norm),

(4)
$$x \wedge_D y = \begin{cases} 0, & \text{if } (x, y) \in [0, 1]^2; \\ min(x, y), & \text{otherwise.} \end{cases}$$
 (drastic product)

These T-Norms cover the range for T-Norms, from the strongest T-Norm \wedge_M to the weakest T-Norm \wedge_D . There are other T-Norms, namely *parametric T-Norms*, which range the spectrum of all possible T-Norms. Examples of these T-Norms are the *Dombi* T-Norms.

Definition 3 (Dombi T-Norm)

The definition of Dombi *T-Norm* is the following:

$$DT^{\lambda}_{\wedge}(a,b) = \left\{ 1 + \left[\left(\frac{1}{a} - 1\right)^{\lambda} + \left(\frac{1}{b} - 1\right)^{\lambda} \right]^{\frac{1}{\lambda}} \right\}^{-1}$$

Where the parameter $\lambda \in [0, +\infty[$.

Example 2 (Basic T-Conorms)

The following are the four basic T-Conorms \lor_M, \lor_P, \lor_L and \lor_D given by, respectively: (1) $x \lor_M y = max(x, y)$ (maximum),

(2) $x \lor_P y = x + y - x \cdot y$ (probabilistic sum),

(3) $x \lor_L y = min(x + y, 1)$ (Lukasiewicz T-Conorm),

(4)
$$x \lor_D y = \begin{cases} 1, & \text{if } (x, y) \in [0, 1]^2; \\ max(x, y), & \text{otherwise.} \end{cases}$$
 (drastic sum)

These T-Conorms define the specific range of T-Conorms, from the strongest T-Conorm \lor_D to the weakest T-Conorm \lor_M .

Definition 4 (Dombi T-Conorm)

The definition of Dombi T-Conorm is the following:

$$DT^{\lambda}_{\vee}(a,b) = \left\{ 1 + \left[\left(\frac{1}{a} - 1\right)^{\lambda} + \left(\frac{1}{b} - 1\right)^{\lambda} \right]^{-\frac{1}{\lambda}} \right\}^{-1}$$

Where the parameter $\lambda \in [0, +\infty[$.

Now we are able to define the transitivity property of a fuzzy relation.

Definition 5 (Transitivity) A fuzzy relation R(X,X) is transitive if

$$R(x,y) \ge \bigvee_{z} (R(x,z) \land R(z,y))$$

is satisfied $\forall x, y, z \in X$.

Definition 5 entails that transitivity depends on the pairs T-Conorm/T-Norm chosen.

Definition 6 (Fuzzy Complement)

A complement c of a fuzzy set satisfies the following axioms:

(c1) c(0) = 1 c(1) = 0 (boundary conditions).

(c2) $\forall a, b \in [0, 1]$ if $a \leq b$, then $c(a) \geq c(b)$ (monotonicity).

The *Complement* of a fuzzy set measures the degree to which a given element of the fuzzy set does not belong to the fuzzy set. Two most desirable requirements, which are usually among of fuzzy complements are:

Definition 7 (Fuzzy Complement)(cont))

_1

A complement c of a fuzzy set satisfies the following axioms:

(c3) c is a continuous function.

(c4) *c* is involutive, which means that c(c(a)) = a for each $a \in [0, 1]$.

In classical set theory, the operations of intersection and union are dual with respect to the complement in the sense that they satisfy the De Morgan laws. It is desirable that this duality be satisfied for fuzzy set as well. We say that a T-Norm \land and a T-Conorm \lor are dual with respect to a fuzzy complement *c* if and only if

$$c(a \wedge b) = c(a) \lor c(b)$$

and

4

$$c(a \lor b) = c(a) \land c(b).$$

Examples of dual T-Norms and T-Conorms with respect to the complement $c_s(a) = (1-a)^s$ are:

$$< min(a,b), max(a,b), c_s >$$

 $< DT^1(a,b), DT^1(a,b), c_s >$

. We can have weaker complements, which only obey to the first two axioms in definition 6 to allow other T-Norm and T-Conorm operators.

Next we follow with composition of fuzzy relations.

Definition 8 (Relation Composition)

Consider two binary fuzzy relations, P(X,Z) and Q(Z,Y) with a common set of Z. The standard composition of these relations, which is denoted by $P(X,Z) \circ Q(Z,Y)$ produces a binary fuzzy relation R(X,Y) on $X \times Y$ defined by

$$R(X,Y) = [P \circ Q] = \bigvee_z (P(x,z) \land Q(z,y)),$$

 $\forall x \in X \text{ and } \forall y \in Y \text{ and } \forall z \in Z$.

When the transitive closure $R^T(X,X)$ uses the T-Conorm $\lor = \text{maximum}$, with any T-Norm \land , κ in eq. 1 is finite and not larger than |X| - 1 (Klir and Yuan, 1995). In other words, the transitive closure converges in finite time and can be easily computed using Algorithm 1 (Klir and Yuan, 1995):

Algorithm 1

- 1. $R' = R \cup (R \circ R)$
- 2. If $R' \neq R$, make R = R' and go back to step 1.
- 3. Stop: $R^T = R'$

It has also been shown that if the semiring formed by $\langle \vee, \wedge \rangle$ on the unit interval is a dioid or a bounded preordered lattice(Gondran and Minoux, 2007), then κ in eq. 1 is also finite (Han and Li, 2004; Han et al., 2007) (see conditions below). In this case, the transitive closure can be computed in finite time using Algorithm 2:

Algorithm 2

R' = R, R_p = R, p = 1
 R_p = R ∘ R_p, p = p + 1
 If R' ≠ (R' ∪ R_p), make R' = R' ∪ R_p and go back to step 2.

4. Stop: $R^{T} = R'$

The union in step 1 must be in accordance with the T-Conorm defined in the relation composition. The resulting relation in step 3 is transitive with respect to the T-Norm, T-Conorm operations used. Moreover, given the last algorithm, a fuzzy graph is transitive if the algorithm stops at the first step. A reflexive, symmetric and transitive fuzzy relation is denominated as a *Similarity* or *Equivalence* relation.

Next we give a more detailed description of T-Norms and T-Conorms.

The intersection of two fuzzy sets *A* and *B* is performed by a binary operation closed on the unit interval. There are an infinite number of T-Norms from definition 1. One important class is that of *Archimedean T-Norms*, see (Klir and Yuan, 1995). Before we introduce one of the fundamental theorems of T-Norms, which provides us a method for generating Archimedean T-Norms we introduce the following definitions:

Definition 9 (Decreasing Generator)

A decreasing generator φ is a continuous decreasing function from the unit interval [0,1] into the real extended interval $[-\infty, +\infty]$.

Definition 10 (Pseudo-Inverse of a decreasing generator)

The pseudo-inverse of a decreasing generator φ is defined by

$$oldsymbol{arphi}^{(-1)}(a) = \left\{egin{array}{cccc} 1 & for & a \in (-\infty,0) \ arphi^{-1}(a) & for & a \in [0, arphi(0)] \ 0 & for & a \in (arphi(0),\infty) \end{array}
ight.$$

Where φ^{-1} is the inverse function of φ .

Theorem 1 (Characterization Theorem of T-Norms)

Let i be a binary operation closed on the unit interval. Then, i is an Archimidean T-Norm iff there exists a decreasing generator φ such

$$a \wedge b = \boldsymbol{\varphi}^{(-1)}(\boldsymbol{\varphi}(a) + \boldsymbol{\varphi}(b))$$

for all $a, b \in [0, 1]$.

With this last theorem we can generate an infinite class of T-Norms. Among many decreasing generators is the *Dombi T-Norm generator*, (see definition 3):

$$\varphi(x) = \left(\frac{1-x}{x}\right)^{\lambda}$$

Parameter λ allow us to obtain the range from the \wedge_D T-Norm ($\lambda \rightarrow 0$) to the \wedge_M T-Norm ($\lambda \rightarrow +\infty$). For many other decreasing generators, see (Klement et al., 2000).

Set unions are generalized by the T-Conorms in definition 2. There are an infinite number of T-Conorms and ways to generate new T-Conorms. One important class of T-Conorms is the *Archimedean T-Conorms*, see (Klir and Yuan, 1995).

Definition 11 (Increasing Generator)

A increasing generator θ is a continuous increasing function from the unit interval [0,1] into the real extended interval $[-\infty, +\infty]$.

Definition 12 (Pseudo-Inverse of a increasing generator)

The pseudo-inverse of a increasing generator θ is defined by

$$\theta^{(-1)}(a) = \begin{cases} 0 & for & a \in (-\infty, 0) \\ \theta^{-1}(a) & for & a \in [0, \theta(0)] \\ 1 & for & a \in (\theta(0), \infty) \end{cases}$$

Where θ^{-1} is the inverse function of θ .

Theorem 2 (Characterization Theorem of T-Conorms)

Let u be a binary operation closed on the unit interval. Then, u is an Archimidean T-Conorm iff there exists an increasing generator θ such

$$a \lor b = \theta^{(-1)}(\theta(a) + \theta(b))$$

for all $a, b \in [0, 1]$.

6

With this last theorem we can generate an infinite class of T-Conorms. Among many increasing generators is the Dombi T-Conorm generator:

$$\boldsymbol{\theta}(x) = \left(\frac{x}{1-x}\right)^{\lambda}$$

Parameter λ allow us to obtain the range from the \vee_M T-Conorm ($\lambda \to 0$) to \vee_D T-Conorm ($\lambda \to +\infty$). For many other decreasing generators the reader can see, (Klement et al., 2000).

A.2 Algebraic Structures Basics

Here we present the basic definitions on algebraic structures used in this work.

The whole class of semirings splits into main disjoint subclasses: (a) rings and (b) canonical ordered semirings or *dioids*. On the following, we consider algebraic structures consisting of a basic set *E*, with two internal operations \oplus and \otimes . All these definitions can be found on (Gondran and Minoux, 2007).

Definition 13 (Semi-Ring)

Let consider the following algebraic structure $L = (E, \oplus, \otimes)$. *L* is called a *semiring* if the following properties hold:

(i) (E, \oplus) is a commutative monoid with zero element ε ,

(ii) (E, \otimes) is a monoid with unit element *e*,

(iii) \otimes is right and left distributive with respect to \oplus ,

(iv) ε is absorbing, i.e. $\varepsilon \otimes a = a \otimes \varepsilon = \varepsilon$, $\forall a \in E$.

Definition 14 (Canonical Order)

 $L = (E, \oplus)$ being a monoid, the binary relation \leq on *E* is defined as: $a \leq b$ iff $\exists c \in E$ such that $b = a \oplus c$, is a *preorder relation* (reflexive and transitive) called the *canonical preorder*. A monoid is called *canonically ordered* iff the canonical preorder is order, or equivalently iff \leq is antisymmetric ($a \leq b$ and $b \leq a \Rightarrow a = b$).

Definition 15 (Dioid)

A semiring (E, \oplus, \otimes) such that (E, \oplus) is canonically orderd is called a *dioid*.

The algebraic structure $I = ([0, 1], \lor, \land)$, where \lor and \land are general T-Conorm/T-Norm, respectively, are not in general a dioid, since they fail property (*iii*) (distributivity) of definition 13 (semiring). However, there are subclasses of the algebraic structure $I = ([0, 1], \lor, \land)$, which are dioids.

For more details about algebraic structures see for example (Gondran and Minoux, 2007; Han and Li, 2004) or any book about Abstract Algebra.

B Proofs to the theorems

In this section we provide the proofs to the theorems in the main text.

Theorem 1

Let $G_P = (X, P)$ be a proximity (symmetric and reflexive) graph and Φ the graph distance function in definition 2, then $G_D = (X, D)$, where $D = \Phi(P)$, is symmetric and anti-reflexive.

Proof

Since G_P is reflexive then $p_{x,x} = 1$ and from definition 2 we have $d_{x,x} = \varphi(p_{x,x}) = \varphi(1) = 0$, therefore G_D is anti-reflexive. Let x and y be two vertices of G_P , because a proximity graph is symmetric we have $p_{x,y} = p_{y,x}$, since φ is bijective $d_{x,y} = \varphi(p_{x,y}) = \varphi(p_{y,x}) = d_{y,x}$, therefore G_D is symmetric. \Box

Theorem 2

If φ is a distance function as in definition 2. For every pair of T-Norm/T-Conorm operations $\langle \wedge, \vee \rangle$, there exists a pair of operations $\langle f, g \rangle$ a TD-conorm/TD-norm (definition 3) and vice versa, obtained via the following constraints:

(1) $\varphi(a \wedge b) = g(\varphi(a), \varphi(b));$ (2) $\varphi(a \vee b) = f(\varphi(a), \varphi(b)).$

Where $a, b \in [0, 1]$.

Proof

Let us assume $a \leq b$.

(1) Suppose $\varphi(a \wedge b) > g(\varphi(a), \varphi(b))$, thus the inequality is true if the maxima of $\varphi(a \wedge b)$ (must be maximum) is bigger than the minimum of $g(\varphi(a), \varphi(b))$ (must be minimum). $\varphi(a \wedge b)$ is maximum for $\wedge \equiv T_D$ (drastic product, see (Klement et al., 2000) (Klir and Yuan, 1995)) and $g(\varphi(a), \varphi(b))$ is minimum for $\varphi(b) = 0$, thus for $\varphi(b) = 0$ we obtain, $\varphi(a) \leq g(\varphi(a), \varphi(b))$, from the other side $\varphi(a \wedge b) \leq \varphi(min(a, b)) = \varphi(a)$. Therefore, $\varphi(a \wedge b) \leq g(\varphi(a), \varphi(b))$.

Suppose $\varphi(a \wedge b) < g(\varphi(a), \varphi(b))$, thus $\varphi(a \wedge b)$ must be minimum and $g(\varphi(a), \varphi(b))$ must be maximum. $\varphi(a \wedge b)$ is minimum for $\wedge \equiv \min$ and $g(\varphi(a), \varphi(b))$ is maximum for a = 0, thus for a = 0 we obtain, $g(\varphi(a), \varphi(b)) \le \varphi(a)$, from the other side $\varphi(a \wedge b) \ge$ $\varphi(\min(a, b)) = \varphi(a)$. Therefore, $\varphi(a \wedge b) \ge g(\varphi(a), \varphi(b))$, and from above this implies $\varphi(a \wedge b) = g(\varphi(a), \varphi(b))$, which proves statement (1).

(2) Suppose $\varphi(a \lor b) > f(\varphi(a), \varphi(b))$, thus $\varphi(a \lor b)$ must be maximum and $f(\varphi(a), \varphi(b))$ must be minimum. $\varphi(a \lor b)$ is maximum for $\lor \equiv max$ and $f(\varphi(a), \varphi(b))$ is minimum for $\varphi(a) = 0$, thus for $\varphi(a) = 0$ we obtain, $f(\varphi(a), \varphi(b)) \ge 0$, from the other side $\varphi(a \lor b) \le \varphi(max(1,b)) = \varphi(1) = 0$. Therefore, $\varphi(a \lor b) \le f(\varphi(a), \varphi(b))$.

Suppose $\varphi(a \lor b) < f(\varphi(a), \varphi(b))$, thus $\varphi(a \lor b)$ must be minimum and $f(\varphi(a), \varphi(b))$ must be maximum. $\varphi(a \lor b)$ is minimum for $\lor \equiv S_D$ (drastic sum, see (Klement et al., 2000) (Klir and Yuan, 1995)) and $f(\varphi(a), \varphi(b))$ is maximum for b = 0, thus for b = 0 we obtain, $f(\varphi(a), \varphi(b)) \le \varphi(a)$, from the other side $\varphi(a \lor b) \ge \varphi(max(a,b)) = \varphi(a)$. Therefore, $\varphi(a \lor b) \ge f(\varphi(a), \varphi(b))$, and from above this implies $\varphi(a \lor b) = f(\varphi(a), \varphi(b))$, which proves statement (2). \Box

Theorem 3

If $G_P = (X, P)$ is a fuzzy proximity graph and $G_D = (X, D)$ is the distance graph obtained from G_P via $D = \Phi(P)$, where Φ is the isomorphism (distance function) in definition 2, then the following statements are true:

1) $\Phi(P) \supseteq \Phi(P^2) \supseteq \Phi(P^3) \supseteq \cdots \supseteq \Phi(P^{\infty})$; 2) $D \supseteq D^2 \supseteq D^3 \supseteq \cdots \supseteq D^{\infty}$.

where $\Phi(P^n) \supseteq \Phi(P^{n+1})$ means that: $\forall x_i, x_j \in X : \varphi(p_{ij}^n) \ge \varphi(p_{ij}^{n+1})$, and $D^n \supseteq D^{n+1}$ means that: $\forall x_i, x_j \in X : d_{ij}^n \ge d_{ij}^{n+1}$.

Proof

1) φ is a monotonic decreasing function and because P is reflexive, from (Mordeson and Nair, 2000) we have $P \subseteq P^2 \subseteq P^3 \subseteq \cdots \subseteq P^{\infty} \Rightarrow \Phi(P) \supseteq \Phi(P^2) \supseteq \Phi(P^3) \supseteq \cdots \supseteq \Phi(P^{\infty})$ which proves the statement.

2) To prove the second statement we first need to prove that $D \supseteq D^2$, which is equivalent to showing that, $\forall x, y, z \in X : d_{x,y}^2 = f\{g(d_{x,z}, d_{z,y})\} \le d_{x,y}$. Lets prove by absurd this statement: suppose $d_{x,y}^2 > d_{x,y}$ then the minimum of $f\{g(d_{x,z}, d_{z,y})\}$ must be $> d_{x,y}$. $f\{g(d_{x,z}, d_{z,y})\}$ is minimum if f and g are minimum. g is minimum if $d_{z,y} = 0$ for all $z \in X - \{x\}$, then $g(d_{x,z}, d_{z,y}) \ge d_{x,z}$. f is minimum if $d_{x,z} \ge d_{x,y}$ for all $z \in X - \{y\}$ then $f(d_{x,y}, d_{x,z}) \le f(d_{x,y}, +\infty) \le d_{x,y}$, which contradicts our assumption, $d_{x,y}^2 > d_{x,y}$. Therefore, $d_{x,y}^2 \le d_{x,y}$.

By induction we can prove the general result.

 $\forall x, y, z \in X : d_{x,y}^{n+1} = f_z \{ g(d_{x,z}^n, d_{z,y}) \} \text{ by hypothesis } d_{x,y}^n \leq d_{x,y}^{n-1}, \text{ thus } d_{x,y}^{n+1} \leq f_z \{ g(d_{x,z}^{n-1}, d_{z,y}) \} = d_{x,y}^n, \text{ which proves the second statement.} \square$

Theorem 4

Given a proximity graph $G_P = (X, P)$, a distance graph $G_D = (X, D)$, and the isomorphism φ and Φ of definition 2, for any algebraic structure $I = ([0, 1], \land, \lor)$ with a T-Conorm/T-Norm pair $\langle \land, \lor \rangle$ used to compute the transitive closure of P, there exists an algebraic structure $II = ([0, +\infty], f, g)$ with a TD-conorm/TD-norm pair $\langle f, g \rangle$ to compute the isomorphic distance closure of $D, D^T = \Phi(P^T)$, which obeys the condition:

$$\forall x_i, x_j, x_k \in X : f_k(g(\varphi(p_{ik}), \varphi(p_{kj}))) = \varphi(\bigvee_k((p_{ik} \land p_{kj})))$$

and vice-versa if we fix $\langle f, g \rangle$ (TD-norm/TD-Conorm) and isomorphism φ , to obtain $\langle \lor, \land \rangle$:

$$\forall x_i, x_j, x_k \in X : \bigvee_k (\varphi^{-1}(d_{ik}) \land \varphi^{-1}(d_{kj})) = \varphi^{-1}(f(g(d_{ik}, d_{kj})))$$

where φ^{-1} is the inverse function of φ .

Proof

The transitive closure of P is given by P^{k_1} and the distance closure of D by D^{k_2} , with k_1 and k_2 integers. Let $n = max(k_1, k_2)$, thus for $\Phi(P^n) = D^n$ to be true, the following must also be true:

$$\forall x, y, z \in X : f_{z}\{g(\varphi(p_{x,z}), \varphi(p_{z,y})\} = \varphi(\bigvee_{z} \{p_{x,z} \land p_{z,y}\})$$

We can prove by induction that $\Phi(P^n) = D^n$ is true if we assume that the condition in this theorem is true.

10

Tiago Simas & Luis M. Rocha

The condition in this theorem is equivalent to:

$$\Phi^{-1}(\Phi(P) \circ \Phi(P)) = P^2 = P \circ P$$

Where $\Phi(P) \circ \Phi(P)$ is the distance composition using f and g, and $P \circ P$ is the transitive composition using \wedge and \vee . We also can define D^n in function of Φ and P.

$$D^n = \underbrace{D \circ \cdots \circ D}_n = \underbrace{\Phi(P) \circ \cdots \circ \Phi(P)}_n$$

Therefore, what we want to prove is:

$$\Phi^n(P) = \Phi(P^n)$$

given the condition on this theorem is true. by induction:

(1) $\Phi(P) \circ \Phi(P) = \Phi(P^2)$ (Basis); (2) $\Phi^n(P) = \Phi(P^n)$ (Hypothesis); (3) $\Phi^{n+1}(P) = \Phi(P^{n+1})$ (Thesis).

Assuming the condition on this theorem $\Phi^{-1}(\Phi(P) \circ \Phi(P)) = P^2$ is true, then it is also true that $\Phi(P) \circ \Phi(P) = \Phi(P^2)$. Thus, $\Phi^{n+1}(P) = \Phi^n(P) \circ \Phi(P) = \Phi(P^n) \circ \Phi(P) = \Phi(P^{n+1})$ from statements (1) and (2), which proves the theorem.

Let us prove that there exist a pair of binary functions f and g per definition 3. From theorem 2 we have

$$g(\varphi(p_{x,z}),\varphi(p_{z,y})) = \varphi(p_{x,z} \wedge p_{z,y})$$

and from the condition in this theorem, we have

$$f_{z}\{g(\varphi(p_{x,z}),\varphi(p_{z,y}))\} = \varphi(\bigvee_{z}\{p_{x,z} \land p_{z,y}\})$$
$$f_{z}\{\varphi(p_{x,z} \land p_{z,y})\} = \varphi(\bigvee_{z}\{p_{x,z} \land p_{z,y}\})$$

Therefore,

$$f(d_{x,z}, d_{z,y}) \equiv \boldsymbol{\varphi}(\boldsymbol{\varphi}^{-1}(d_{x,z}) \lor \boldsymbol{\varphi}^{-1}(d_{z,y}))$$

The conditions of this theorem leads to the equations of theorem 2:

$$g(d_{x,z}, d_{z,y}) = \varphi(\varphi^{-1}(d_{x,z}) \land \varphi^{-1}(d_{z,y}))$$
$$f(d_{x,z}, d_{z,y}) \equiv \varphi(\varphi^{-1}(d_{x,z}) \lor \varphi^{-1}(d_{z,y}))$$

From these last equations we can also find \lor and \land given f, g and the isomorphism φ :

$$p_{x,z} \lor p_{z,y} = \varphi^{-1}(f(\varphi(p_{x,z}), \varphi(p_{z,y})))$$
$$p_{x,z} \land p_{z,y} = \varphi^{-1}(g(\varphi(p_{x,z}), \varphi(p_{z,y})))$$

Theorem 5

Given a finite proximity graph $G_P(X, P)$, and an algebraic structure $I = ([0, 1], \lor, \land)$, with a T-Conorm/T-Norm pair $\langle \land, \lor \rangle$ used to compute the transitive closure of G_P , if I is a dioid, then the transitive closure $G_P^T(X, P^T)$ can be computed by equation 1 for a finite κ .

See (Gondran and Minoux, 2007) for proof; further discussion and examples also see (Han and Li, 2004; Han et al., 2007; Pang, 2003; Klir and Yuan, 1995).

Theorem 6

Given a finite distance graph $G_D(X,D)$, and an algebraic structure $II = (\{[0,+\infty], f,g),$ with a TD-Conorm/TD-Norm pair $\langle f, f \rangle$ used to compute the distance closure of G_D , if II is a dioid, then the distance closure $G_D^T(X,D^T)$ can be computed in finite time via the transitive closure of isomorphic graph $G_P(X,P)$ with algebraic structure I obtained by an isomorphism satisfying Theorem 4. In other words, if II is a dioid, via an isomorphism satisfying Theorem 4 we obtain an algebraic structure I which is also a dioid.

This theorem can be easily proven from theorems 3, 4 and 5, by evoking the isomorphism to proximity space.

Corollary 1

Given the isomorphism constraint on the T-Norm from algebraic structure *I* (eq. 7) from theorem 4, let $f \equiv \min$, $g \equiv +$ and φ a distance function, per definition 2. If $\lor \equiv \max$ as T-Conorm, then the T-Norm operator \land exists and φ is its generator function.

Proof

We have seen in theorem 2 that $\varphi(x \wedge y) = g(\varphi(x), \varphi(y))$ therefore $\forall x, y, z \in P$ and by theorem 4:

$$\varphi^{-1}(\min_{z} \{\varphi(p_{x,z}) + \varphi(p_{z,y})\}) = \max_{z} \{p_{x,z} \land p_{z,y}\}$$
$$\max_{z} \{\varphi^{-1}(\varphi(p_{x,z}) + \varphi(p_{z,y}))\} = \max_{z} \{p_{x,z} \land p_{z,y}\}$$
$$\Rightarrow$$
$$\varphi^{-1}(\varphi(p_{x,z}) + \varphi(p_{z,y})) = p_{x,z} \land p_{z,y}$$

This last result is the characterisation function of T-Norms, according to theorem 7 (Klir and Yuan, 1995), which states that \land is a T-Norm and φ is the decreasing generator function (obeying definition 2).

Theorem 8

Given the isomorphism φ , if D^{mc} is the metric closure with $f \equiv \min$ and $g_1 \equiv +$, and D^{um} is the ultra-metric closure with $f \equiv \min$ and $g_2 \equiv \max$ then $D^{mc} \supseteq D^{um}$ is equivalent to $P^{mc} \subseteq P^{um}$, where $D^{mc} = \Phi(P^{mc})$ and $D^{um} = \Phi(P^{um})$. Therefore, $\Delta(P^{um}) \ge \Delta(P^{mc})$.

Proof

We can prove by induction that:

1)
$$D^2 \stackrel{i}{\supseteq} \Phi(P^2)$$
;
2)
$$\begin{cases}
H : D^n \stackrel{i}{\supseteq} \Phi(P^n) \\
T : D^{n+1} \stackrel{i}{\supseteq} \Phi(P^{n+1}) \\
\text{Let's prove 1} \\
\forall x, y, z \in X : D^2_{mc} = f(d_{x,z} + d_{z,y}) = f(\varphi(p_{x,z}) + \varphi(p_{z,y})) \ge f(g_2(\varphi(p_{x,z}), \varphi(p_{z,y}))) = D^2_{um}, \text{ therefore } D^2_{mc} \stackrel{i}{\supseteq} D^2_{um}.$$

2) by the hypothesis we know that $\forall x, y, z \in X : D^n \ge \Phi(P^n)$, then using this result we have $\forall x, y, z \in X : D^{n+1} = f\{d_{x,z}^n + d_{z,y}\} \ge f\{\varphi(p_{x,z}^n) + \varphi(p_{z,y})\}$, because $f\{\varphi(p_{x,z}^n) + \varphi(p_{x,y})\} \ge f\{\varphi(p_{x,z}^n) \lor \varphi(p_{z,y})\}$ and using theorem 2, $f\{g_2(\varphi(p_{x,z}^n), \varphi(p_{z,y}))\} = \varphi(\bigvee_z \{p_{x,z}^n \land p_{z,y}\}) = \Phi(P^{n+1})$, so $\forall x, y, z \in X : D^{n+1} \ge \Phi(P^{n+1})$, which proves that $D^{mc} \equiv D^n \supseteq \Phi(P^n) \equiv D^{um}$. \Box

Theorem 9

Given a fuzzy complement c(x), a T-Norm $DT^1_{\wedge} = \frac{ab}{a+b-ab}$ and a T-Conorm max(a,b), then the triple has no involutive complement, which satisfies the De Morgan's laws.

Proof

12

A complement is involutive if c(c(x)) = x. If the complement c(x) satisfies the De Morgan's laws we have:

$$a \lor b = \bar{a} \land b$$
$$c(max(a,b)) = \frac{c(a)c(b)}{c(a) + c(b) - c(a)c(b)}$$

without loss of generality let $a \ge b$

$$c(a) = \frac{c(a)c(b)}{c(a) + c(b) - c(a)c(b)}$$
$$c(a)(1 - c(b)) = 0$$
$$c(a) = 0 \lor c(b) = 1$$

the only function that satisfies this condition is the threshold function, which is not involutive (Klir and Yuan, 1995). \Box

C Optimal Dombi T-Norm for a characteristic path length

We have seen that we can apply an infinity of pairs of T-Norms and T-Conorms to calculate distance closure, and compute shortest paths in distance graphs. In this formulation (see corollary 1), we fix the T-Conorm with $\forall \equiv max$, allowing us to explore many options for the T-Norm \land . The T-Norm is defined via the T-Norm generator isomorphism φ (corollary 1). Then, using $\langle f \equiv min, g \equiv + \rangle$ as the TD-norm/TD-conorm pair for computing the metric closure, via the APSP/Dijkstra, distance product or equivalent, we can sweep the space of possible T-Norms, thus simultaneously exploring the range of possible isomorphisms. In this section we explore the Dombi T-Norm family, where the Dombi T-Norm generator is:

$$\varphi(x) = \left(\frac{1}{x} - 1\right)^{\lambda} \tag{C1}$$

where λ is the sweeping parameter. The parameter λ in the T-Norm generator takes values in $]0, +\infty[: \lambda \to 0$ lower bound (*drastic product*) and $\lambda \to \infty$ is the upper bound (*minimum*). The reason we choose this T-Norm generator is because it yields the more commonly used isomorphism from proximity to distance; when $\lambda = 1$, (Eckhardt et al., 2009) (Strehl, 2002), the generator of eq. C 1, becomes the isomorphism of formulae 2, which we have used in the previous section:

$$\varphi(x) = \frac{1}{x} - 1.$$

We have seen that when T-Norm and T-Conorm (\lor, \land) are fixed, the transitive closure and the distance closure are equivalent via isomorphism φ .

For empirical analysis of complex networks it is desirable that properties of the graphs obtained via specific closures, such as *average shortest path*, be simultaneously characteristic in both spaces (proximity and distance). That is, the fluctuations of the mean, must be constrained on both spaces (average shortest path and average strongest path). In order to have a characteristic average path length, the shortest paths distribution must follow approximately a normal distribution. We want to find the best λ , using the Dombi T-Norm generator, which guarantees these assumptions, while fixing $\vee = \max$.

Assuming that the shortest path distribution of a distance graph follows a normal distribution, the probability density function for a normal random variable X, here the shortest path, is given by:

$$h_X(x) = \frac{1}{\sqrt{2\pi\sigma^2}} e^{\frac{-(x-\mu)^2}{2\sigma^2}}$$
(C2)

where μ and σ are the mean and standard deviation of the normal distribution.

The mean of a random variable Y = j(X), which is a monotonic function of X, where X is the random variable representing shortest path in a distance graph, and Y the random variable representing the strongest path in the isomorphic distance graph, is given by:

$$\langle Y \rangle = \int_0^\infty j(x)h_X(x)dx$$
 (C 3)



Fig. C1. Study of the fluctuations in proximity space, CV_p as function of λ for $\mu = 10$ (average path length in distance space) with $CV_d = 0.2$.

In our case,

14

$$j(x) = \varphi^{-1}(x) = \frac{1}{x^{\frac{1}{\lambda}} + 1}$$

Therefore, the fluctuations of the mean, in the proximity space are given by:

$$CV_p = \frac{\sigma_p}{\mu_p} = \frac{\sqrt{\langle Y^2 \rangle - \langle Y \rangle^2}}{\langle Y \rangle}$$
 (C4)

where CV_p is the *coefficient of variability*¹, and σ_p and μ_p are the standard deviation and mean of the strongest path in the proximity space and $\langle Y^2 \rangle$ is given by:

$$\langle Y^2 \rangle = \int_0^\infty j^2(x) h_X(x) dx$$
 (C 5)

The fluctuations in the distance space of the shortest path, are given by the *coefficient of* variability, CV_d :

$$CV_d = \frac{\sigma}{\mu} \tag{C6}$$

The dependence of CV_p on CV_d comes from equations C 2, C 3 and C 5. In figure C 1 we plot the theoretical relation between λ and CV_p for $\mu = 10$ (average shortest path in distance space is normally distributed) and $CV_d = 0.2$, using equation C 4; the shape is preserved for different parameter values. We can see from this figure that the coefficient of variability in the proximity space is minimum when λ converges to the *min* T-Norm $(\lambda \to +\infty)$; the ultra-metric closure. However, from our assumptions we require that $CV_p \approx$ $CV_d = 0.2$, in this case. The marked point in the figure C 1 shows the point where the assumptions are met. We observe that $\lambda \approx 1$ in this scenario.

¹ The coefficient of variability is scale invariant.



Fig. C 2. λ versus μ for several coefficients of variability CV_d and CV_p

To inspect in more detail the best value or values for λ , using the metric closure we plot, in figure C 2 the theoretical λ versus μ (average shortest path), for several acceptable coefficients of variability in both spaces, assuming that the optimal value should share a controlled $CV_d \approx CV_p \leq 0.6$. The results from this figure are obtained by finding the root (λ) of the equation:

$$CV_p^{theoretical}(\lambda) - CV_p = 0$$

 $CV_p^{theoretical}(\lambda) = rac{\sqrt{\langle Y^2 \rangle - \langle Y \rangle^2}}{\langle Y \rangle}$

Where $\langle Y^2 \rangle$ and $\langle Y \rangle$ are given by equations C2, C3 and C5 with $j(x) = \frac{1}{x^{\frac{1}{\lambda}} + 1}$ and we assume $h_X(\mu, \sigma)$ is normally distributed with $\sigma = \mu \times CV_d$ (μ is the average shortest path) with $CV_d \approx CV_p$ the real data fluctuations. We use *Mathematica* 7 to find the roots of this equation. From this figure we can see that when we increase the coefficients of variability, λ also increases. However, λ remains contained in the interval [0.8, 1.9]. For small average shortest paths the best $\lambda \in [0.8, 1.2]$, where after a transient $(\mu \approx 25)$, λ reaches an equilibrium, independent of scale factors (λ becomes invariant). The scale factor associated to the average shortest path length (characteristic for each network), depends mainly on the weights distribution. We can also observe that for very small fluctuations ($CV_d = CV_p = 0.1$), λ becomes invariant for values ≈ 1 . $\lambda = 1$ is an optimal asymptotic value for small fluctuations, since $CV \ge 0$. In real data in order to guarantee a characteristic mean (average strongest and shortest path), in both spaces (proximity and distance), the fluctuations should be as small as possible. However in real data the shortest path distribution only approximates to the normal distribution, which is one of our assumptions, resulting in higher fluctuations, for both spaces. For fluctuations $CV_d \approx CV_p \in [0, 0.4]$ we should use an isomorphism with $\lambda \in [0.8, 1.9]$. For $CV \approx 0$ the asymptotical optimal value is $\lambda = 1$ (see figure C2). This gives us a lower bound to calculate the desired metric closure in a distance graph to minimize fluctuations, λ should be larger or equal than 1 ($\lambda \ge 1$). To control fluctuations in both spaces (proximity,

16

Tiago Simas & Luis M. Rocha

distance) we should choose λ according to the fluctuations obtained in the distance or proximity spaces (this can be seen as an optimization problem).

In most applications, researchers use mappings between proximity and distance spaces similar to $\lambda = 1$, using isomorphisms $\varphi = \frac{1}{x}$ or $\varphi = \frac{1}{x} - 1$. We have to alert that the first choice $\varphi = \frac{1}{x}$ is not mathematically correct, since it maps $\varphi : [0,1] \rightarrow [1,+\infty]$, which is not a distance space. $\lambda = 1$ leads to the more common φ and asymptotical optimal value, assuming small fluctuations. However, to constrain fluctuations we may want to use other values of $\lambda \ge 1$, depending on the level real data fluctuations.

D Community Structure in Example Networks



Fig. D1. Community Structure of Toy Network with Newman's Fast Algorithm.



Fig. D 2. Community Structure of Toy Network with Hierarchical Clustering.

18

15:18

Tiago Simas & Luis M. Rocha



Fig. D3. Community Structure of Flu Network with Newman's Fast Algorithm.



Fig. D4. Community Structure of Flu Network with Hierarchical Clustering.

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ZU064-05-FPR Supplementary Materials 6 February 2015 15:18