ON PROXIMITY MEASURES FOR GRAPH VERTICES¹

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We study the properties of several proximity measures for the vertices of weighted multigraphs and multidigraphs. Unlike the classical distance for the vertices of connected graphs, these proximity measures are applicable to weighted structures and take into account not only the shortest, but also all other connections, which is desirable in many applications. To apply these proximity measures to unweighted structures, every edge should be assigned the same weight which determines the proportion of taking account of two routes, from which one is one edge longer than the other. A topological interpretation is obtained for the Moore–Penrose generalized inverse of the Laplacian matrix of a weighted multigraph.

1. INTRODUCTION

Proximity measures for the vertices of directed and undirected graphs arise in many applied settings. The range of applications of such functions is rather wide, including chemistry [1–7], crystallography [8], epidemiology [9], urban planning [10], organizational management [11], political sciences [12], aggregation of preferences [13, 14], etc. The most steadfast interest in them is displayed in mathematical sociology [15–25] in connection with the problem of measuring centrality in social networks. This important concept is multifarious, and a great variety of model and heuristic approaches were proposed to define its numerical representation. Note that graph theorists mainly dealt with the classical distance between the vertices of a connected graph [26], which is the length of the shortest path between them. At the same time, the presence of additional, even longer paths is of practical importance in many applications. For example, if the shortest road between two places is congested, a portion of goods can be delivered by a longer path (detour).

In this paper, we study the properties of several "sensitive" proximity measures that take into account all connections in a multigraph. Their common feature is the calculation (with appropriate weights) of all structures of a certain type that connect two vertices: paths, routes, routes with drains, trees, and so forth. For these measures, the weights of edges determine the proportion of taking account of longer paths in comparison with shorter ones. In some cases, the weight of an edge has the meaning of a "transfer factor" that specifies the losses (of substance, influence, reliability, etc.) when moving through a graph.

2. SOME NORMATIVE PROPERTIES OF PROXIMITY MEASURES

Suppose that G is a weighted multigraph with vertex set $V(G) = \{1, ..., n\}$ and edge set E(G); Γ is a weighted multidigraph with vertex set $V(\Gamma) = \{1, ..., n\}$ and arc set $E(\Gamma)$; the weights of edges and arcs are denoted by ε_{ij}^p (the pth edge/arc from i to j) and are strictly positive. The terms "graph" and "subgraph" will be used as

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generic ones (allowing multiple, weighted, and directed arcs).

Suppose that $E = (\varepsilon_{ij})$ is the matrix of total weights of edges (arcs) for all pairs of vertices:

$$\varepsilon_{ij} = \sum_{p=1}^{a_{ij}} \varepsilon_{ij}^p, \ i, j = 1, \dots, n,$$

where a_{ij} is the number of edges (arcs) that connect i to j. Let H be a subgraph of G. The product of the weights of all edges of H will be termed the weight of H and denoted by $\varepsilon(H)$. The weight of a directed subgraph of Γ is defined similarly. The weight of a subgraph without edges/arcs is set to be 1. For any nonempty set of subgraphs \mathcal{G} , its weight is

$$\varepsilon(\mathcal{G}) = \sum_{H \in \mathcal{G}} \varepsilon(H). \tag{1}$$

The weight of the empty set is zero. $P=(p_{ij})$ will designate various $n\times n$ -matrices of proximity (accessibility, connectedness) measures for the vertices of G or Γ .

Let us formulate a number of conditions whose fulfillment is rather natural to the proximity measures under consideration. Most of them were introduce in connection with the *relative forest accessibility* of graph vertices [25].

Symmetry. For every multigraph, the matrix P is symmetric.

This condition is hardly natural as applied to directed graphs. In the statements below, symmetry always stands for that applied in the undirected case.

Nonnegativity. For any multigraph (multidigraph), $p_{ij} \geq 0, i, j = 1, \dots, n$.

Reversal property. For any multidigraph, the reversal of all its arcs (provided that their weights are preserved) results in the transposition of the proximity matrix.

Diagonal maximality. For any multigraph (multidigraph) and any i, j = 1, ..., n such that $i \neq j$, $p_{ii} > p_{ij}$ and $p_{ii} > p_{ji}$ hold.

This condition requires a stronger relation of each vertex to itself than to any other vertex. If a proximity measure has the reversal property, then the two inequalities of the diagonal maximality are equivalent in the case of directed graphs as well as in the undirected case. Since all the measures applicable to directed graphs hereinafter possess the reversal property, we will prove only the first inequality of diagonal maximality.

Triangle inequality for proximities. For any multigraph and for any i, j, k = 1, ..., n, $p_{ij} + p_{ik} - p_{jk} \le p_{ii}$ holds. If, in addition, j = k and $i \ne j$, then the inequality is strict.

The triangle inequality for proximities is also meaningful as applied to directed graphs. However, in this case it requires special consideration, since different orders of subscripts $(p_{ij} \text{ or } p_{ji}, \text{ etc.})$ give rise to several modifications. In this paper, a "directed" triangle inequality for proximities is used in some proofs, but in the main text we deal with its undirected version only.

Consider the index¹

$$d_{ij} = p_{ii} + p_{jj} - p_{ij} - p_{ji}, \quad i, j = 1, \dots, n.$$
(2)

Metric representability of proximity. The index d_{ij} is a distance between the vertices of a multigraph, i.e., it satisfies the axioms of a metric.

This condition is always satisfied, provided that symmetry and the triangle inequality for proximities hold true [29]; the latter condition turns out to be closely related to the usual triangle inequality for the distance d_{ij} . Moreover, some kind of duality has been established between the metrics defined on an arbitrary set and the functions that satisfy the triangle inequality for proximities and an additional normalization condition [29].

Let us adduce an example not dealing with graphs to illustrate the triangle inequality for proximities and the metric (2). Let p(x, y) be the function, defined on the pull-back of some family \mathcal{X} of finite sets, that takes every pair of sets (x, y) to the number $|x \cap y|$ of elements in their meet. Then, for any $x, y, z \in \mathcal{X}$,

$$p(x,x) = |x| \ge |x \cap y| + |x \cap z| - |x \cap y \cap z| \ge |x \cap y| + |x \cap z| - |y \cap z|$$

= $p(x,y) + p(x,z) - p(y,z),$ (3)

¹Transformations of the form of (2) in either explicit or implicit form appear in many papers, e.g., [3, 6, 7, 9, 19, 25, 27, 28], and also in the theory of linear statistical models.

i.e., the triangle inequality for proximities is fulfilled (since the first inequality in (3) is strict at $x \neq y$ and y = z). The transformation (2) applied to p(x,y) generates the usual metric on finite sets: the distance between x and y is the number of elements in their symmetric difference.

In the sequel, we assume that there is one path of length 0 from any vertex to itself.

Disconnection condition. For any multigraph G (multidigraph Γ) and for any $i, j = 1, ..., n, p_{ij} = 0$ iff there is no path from i to j in G (in Γ).

Connectivity condition (a consequence of the disconnection condition).

- (1) For any multigraph, the matrix P can be reduced to a block-diagonal form, where all block entries are strictly positive, all other entries being zero. The matrix P is strictly positive iff G is connected.
 - (2) For any $i, j, k \in V(G)$, $p_{ij} > 0$ and $p_{jk} > 0$ imply $p_{ik} > 0$.

The following normative property can be considered as an extension of diagonal maximality.

Transit property. For any multigraph G and any $i, k, t \in V(G)$, if G contains a path from i to $k, i \neq k \neq t$, and each path from i to t includes k, then $p_{ik} > p_{it}$. The same applies to multidigraphs.

Monotonicity. Suppose that the weight of some edge (arc) ε_{kt}^p in a multigraph G (multidigraph Γ) increases or a new edge (arc) from k to t appears. Then

- (1) $\Delta p_{kt} > 0$, and for any $i, j = 1, \ldots, n$, $\{i, j\} \neq \{k, t\}$ implies $\Delta p_{kt} > \Delta p_{ij}$; in the directed case, the hypothesis is weakened to $[i \neq k \text{ or } j \neq t]$;
 - (2) for any $i=1,\ldots,n$, if there is a path from i to k, and each path from i to t includes k, then $\Delta p_{it}>\Delta p_{ik}$;
- (3) for any $i_1, i_2 = 1, ..., n$, if i_1 and i_2 can be substituted for i in the hypothesis of item 2, then $p_{i_1 i_2}$ does not increase.

Item 3 can be interpreted as follows: the proximity between two vertices does not increase whenever the bond that appears or becomes stronger is extraneous for the connection of these two vertices.

3. PATH ACCESSIBILITY

The simplest proximity measure that takes into account not only the shortest path between vertices is path accessibility. The path accessibility of j from i is defined as the total weight of all paths from i to j. There are two ways of defining this measure at j=i. First, "paths from i to i" can be interpreted as simple cycles from i to i plus the path of length 0 whose weight is unity. The second possibility is to assume that the latter trivial path is the only path from i to i. Note that discarding this trivial path leaves no chance of meeting diagonal maximality. We adopt the first definition, which is more informative, though more disputable, but the subsequent discussion is applicable to the second definition too.

Path accessibility can serve as a proximity measure only if a shorter path is assigned a greater weight than a covering longer path (cf. transit property). If the weight of a path is the product of the weights of the constituent edges/arcs (as we assume hereinafter), this requires that the edge/arc weights belong to the interval [0,1]. In this way, path accessibility (as well as the subsequent indices) corresponds to the models where every edge weight is a "transfer factor" that determines the weakening of "vertex influence" with movement away from the vertex along the edge. In some cases, such a model can be applicable to transformed data that result after multiplying each edge (arc) weight by a constant factor τ , $0 < \tau < (\max_{i,j,p} \varepsilon_{ij}^p)^{-1}$. With the same effect, the weight of a path can be defined as $\prod(\tau\varepsilon(e))$, with the product over all edges (arcs) e in the path. In the same manner, each edge/arc of an unweighted graph can be assigned the same weight τ . While talking about edge/arc weights, we will have in mind the weights so obtained too.

To choose τ for unweighted graphs, one has to estimate the proximity of two vertices connected by an edge compared to the proximity of two vertices connected by a two-edge path. If the latter vertices appear to be two times "farther," then $\tau=1/2$ can be chosen. In this case, two vertices connected by a three-edge (four-edge) path are four times (respectively, eight times) farther. If the respective decrements of 3 and 4 seem to be more natural, one has to take another model, which the reader can easily construct. Here, the reciprocal weight of a path is the sum of the reciprocal weights of the constituent edges (harmonic rather than geometric decrease). The original concept in such models is distance, whereas proximity can be introduced as the reciprocal value. Undoubtedly, these models are natural, but we do not consider them in this paper. Some of their properties are discussed in [9, 30].

Let P be the matrix whose entries are the values of path accessibility for all pairs of vertices.

Proposition 1. Path accessibility has the following properties: symmetry, nonnegativity, reversal property, and disconnection condition. Moreover, if $\varepsilon_{ij}^p < \varepsilon_0$ for all $i, j = 1, ..., n, p \le a_{ij}$ (where ε_0 is a specific constant

dependent on n and the greatest possible number m of multiple edges/arcs), then diagonal maximality, the triangle inequality for proximities, the transit property, and monotonicity are true.

The proofs of all statements are given in the Appendix.

Since the changes in proximities under special modifications of graphs are of interest, restrictions on the edge/arc weights are introduced for certain families of graphs rather than for individual graphs. Here, such a family is determined by n and m.

4. CONNECTION RELIABILITY AS A VERTEX PROXIMITY MEASURE

Let us assume that all edge/arc weights belong to the interval [0,1], and consider them as the probabilities of edge/arc intactness. Define p_{ij} to be the reliability of connections between i and j, i.e., the probability that at least one intact path between i and j survives, provided that all edge/arc failures are independent; let $P=(p_{ij})$ be the matrix of connection reliabilities for all pairs of vertices. Connection reliability can be considered as a proximity measure for graph vertices. Let us point out some advantages of this measure. First, it is based upon a natural model. Second, it is not always appropriate that the proximity be doubled as all paths between a pair of vertices are duplicated (this is the case when path accessibility is used); in some cases, the increase should be more moderate. This property features connection reliability.

According to a well-known theorem (see, e.g., [31, p. 10]),

$$p_{ij}(G) = \sum_{k} \Pr(R_k) - \sum_{k < t} \Pr(R_k R_t) + \sum_{k < t < l} \Pr(R_k R_t R_l) - \dots + (-1)^{h+1} \Pr(R_1 R_2 \cdots R_h), \tag{4}$$

where R_1, R_2, \ldots, R_h are all paths between i and j; $\Pr(R_k R_t) = \varepsilon(R_k \cup R_t)$, where $R_k \cup R_t$ is the subgraph that contains those edges (arcs) that belong to R_k or R_t , and so forth. By virtue of (4), connection reliability is a natural modification of path accessibility that takes into account the *degree of overlapping* for different paths between two vertices.

Connection reliability possesses all the normative properties listed in Sec. 2, though for some of them the strict inequality $\varepsilon_{ij}^p < 1$ is necessary.

Proposition 2. Connection reliability has the following properties: symmetry, nonnegativity, reversal property, disconnection condition, and item 3 of monotonicity. Diagonal maximality, the triangle inequality for proximities, the transit property, and items 1 and 2 of monotonicity hold true, provided that the intactness probability of each edge/arc is strictly less than 1; otherwise they are satisfied in a nonstrict form.

5. ROUTE ACCESSIBILITY

A special feature of path accessibility (which also applies to connection reliability) is the necessity of a logical algorithm for its calculation. The replacement of paths by routes reduces the problem to the inversion of a matrix (see, e.g., [8]). Moreover, the route accessibility of j from i has some relation to the following problem: find the probability that a random walk started at i is located at j at a "randomly chosen" moment. Note that the proximity measures originating from the analysis of Markov chains require special consideration. Interesting information on them can be found in [7, 9, 20, 32].

Consider the matrix $P = (I - E)^{-1}$, where $E = (\varepsilon_{ij})$ is the matrix of total weights of edges (arcs) introduced above. Expand P as the sum of an infinitely decreasing geometric progression (not specifying the conditions of its validity so far):

$$P = (I - E)^{-1} = I + E + E^{2} + \dots . (5)$$

Let \mathcal{N}_{ij} be the set of routes from i to j. Since the entries of E^k are the total weights of k-length routes, (5) implies

$$p_{ij} = \sum_{N \in \mathcal{N}_{ij}} \varepsilon(N),\tag{6}$$

i.e., p_{ij} is the total weight of routes from i to j (at j = i, the route of length 0 weighted by 1 is naturally taken into account). Therefore, P is the matrix of route accessibilities in a multigraph (multidigraph).

Equation (5) is valid if and only if

$$|\lambda_1| < 1, \tag{7}$$

where $|\lambda_1|$ is the spectral radius of E [33, Corollary 5.6.16].

Consider the upper bound for $|\lambda_1|$ provided by the Geršgorin theorem (see [33]):

$$|\lambda_1| \le \max_{1 \le i \le n} \sum_{j=1}^n |\varepsilon_{ij}|. \tag{8}$$

Let ε_{max} be an imposed upper bound for the edge/arc weights; suppose that m is the greatest possible number of multiple edges (arcs) incident to the same pair of vertices. Then

$$|\lambda_1| \le \max_{1 \le i \le n} \sum_{i=1}^n |\varepsilon_{ij}| \le m(n-1)\varepsilon_{\max}.$$
(9)

Therefore, the validity of (7) (and thus of (5)) is provided by

$$\varepsilon_{\max} < \left(m(n-1) \right)^{-1}. \tag{10}$$

While on the subject of route accessibility, we will assume that the constraint (10) is satisfied (possibly, after the transformation of edge/arc weights mentioned in Sec. 3). A representation of the entries of P through the weights of specific connections in a digraph (this representation involves finite sums only and thus does not require any restrictions on the edge/arc weights) can be found in [34]. A useful review of results related to the calculation of routes in graphs is given in [35].

Proposition 3. Route accessibility has the following properties: symmetry, nonnegativity, reversal property, diagonal maximality, the triangle inequality for proximities (for the edge/arc weights not exceeding $(mn)^{-1}$), the disconnection condition, the transit property, and items 1 and 2 of monotonicity. Item 3 of monotonicity is not valid for it.

The triangle inequality has not yet been proved in the general case. The following proposition is used in the proofs of other properties and is worth mentioning in itself.

Proposition 4 (on one-step increment of route accessibility for multidigraphs). Suppose that some arc weight ε_{kt}^p in Γ increases by $\Delta \varepsilon_{kt} > 0$ or an extra arc from k to t with a weight $\Delta \varepsilon_{kt}$ is added to Γ . Let Γ' be the new multidigraph and $P' = P(\Gamma')$. Then

$$\Delta P = hR$$

where $\Delta P = P' - P$, $h = \frac{\Delta \varepsilon_{kt}}{1 - \Delta \varepsilon_{kt} p_{tk}}$, and $R = (r_{ij})$ is the $n \times n$ -matrix with entries $r_{ij} = p_{ik} p_{tj}$.

6. RELATIVE FOREST ACCESSIBILITY FOR MULTIGRAPHS

The notion of relative forest accessibility for multigraphs and multidigraphs was introduced in [25, 36], where we studied its properties in the case of multigraphs. In the present paper, we consider the undirected case too. Relative forest accessibility for multidigraphs is not one, but two complementary indices, calculated by counting the weights of converging and diverging spanning forests, respectively. None of the two possesses the reversal property of Sec. 2, but they have it "together": the matrix of the first index for the multidigraph with reversed arcs equals the transposed matrix of the second index for the original multidigraph, and vice versa. Some other properties are also natural to apply to the pair of indices. Thereby, the consideration of the above-mentioned indices in this paper could excessively complicate its structure. In the next two sections, we study the limit properties of the relative forest accessibility measure for multigraphs. The corresponding limit properties for multidigraphs are substantially different, and they should be considered elsewhere.

All assertions of Proposition 5 stated below, except for item 1 of monotonicity, are proved in [25]. Item 1 of monotonicity is proved in the Appendix.

Recall that the Laplacian matrix (also called the Kirchhoff or the admittance matrix) of a multigraph G is the $n \times n$ -matrix $L = L(G) = (\ell_{ij})$ with entries

$$\ell_{ij} = -\sum_{p=1}^{a_{ij}} \varepsilon_{ij}^p, \quad j \neq i, \quad i, j = 1, \dots, n,$$

$$(11)$$

$$\ell_{ii} = -\sum_{j \neq i} \ell_{ij}, \quad i = 1, \dots, n, \tag{12}$$

where a_{ij} is the number of (multiple) edges incident to i and j simultaneously. By (11) and (12), ℓ_{ii} is the total weight of edges incident to i (exclusive of loops).

The matrix

$$Q = (q_{ij}) = (I + L(G))^{-1}.$$

is the matrix of relative forest accessibilities of vertices in G.

This term is suggested by the matrix-forests theorem [13, 25, 28, 36]. Suppose that $\mathcal{F}(G) = \mathcal{F}$ is the set of all spanning rooted forests of multigraph G, and $\mathcal{F}^{ij}(G) = \mathcal{F}^{ij}$ is the set of those spanning rooted forests, in which i and j belong to the same tree rooted at i. A spanning rooted forest is an acyclic subgraph of G that has the same vertex set as G and one marked vertex (a root) in each component.

THEOREM 1 (matrix-forest theorem for weighted multigraphs) [25, 36]. For any weighted multigraph G, the matrix $Q = (I + L(G))^{-1}$ exists and $q_{ij} = \varepsilon(\mathcal{F}^{ij})/\varepsilon(\mathcal{F})$, $i, j = 1, \ldots, n$.

Recall that, according to (1), $\varepsilon(\mathcal{F}^{ij})$ and $\varepsilon(\mathcal{F})$ are the total weights of forests that belong to \mathcal{F}^{ij} and \mathcal{F} , respectively. For the sake of unification, in the sequel we denote the matrix Q by $P = (p_{ij})$ (as well as other matrices of proximity measures).

The characteristic features of relative forest accessibility are *doubly stochastic normalization* (more precisely, its second condition) and *macrovertex independence*.

Doubly stochastic normalization. For any multigraph G,

(1) $p_{ij} \ge 0$, i, j = 1, ..., n, and

(2)
$$\sum_{i=1}^{n} p_{ij} = \sum_{i=1}^{n} p_{ji} = 1, i = 1, \dots, n.$$

According to this condition, p_{ij} can be interpreted as the share of the connectivity of i and j in the total connectivity of i (or j) with all vertices. This interpretation requires some explanation. Indeed, by virtue of symmetry, it requires that the "total connectivity" of all vertices be identical, irrespective of the difference in their position within a multigraph. This is realized with the aid of the diagonal entries of the matrix: if i is poorly connected with other vertices, then p_{ii} (which expresses the "solitariness" of i) is great, and hereby the "total connectivity" is the same as for all other vertices.

Let D be a subset of the vertex set V(G). We say that D is a macrovertex in G, if for every $i, j \in D$ and $k \notin D$, $\varepsilon_{ik} = \varepsilon_{jk}$ holds.

The following property is a sufficient condition for the equality and stability of proximities.

Macrovertex independence. Suppose that D is a macrovertex in G and $i \in D$, $j \in D$, $k \notin D$. Then $p_{ik} = p_{jk}$, and p_{ik} does not vary when any new edges appear or the weights of any existing edges change inside D.

Macrovertex independence substantially strengthens the following simple condition (which is not included in the list of Sec. 2, since it is obviously met by all proximity measures under consideration).

Independence of other components. Let A and B be two different components of a multigraph. Then any addition, removal, or reweighting of edges (arcs) within B does not alter the values of proximity for the vertices that belong to A.

Proposition 5. Relative forest accessibility for multigraphs has the following properties: symmetry, nonnegativity, diagonal maximality, the triangle inequality for proximities, the disconnection condition, the transit property, monotonicity, doubly stochastic normalization, and macrovertex independence.

Thereby, relative forest accessibility for multigraphs possesses all normative properties of Sec. 2 without any restrictions on the weights of edges, and it features macrovertex independence and doubly stochastic normalization. Certainly, this does not raise relative forest accessibility over other proximity measures. Rather, this index perfectly corresponds to one possible concept of proximity specified by the properties listed in Proposition 5.

7. COMPONENTS OF RELATIVE FOREST ACCESSIBILITY

In this section, the relative forest accessibility for multigraphs is decomposed into components that correspond to the sets of forests with a varying number of trees. Next, we consider the notions of proximity that correspond to each component. Let v be the number of connected components in G; by V_i we denote the set of vertices of the component of G that contains vertex i (i = 1, ..., n).

THEOREM 2 (a parametric version of the matrix-forest theorem for multigraphs). For any weighted multigraph G and any $\tau \geq 0$, let $Q(\tau) = (q_{ij}(\tau))$ be the matrix $(I + \tau L)^{-1}$. Then $Q(\tau)$ exists and

$$q_{ij}(\tau) = \sum_{k=0}^{n-v} \tau^k \varepsilon(\mathcal{F}_k^{ij}) / \sum_{k=0}^{n-v} \tau^k \varepsilon(\mathcal{F}_k), \quad i, j = 1, \dots, n,$$
(13)

where \mathcal{F}_k is the set of spanning rooted forests in G that consist of k edges, and $\mathcal{F}_k^{ij} \subseteq \mathcal{F}_k$ is its subset comprising those forests in which j belongs to a tree rooted at i.

By Proposition 5, the matrix of relative forest accessibilities is doubly stochastic, whence $\sum_{j=1}^{n} q_{ij}(\tau) = 1$, $i = 1, \ldots, n, \ \tau \ge 0$. The following proposition states a stronger fact, namely, the stochastic property is true for the coefficients at every exponent of τ in (13).

Proposition 6. For any i = 1, ..., n and k = 0, ..., n - v, we have

$$\sum_{j=1}^{n} \varepsilon(\mathcal{F}_{k}^{ij}) = \varepsilon(\mathcal{F}_{k}). \tag{14}$$

The matrices $Q(\tau)$, $\tau > 0$, make up a parametric family of relative forest accessibility indices which obviously have the same basic properties as Q = Q(1). By (13), $Q(\tau)$ can be represented as

$$Q(\tau) = \frac{1}{s(\tau)} \left(\tau^0 Q_0 + \tau^1 Q_1 + \dots + \tau^{n-v} Q_{n-v} \right), \tag{15}$$

where
$$s(\tau) = \sum_{k=0}^{n-v} \tau^k \varepsilon(\mathcal{F}_k)$$
, $Q_k = (q_{k,ij})$, and $q_{k,ij} = \varepsilon(\mathcal{F}_k^{ij})$, $k = 0, \ldots, n-v$, $i, j = 1, \ldots, n$.

Every matrix Q_k , $k=0,\ldots,n-v$, reflects a specific vertex proximity. Let us consider them in some detail. First, $Q_0=I$, i.e., the "proximity" specified by Q_0 is simply identity. Further, the entry $q_{1,ij}$, $j\neq i$, of Q_1 is equal to the total weight of the edges in G that are incident to i and j. Generally, the entry $q_{k,ij}$ of Q_k is distinct from zero if and only if G contains some paths of length k or shorter between i and j. The corresponding notion of proximity ignores all paths of length k+1 or longer. Whenever $k\geq |V_i|_{\max}-1$ (where $|V_i|_{\max}$ is the maximum number of vertices among the components of G), the proximity corresponding to Q_k takes into account all paths in G.

Recall that V_i is the set of vertices in the component of G that contains i. To examine the proximity corresponding to Q_{n-v} , we introduce the matrix $\bar{J}(G) = \bar{J} = (\bar{J}_{ij})$:

$$\bar{J}_{ij} = \begin{cases} \frac{1}{|V_i|}, & \text{if } j \in V_i, \\ 0, & \text{otherwise} \end{cases}$$

and prove the following lemma.

LEMMA 1.

$$Q_{n-v} = \varepsilon(\mathcal{F}_{n-v})\bar{J}. \tag{16}$$

As mentioned above, the "proximity" that corresponds to Q_0 is identity. By Lemma 1, the matrix Q_{n-v} represents an opposite concept of proximity: all vertices that belong to the same component of G are equally "close" to each other, and the value of their proximity is inversely proportional to the number of vertices in the component. Thus, the proximity to vertex i is uniformly distributed over the component of G that contains i. If G is connected, then $\bar{J} = (1/n)J$, where J is the $n \times n$ -matrix having all entries one, and so all entries of Q_{n-v} are $\varepsilon(\mathcal{F}_{n-v})/n$. For all matrices Q_k , $k = 0, \ldots, n-v$, the proximity of two vertices from different components of G is zero.

COROLLARY 1.
$$\lim_{\tau \to \infty} Q(\tau) = \bar{J}$$
.

Corollary 1 follows directly from Theorem 2 and Lemma 1.

Remark 1. The matrix Q_{n-v-1} is of special interest. Its entry $q_{n-v-1,ij}$ is the total weight of those spanning rooted forests in G that

- (1) have two trees in one component of G and one tree in each of the others, and
- (2) have i and j in the same tree rooted at i.

Among the matrices Q_k , k = 0, ..., n - v, the matrix Q_{n-v-1} is the most similar (in the properties) to the matrices $Q(\tau)$ of relative forest accessibility. Indeed, by (15)–(16), the comparison of two entries of $Q(\tau)$ at a large τ

is determined by the comparison of the corresponding entries of Q_{n-v-1} . Only when the latter entries are equal do the corresponding entries of Q_k at k < n-v-1 matter. Dealing with examles convinces us that the situations where two entries of Q_{n-v-1} are equal, whereas the corresponding entries of Q_k , k < n-v-1, vary, are not frequent, and indeed it is not easy to intuitively discriminate between the compared proximities in these cases. Still, an important exception exists. As mentioned above, $k \ge |V_i|_{\max} - 1$ is necessary and sufficient for Q_k to take into account all paths in G. If all components of G, except one, are separate vertices or G is connected, then $|V_i|_{\max} - 1 = n - v$. In this case, if a pair of vertices in the nontrivial component is connected only by paths of length n-v (a chain graph), then the corresponding entry of Q_{n-v-1} is zero, and so Q_{n-v-1} violates the disconnection condition. Note that some weighted sums of Q_{n-v-1} and Q_{n-v} are free of this flaw. Such linear combinations are studied in the following section. Moreover, we show that Q_{n-v-1} is closely connected with the matrix L^+ , the Moore–Penrose generalized inverse of L. More precisely, L^+ is the sum of Q_{n-v-1} and Q_{n-v} with definite coefficients.

8. ACCESSIBILITY VIA DENSE FORESTS CONNECTED WITH THE GENERALIZED INVERSION OF THE LAPLACIAN MATRIX

This section is devoted to weighted sums of matrices Q_{n-v-1} and $Q_{n-v} = \varepsilon(\mathcal{F}_{n-v})\bar{J}$. A number of papers [6, 7, 9, 19] use, either explicitly or implicitly, proximity matrices whose generalization to multicomponent graphs can be represented as $(L + \alpha \bar{J})^{-1}$, where $\alpha > 0$. The aims of this section are as follows:

- (1) to provide a topological interpretation of such a proximity in the case of arbitrary multigraphs (it is based on the matrices Q_{n-v-1} and Q_{n-v});
 - (2) to establish its relation with the matrix L^+ , the Moore-Penrose generalized inverse of L, and
 - (3) to ascertain its properties.

We will show that $(L + \alpha \bar{J})^{-1}$ with a sufficiently small α is a weighted sum of Q_{n-v-1} and Q_{n-v} with positive coefficients and satisfies a number of conditions of Sec. 2.

To solve the foregoing problems, we will need the matrix

$$\widetilde{Q} = (L + \overline{J})^{-1} - \overline{J},\tag{17}$$

which has many remarkable properties. Four representations for \widetilde{Q} are stated below (Proposition 7–9 and Theorem 3).

Proposition 7. For any
$$\alpha \neq 0$$
, the matrix $(L + \alpha \bar{J})$ is invertible, and $\widetilde{Q} = (L + \alpha \bar{J})^{-1} - \alpha^{-1} \bar{J}$.

By Proposition 7, the difference between \widetilde{Q} and $(L + \alpha \overline{J})^{-1}$ is represented by a matrix whose entries are constant within each component of G. In [6, 7, 9, 19], matrices of the form of $(L + \alpha \overline{J})^{-1}$ are mainly used for transformations such as (2), where, if one pays no regard for intercomponent entries, they can be equivalently replaced by \widetilde{Q} .

Recall that for any rectangular complex matrix A, the Moore–Penrose generalized inverse of A is the unique matrix A^+ such that

- (1) AA^+ and A^+A are Hermitian matrices,
- (2) $AA^{+}A = A$, and
- (3) $A^+ A A^+ = A^+$.

Proposition 8. For any weighted multigraph G, the matrix \widetilde{Q} is the Moore–Penrose generalized inverse of L = L(G), that is, $\widetilde{Q} = L^+$.

Since L is a square matrix, and $AA^+ = A^+A$ (which follows from the proof of Proposition 8), the matrix \widetilde{Q} is the group inverse of L (cf. [30]). Geometric interpretations for L^+ are given in [27].

It turns out that L^+ can be obtained by a passage to the limit from the parametric matrix $Q(\tau)$ of relative forest accessibilities (cf. Corollary 1).

Proposition 9.
$$L^+ = \lim_{\tau \to \infty} \tau(Q(\tau) - \bar{J}).$$

Proposition 9 and Theorem 2 enable one to obtain a topological interpretation for $L^+ = (\ell_{ij}^+)$.

THEOREM 3 (a topological interpretation for the matrix L^+ , the Moore–Penrose generalized inverse of L):

$$\ell_{ij}^{+} = \begin{cases} \frac{\varepsilon(\mathcal{F}_{n-v-1}^{ij}) - \frac{1}{|V_i|} \cdot \varepsilon(\mathcal{F}_{n-v-1})}{\varepsilon(\mathcal{F}_{n-v})}, & \text{if } j \in V_i, \\ 0, & \text{otherwise.} \end{cases}$$
(18)

Here, the numerator is the result of centralization: the ij-entry minus the ith-row mean of Q_{n-v-1} (see (14)). By Theorem 3, the definition of \bar{J} , and Lemma 1, one has

$$L^{+} = \frac{\varepsilon(\mathcal{F}_{n-v-1})}{\varepsilon(\mathcal{F}_{n-v})} \left(\frac{1}{\varepsilon(\mathcal{F}_{n-v-1})} Q_{n-v-1} - \frac{1}{\varepsilon(\mathcal{F}_{n-v})} Q_{n-v} \right)$$
$$= \frac{1}{\varepsilon(\mathcal{F}_{n-v})} \left(Q_{n-v-1} - \varepsilon(\mathcal{F}_{n-v-1}) \bar{J} \right). \tag{19}$$

Another representation of L^+ for connected weighted graphs was obtained in [30].

Can L^+ be considered as a matrix of vertex proximities? By (18), this "proximity" equals zero for vertices from different component of G, and so does the sum of "proximities" of each vertex with the vertices of the same component. The latter does not match an intuitive idea of proximity. First, nonnegativity is violated; second, the "proximity" of poorly connected vertices from the same component turns out to be less than that for any vertices from different components.

Now, let us return to the matrices $(L + \alpha \bar{J})^{-1}$. Propositions 7–9 and Eq. (19) imply the following identities:

$$(L + \alpha \bar{J})^{-1} = L^{+} + \alpha^{-1} \bar{J}$$
 (20)

$$= \lim_{\tau \to \infty} \tau(Q(\tau) - \bar{J}) + \alpha^{-1} \bar{J} \tag{21}$$

$$= \frac{1}{\varepsilon(\mathcal{F}_{n-v})} \left(Q_{n-v-1} + \left(\alpha^{-1} - \frac{\varepsilon(\mathcal{F}_{n-v-1})}{\varepsilon(\mathcal{F}_{n-v})} \right) Q_{n-v} \right)$$
 (22)

$$= \frac{1}{\varepsilon(\mathcal{F}_{n-v})} Q_{n-v-1} + \left(\alpha^{-1} - \frac{\varepsilon(\mathcal{F}_{n-v-1})}{\varepsilon(\mathcal{F}_{n-v})}\right) \bar{J}.$$
 (23)

Thus, whenever $0 < \alpha < \varepsilon(\mathcal{F}_{n-v})/\varepsilon(\mathcal{F}_{n-v-1})$, the matrix $(L + \alpha \bar{J})^{-1}$ is the sum of Q_{n-v-1} and Q_{n-v} with positive coefficients. Let a *dense forest* be a spanning rooted forest in G with n-v or n-v-1 edges. Then the proximity measure (22) with $0 < \alpha < \varepsilon(\mathcal{F}_{n-v})/\varepsilon(\mathcal{F}_{n-v-1})$ can be referred to as *accessibility via dense forests*.

Proposition 10. The accessibility via dense forests in the case of multigraphs has the following properties: symmetry, nonnegativity, diagonal maximality, the triangle inequality for proximities, the disconnection condition, and the transit property. It does not satisfy monotonicity.

It is interesting to examine the nature of the violation of monotonicity. It follows from (21) that whenever k and t belong to the same component of the original multigraph, monotonicity is valid in a nonstrict form, i.e., all strict inequalities are replaced by nonstrict ones, which can be regarded as acceptable. Rough violations of monotonicity (namely, $\Delta p_{kt} < \Delta p_{ij}$ and $\Delta p_{kt} < 0$) only occur when k and t originally belong to different components of G. This suggests an idea of searching for a better modification of accessibility via dense forests. The scrutiny of this question, as well as the examination of the metric corresponding (in the sense of [29]) to this proximity measure (see [6, 7, 9, 30]), is beyond the scope of this paper.

9. ON SOME PECULIARITIES OF THE PROXIMITY MEASURES

A specific feature of path and route accessibilities is the necessity of imposing rather strong restrictions on the weights of edges (arcs) to guarantee the properties of Sec. 2 convergence (in the case of route accessibility). These restrictions imply a fast decrease of proximity with movement away from a vertex along an edge chain. A characteristic feature of connection reliability is the effect of saturation. If, for example, two vertices are connected by an edge, the weight of which is close to 1, then the addition of other paths between them leaves the value of proximity almost the same. In addition, all diagonal entries are ones, i.e., they do not characterize self-relations of any kind. Accessibility via dense forests violates monotonicity when two components of a graph get a connection; it only satisfies the nonstrict version of monotonicity, when a graph is changed within components. Unlike relative forest accessibility, here the triangle inequality is also satisfied in a nonstrict form, provided that i, j, and k are distinct. On the other hand, the metric derived from this proximity measure by (2) coincides with the classical graph metric in the case of trees [6]. For a further study of this metric, see [30]. The relative forest accessibility differs from the other proximity measures by the very fact of its relativeness. A manifestation of this is the stochastic normalization property of the matrices Q and $Q(\tau)$ for digraphs and doubly stochastic normalization in the case of undirected graphs. As a corollary, the addition of new edges (arcs) in a graph does not increase all proximities; some of them will necessarily decrease. The corresponding "absolute" proximity measure can be obtained by considering the adjugate of the matrix $(I + \tau L)$ instead of $Q(\tau) = (I + \tau L)^{-1}$. In addition, relative forest accessibility features

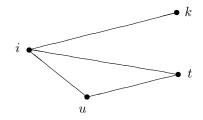


Figure 1: Example 1.

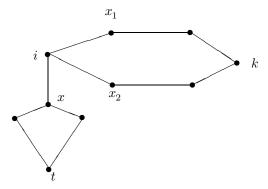


Figure 2: Example 2.

macrovertex independence, which is not always desirable. To illustrate these and some other peculiarities of the proximity measures under study, we shall consider a few simple examples.

For the graph in Fig. 1, path accessibility, connection reliability, and route accessibility give $p_{ik} < p_{it}$. Seemingly, it would otherwise be unnatural, since i and t are connected not only by an edge (as i and k are), but also by a path of length 2 (iut). Nevertheless, the relative forest accessibility gives $p_{ik} = p_{it} = p_{iu}$ (this follows from macrovertex independence: $\{k, t, u\}$ is a macrovertex). The same result is provided by the accessibility via dense forests. Macrovertex independence is appropriate when any connections within a macrovertex can be regarded as its "domestic affairs." For example, if each professor gives his/her lectures to all students (then the students form a macrovertex), and the students write them down verbatim, then no reading or rewriting of the notes of each other can help them learn anything more (i.e., to approach the knowledge of the professors).

The following example illustrates some peculiarities of the path and route accessibilities. In Fig. 2, i is connected with k by two paths, as well as with t, and the weights of these paths are equal (provided that the weights of all edges are equal). Hence, the path accessibilities p_{ik} and p_{it} are also equal. But the paths that connect i to t have a common edge. Therefore, connection reliability gives $p_{ik} > p_{it}$. The same result holds for relative forest accessibility and accessibility via dense forests. In contrast, route accessibility provides $p_{ik} < p_{it}$. This is because there exist two paths of length two from x to t and only one path of length two from x_1 (or from x_2) to k. As a result, there are eight routes of length seven from i to t and only four routes of length seven from i to k.

Furthermore, the proximity measures at hand behave differently as applied to cycles. The cycle in Fig. 3 has no influence on the values of path accessibility and connection reliability between i and t, i.e., $p_{it} = p_{ik}$ (if all edge weights are equal). Using route accessibility, we have $p_{it} > p_{ik}$. At the same time, relative forest accessibility provides $p_{it} < p_{ik}$, as the approach of i and t to the vertices of the cycle (owing to its appearance) moves them away (in the relative account) from each other. The same holds for the accessibility via dense forests.

Note finally that for path accessibility, connection reliability, and the measures representable by weighted sums of the matrices Q_1, \ldots, Q_{n-v} with fixed weights, the values of proximity linearly depend on the weights of edges (arcs), whereas for the other measures at hand, this is not the case.

Thus, the proximity measures under discussion have significantly different properties. At the same time, "almost all" of them possess "almost all" of the "basic" properties formulated in Sec. 2

10. CONCLUSION

In this paper, we have dealt with several proximity measures for the vertices of directed and undirected

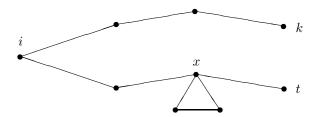


Figure 3: Example 3.

Property	Paths	Reliability	Routes	Forests (undirected)	Dense forests (undirected)
Symmetry	+	+	+	+	+
Nonnegativity	+	+	+	+	+
Reversal property	+	+	+	×	×
Diagonal maximality	+*	+*	+	+	+
Triangle inequality for proximities	+*	+*	+**	+	+
Disconnection condition	+	+	+	+	+
Transit property	+*	+*	+	+	+
Monotonicity (1)	+*	+*	+	+	_
Monotonicity (2)	+	+*	+	+	_
Monotonicity (3)	+	+	_	+	

^{+*} is valid under some restriction and/or in the nonstrict form.

Table 1: Some properties of proximity measures for graph vertices.

multigraphs and considered their properties. These properties and the informal discussion of the previous section can help one choose adequate proximity measures when exact mathematical models are lacking.

A common feature of the indices considered in this paper is the measurement of the proximity (accessibility, connectivity) of two vertices by the total weight of certain substructures that "connect" these vertices. As such substructures, we examined paths (in particular, taking into account their overlaps), routes, spanning rooted forests, and "dense" spanning rooted forests. The weight of a substructure was defined as the product of the weights of the constituent edges (arcs). Within this approach, a proportional modification of all edge weights is needed in some cases, as well as assigning the same weight to all edges (arcs) of unweighted graphs. In conclusion, let us indicate some proximity measures that do not enter into the scope of the present paper. These are the indices dual (in the sense of [29]) to the classical distance for connected graphs and to some nonclassical graph metrics [7], maximum flow (minimum cut) between vertices [9], and a number of measures related to random walks in graphs (see [32, 9, 7]).

APPENDIX

Proof of Proposition 1. Symmetry, nonnegativity, reversal property, and disconnection condition immediately follow from the definition of path accessibility. To prove the remaining properties, let us find ε_0 guaranteeing that whenever the weights of all edges (arcs) are less than ε_0 , $p_{ij} < 1$ holds for all i and $j \neq i$. Let m be the greatest possible number of edges (arcs) incident to the same pair of vertices. Note that when a multigraph G is complete (i.e., exactly m edges are incident to each pair of vertices), and the weights of all edges are ε , then at $j \neq i$, $p_{ij} = \sum_{k=1}^{n-1} A_{n-2}^{k-1}(\varepsilon m)^k$, where A_{n-2}^{k-1} is the number of permutations of n-2 things taken k-1 at a time. Now,

we equate this expression to unity and assign to ε_0 the positive root of the equation obtained. Henceforth, we will assume that $\varepsilon_{ij}^p < \varepsilon_0$ for all edge weights ε_{ij}^p . As p_{ij} is maximal in a complete multigraph, this will guarantee

$$p_{ij} < 1, \quad i, j = 1, \dots, n, \ i \neq j,$$
 (24)

^{+**} was proved under an additional constraint.

[×] inapplicable, as only undirected graphs were considered.

for all weighted multigraphs on n vertices with the number of multiple edges not greater than m. The same constraint can be obtained for the weights of arcs in multidigraphs.

Diagonal maximality follows from the inequalities $p_{ii} \geq 1$ and (24).

Prove the triangle inequality for proximities. At i=j or i=k, the inequality reduces to equality. Suppose that $i\neq j$ and $i\neq k$. Note that whenever all paths from j to k pass through i, $p_{jk}=p_{ji}\,p_{ik}$ holds; otherwise $p_{jk}\geq p_{ji}\,p_{ik}$. Let C be the total weight of simple cycles from i to i; then $p_{ii}=1+C$. Using (24), one obtains the triangle inequality for proximities:

$$p_{ij} + p_{ik} - p_{jk} - p_{ii} \le p_{ji} + p_{ik} - p_{ji} p_{ik} - 1 - C = (p_{ji} - 1)(1 - p_{ik}) - C < 0.$$

To prove the transit property, note that $p_{it} = p_{ik} \, p_{kt}$, and using (24), we have $p_{it} < p_{ik}$.

Now prove monotonicity. Item 1. Suppose that $\Delta \varepsilon_{kt}$ is the increment of the weight of an existing edge or the weight of a new edge between k and t. Then $\Delta p_{kt} = \Delta \varepsilon_{kt} > 0$. Let us show that whenever all edge weights are smaller than ε_0 and $\{i,j\} \neq \{k,t\}$, $\Delta p_{ij} < \Delta \varepsilon_{kt}$ holds. If i=k, then $\Delta p_{ij} = \Delta p_{kj} \leq \Delta \varepsilon_{kt} \, p_{tj}$, and the required inequality follows from (24). The cases i=t,j=k, and j=t are similar. It remains to consider the case $\{i,j\} \cap \{k,t\} = \varnothing$, in which $n \geq 4$. Obviously, $\Delta p_{ij} = \Delta \varepsilon_{kt} \, w$, where w is the total $\overline{(k,t)}$ -weight of the paths from i to j that contain the new (reweighted) edge (kt), and the " $\overline{(k,t)}$ -weight" of a path is the product of the weights of all its edges, except for the edge (kt). Prove that w < 1. Obviously, w is maximal in a complete multigraph, where, as is easy to check, $w = 2\sum_{k=2}^{n-2}(k-1)A_{n-4}^{k-2}(\varepsilon_0 \, m)^k$. Let us show that in this case, w is less than the value $p = \sum_{k=1}^{n-1}A_{n-2}^{k-1}(\varepsilon_0 \, m)^k$ of the proximity for two distinct vertices in a complete multigraph, which equals 1 by the definition of ε_0 . Juxtapose the coefficients at the same exponents of $(\varepsilon_0 \, m)$ in the expressions for w and p. It is easy to verify that the inequality $2(k-1)A_{n-4}^{k-2} \geq A_{n-2}^{k-1}$ has a unique solution: n=4, k=2. Thereby, the statement is proved in the case of n>4. Finally, for n=4 we have $p=\varepsilon_0 \, m+2(\varepsilon_0 \, m)^2+2(\varepsilon_0 \, m)^3$ and $w=2(\varepsilon_0 \, m)^2$; therefore, w< p as well. A similar proof applies to multidigraphs.

Item 2. The statement follows from $\Delta p_{ik} = 0$ and $\Delta p_{it} > 0$.

Item 3. We have $\Delta p_{i_1 i_2} = 0$, as the edge (arc) (kt) does not belong to any path from i_1 to i_2 .

Proof of Proposition 2. Symmetry, nonnegativity, reversal property, and disconnection condition follow easily from the definition of connection reliability. Diagonal maximality in a nonstrict version follows from the facts that $p_{ii}=1$ and $p_{ij}\leq 1,\ i,j=1,\ldots,n$. If all edge/arc weights are less than 1, then, obviously, $p_{ij}<1$ at $j\neq i$; therefore $p_{ij}< p_{ii}$.

The proof of the triangle inequality for proximities mimics the corresponding proof for path accessibility.

Transit property (in the form specified in Proposition 2) follows from the equality $p_{it} = p_{ik} p_{kt}$, which is valid under the hypothesis of this property.

Prove item 1 of monotonicity for multidigraphs. This proof will also be applicable to multigraphs. Let a state of a multidigraph, all of whose arcs are assigned some intactness probabilities, be any of its spanning subgraphs. The arcs of the subgraph are interpreted as the only intact arcs of the original multidigraph. By the assumption of independence of failures, the probability of a state is the product of the intactness probabilities of the arcs entering into the state and the failure probabilities of the lacking arcs. Let a new arc from k to t be added. Note that Δp_{ij} is the total probability of those states in which

- (1) the new arc (kt) is present,
- (2) there is a path from i to j, and
- (3) the removal of the arc (kt) leaves no path from i to j.

Note that in all these states, the removal of (kt) does not leave any path from k to t either (otherwise the removal of this arc would not have broken a path from i to j). Therefore, the specified total probability is a summand of Δp_{kt} , and hence, $\Delta p_{kt} \geq \Delta p_{ij}$. Whenever all arc weights are strictly less than 1, there is at least one state whose nonzero probability is a summand of Δp_{kt} , but does not enter into Δp_{ij} : in this state the new arc (kt) is solely intact, and the desired inequality is strict. All these conclusions are preserved when the weight of an arc (kt) increases. This is because the connection reliability is affinely related with each arc weight.

Item 2 of monotonicity is true, since $\Delta p_{ik} = 0$, $\Delta p_{it} \geq 0$, and $\Delta p_{it} > 0$ when all arc/edge weights are strictly less than one. Item 3 is valid, as the edge (arc) (kt) does not belong to any path from i_1 to i_2 .

Proof of Proposition 3. Symmetry, nonnegativity, reversal property, and disconnection condition follow from the definition of route accessibility.

Prove diagonal maximality for multidigraphs. In talking about route accessibility, we always consider a family of graphs with a specified greatest possible number of multiple edges (arcs) m and with edge/arc weights smaller than $\varepsilon_{\max} = (m(n-1))^{-1}$. Suppose that Γ is a weighted multidigraph that belongs to such a family; i and

 $j \neq i$ are arbitrary vertices of Γ ; $\varepsilon < \varepsilon_{\max}$ is the maximum among the arc weights in G. Consider the multidigraph Γ' constructed by removing all arcs directed to i from the complete multidigraph with the multiplicity of all arcs m and the weight of all arcs ε . Obviously, for Γ' , $p'_{ii} = 1$, and $p'_{ij} = p'_{ik}$ for any $k \neq i$. Particularizing the equality P'(I - E') = I for the ij-entry of P'(I - E'), we derive $p'_{ij} = \frac{\varepsilon m}{1 - (n - 2)\varepsilon m}$, and consequently, $p'_{ii} > p'_{ij}$, since $\varepsilon < (m(n-1))^{-1}$. If some arcs are removed from Γ' or some weights of arcs are reduced (let the resulting graph be Γ''), then p_{ii} does not change, whereas p_{ij} can only decrease. Now, let an arc from $k \neq i$ to i be added to Γ'' . By virtue of Proposition 4 (the proof of which is given below), in this case $\Delta p_{ii} - \Delta p_{ij} = hp''_{ik}(p''_{ii} - p''_{ij}) > 0$, and thus, $p_{ii} > p_{ij}$ remains true. Similarly, $p_{ii} > p_{ij}$ is preserved at the consecutive addition of other arcs directed to i. Hence, $p_{ii} > p_{ij}$ is also valid for Γ , and the diagonal maximality is proved. The fulfillment of this property for any multigraph G is ensured by its validity for the symmetric multidigraph Γ with the same matrix E.

Now we prove triangle inequality for proximities in the case where the weights of all edges (arcs) do not exceed $(mn)^{-1}$. First, consider the digraph Γ' that differs from the complete digraph by the lack of all arcs directed to i. At j=i or k=i, the triangle inequality for proximities reduces to equality, so assume that $j\neq i$ and $k\neq i$. Let each arc of Γ' have weight $\varepsilon=1/n$. Using the equality (I-E')P'=I for the entries ij, ik, and ii of (I-E')P', one obtains

$$p'_{ij} = p'_{ik} = \frac{\varepsilon}{1 - (n-2)\varepsilon} = \frac{1}{2},$$

 $p'_{ii} = 1,$

hence, $p'_{ii}-p'_{ij}-p'_{ik}+p'_{jk}>p'_{ii}-p'_{ij}-p'_{ik}=0$. We shall prove now that no change of Γ' can decrease $p_{ii}-p_{ij}-p_{ik}$. Indeed, if some arcs are removed from Γ' and/or the weights of some arcs are reduced, p_{ii} does not change, whereas p_{ij} and p_{ik} can only decrease; therefore, $p_{ii}-p_{ij}-p_{ik}\geq 0$ is preserved. Furthermore, if for some digraph Γ this inequality is valid, then the addition of any arc ti to Γ cannot violate it, since, by Proposition 4,

$$\Delta p_{ii} - \Delta p_{ij} - \Delta p_{ik} = h(t) p_{it} (p_{ii} - p_{ij} - p_{ik}) \ge 0.$$

Thus, the triangle inequality for proximities is valid for any digraph. The fulfillment of this property for multidigraphs is proved by replacing the set of arcs between a pair of vertices with a single arc with the total weight, which reduces the problem to digraphs. The fulfillment of the property for any multigraph is ensured by its validity for the symmetric multidigraph with the same matrix E.

Transit property for multidigraphs will be proved by contradiction. Let Γ be the multidigraph with the minimum number of arcs among the multidigraphs that violate the transit property. Then Γ has a path from i to $k, t \neq k$, and any path from i to t contains t, but t be the multidigraph obtained by removing the arcs t from t. Then, after adding the arc t or t one has t be the multidigraph obtained by removing the arcs t from t. Then, after adding the arc t or t one has t be the multidigraph obtained by removing the arcs t from t. Then, after adding the arc t or t one has t be the multidigraph obtained by removing the arcs t from t to t and t be the multidigraph obtained by removing the arcs t be the first arc of an arbitrary path from t to t one has t be the multidigraph obtained by removing the arcs t be the first arc of an arbitrary path from t to t be the multidigraph obtained by removing the arcs t be the first arc of an arbitrary path from t to t be the multidigraph obtained by removing the arcs t be the first arc of an arbitrary path from t to t be the multidigraph obtained by removing the arcs t be the first arc of an arbitrary path from t to t be the multidigraph obtained by removing the arcs t be the multidigraph obtained by removing the arcs t be the first arc of an arbitrary path from t be the multidigraph obtained by removing the arc t be the multidigraph obtained by removing the arc t be the multidigraph obtained by removing the arc t be the multidigraph obtained by removing the arc t be the multidigraph obtained by removing the arc t be the multidigraph obtained by removing the arc t be the multidigraph obtained by removing the arc t be the multidigraph obtained by removing the arc t by the arch t by the t be the multidigraph obtained by removing the arc t by the arch t by t

To prove item 1 of monotonicity in the case of multidigraphs, note that, by virtue of Proposition 4, $\Delta p_{kt} = hp_{kk}\,p_{tt}$ and $\Delta p_{ij} = hp_{ik}\,p_{tj}$. Now, the required statement follows from the diagonal maximality and can be extended to multigraphs by a standard trick. Similarly, item 2 of monotonicity follows from the formula $\Delta p_{it} - \Delta p_{ik} = h(p_{ik}\,p_{tt} - p_{ik}\,p_{tk})$ and diagonal maximality. Item 3 is not true, since under the hypothesis of monotonicity, some routes from i_1 to i_2 that contain the edge (arc) (kt) can appear or increase their weight.

Proof of Proposition 4. Let $\Delta(I-E)=(I-E')-(I-E)$. Note that $\Delta(I-E)=XY$, where $X=(x_{i1})$, $i=1,\ldots,n$, is the column vector with entries $x_{k1}=-\Delta\varepsilon_{kt}$ and $x_{i1}=0$ for all $i\neq k;\ Y=(y_{1j}),\ j=1,\ldots,n$, is the row vector with entries $y_{1t}=1$ and $y_{1j}=0$ for all $j\neq t$. According to [33, Sec. 0.7.4],

$$P' = P - \frac{1}{1 + YPX}PXYP.$$

It is straightforward to verify that $(-\frac{1}{1+YPX}) = -h/\Delta\varepsilon_{kt}$ and $PXYP = -\Delta\varepsilon_{kt} R$, and thereby the proposition is proved.

Proof of Proposition 5. Let us prove item 1 of monotonicity (all the other statements are proved in [25]). By item 1 of Proposition 7 from [25], $\Delta p_{kt} = h(p_{kk} - p_{kt})(p_{tt} - p_{tk})$ and $\Delta p_{ij} = h(p_{ik} - p_{it})(p_{jt} - p_{jk})$, where

h>0. Diagonal maximality implies $\Delta p_{kt}>0$. If $\Delta p_{ij}>0$, then $(p_{ik}-p_{it})(p_{jt}-p_{jk})>0$. For definiteness, we assume that $p_{ik}-p_{it}>0$ and $p_{jt}-p_{jk}>0$ (the complementary case is treated similarly). Then, by item 2 of Proposition 6 from [25], if $i\neq k$, then G contains a path from i to k, such that the difference $(p_{uk}-p_{ut})$ strictly increases as u progresses from i to k along the path. Hence, $p_{kk}-p_{kt}>p_{ik}-p_{it}$. Similarly, $p_{tt}-p_{tk}>p_{jt}-p_{jk}$ whenever $j\neq t$. Using the above expressions for Δp_{kt} and Δp_{ij} , we get $\Delta p_{kt}>\Delta p_{ij}$.

Proof of Theorem 2. Equation (13) follows from the matrix-forest theorem [25] applied to the weighted multigraph G' that differs from G by the weights of edges only: for all i, j = 1, ..., n and $p = 1, ..., a_{ij}$, $(\varepsilon_{ij}^p)' = \tau \varepsilon_{ij}^p$.

Proof of Proposition 6. This equality holds by virtue of the following three facts, which are true for any k = 0, ..., n - v and for any $i, j, i_1, i_2 = 1, ..., n$ such that $i_1 \neq i_2$: (1) $\mathcal{F}_k = \bigcup_{i=1}^n \mathcal{F}_k^{ij}$, (2) $\mathcal{F}_k^{i_1 j} \cap \mathcal{F}_k^{i_2 j} = \emptyset$, and (3) $\varepsilon(\mathcal{F}_k^{ij}) = \varepsilon(\mathcal{F}_k^{ji})$.

Proof of Lemma 1. Let $j \in V_i$. The desired statement follows from the following fact: each spanning rooted forest from \mathcal{F}_{n-v}^{ij} can be put into correspondence with $|V_i|$ spanning rooted forests from \mathcal{F}_{n-v} : the latter forests have the same weight each and only differ by the root in the component that contains i; each element of \mathcal{F}_{n-v} enters the correspondence exactly once. For $j \notin V_i$, the statement follows from $\mathcal{F}_{n-v}^{ij} = \varnothing$.

Proof of Proposition 7. First, we prove that $\forall \alpha \neq 0$, $\det(L + \alpha \bar{J}) \neq 0$. As the matrix $L + \alpha \bar{J}$ is reducible to a block-diagonal form, where the blocks correspond to the connected components of G, it suffices to prove its nonsingularity in the case of connected multigraphs (including the multigraph with one vertex and without edges — the point graph). Assume, on the contrary, that for some connected multigraph G, $\det(L + \alpha \bar{J}) = 0$. Then there exists a vector $\mathbf{b} = (b_1, \dots, b_n)^T \neq \mathbf{0}$ such that $(L + \alpha \bar{J})\mathbf{b} = \mathbf{0}$, where $\mathbf{0} = (0, \dots, 0)^T$. Note that the entries of $L\mathbf{b}$ sum to zero, whereas the entries of $\alpha \bar{J}\mathbf{b}$ are all equal. Therefore, $L\mathbf{b} = \alpha \bar{J}\mathbf{b} = \mathbf{0}$. It follows from $L\mathbf{b} = \mathbf{0}$ that $b_1 = b_2 = \dots = b_n$, hence, by $\alpha \bar{J}\mathbf{b} = \mathbf{0}$, we have $\mathbf{b} = \mathbf{0}$. This contradiction proves the invertibility of $L + \alpha \bar{J}$. To complete the proof, we will need a simple lemma.

LEMMA 2. For any matrices A and B, if A and B are invertible and $A\bar{J} = \bar{J}B = \alpha \bar{J} \ (\alpha \in \mathbb{R}, \ \alpha \neq 0),$ then $A^{-1}\bar{J} = \bar{J}B^{-1} = \alpha^{-1}\bar{J}$.

Proof of Lemma 2. Premultiplying $A \bar{J} = \alpha \bar{J}$ by A^{-1} yields $\bar{J} = \alpha A^{-1} \bar{J}$. The statement regarding the matrix B is proved similarly.

Note that the following equalities hold true:

$$\bar{J}L = L\bar{J} = 0, \tag{25}$$

$$\bar{J}^2 = \bar{J},\tag{26}$$

and, by Lemma 2 and Theorem 2, for any $\tau > 0$,

$$(I + \tau L)^{-1} \bar{J} = \bar{J},$$
 (27)

$$\left(L + \bar{J}\right)^{-1} \bar{J} = \bar{J}. \tag{28}$$

Using Eqs. (25), (26), and (28), we obtain

$$\widetilde{Q}L = (L + \bar{J})^{-1}L - \bar{J}L = (L + \bar{J})^{-1}(L + \bar{J} - \bar{J}) = I - (L + \bar{J})^{-1}\bar{J} = I - \bar{J},\tag{29}$$

$$\widetilde{Q}\,\bar{J} = (L+\bar{J})^{-1}\,\bar{J} - \bar{J}^2 = 0.$$
 (30)

Consequently, for any $\alpha \neq 0$, we have

$$(\widetilde{Q} + \alpha^{-1} \,\overline{J})(L + \alpha \,\overline{J}) = I - \overline{J} + \overline{J} = I,$$

whence $\widetilde{Q} + \alpha^{-1} \overline{J} = (L + \alpha \overline{J})^{-1}$.

Proof of Proposition 8. By (29), $\widetilde{Q}L = I - \overline{J}$. Similarly, $L\widetilde{Q} = I - \overline{J}$. Thus, the first condition in the definition of the Moore–Penrose generalized inverse is checked. Next, using Lemma 2, (25), and (26), we have

$$L\widetilde{Q}L = L(I - \bar{J}) = L,$$

 $\widetilde{Q}L\widetilde{Q} = (I - \bar{J})Q = Q - \bar{J}Q = Q - \bar{J}(L + \bar{J})^{-1} + \bar{J}^2 = Q - \bar{J} + \bar{J} = Q,$

Proof of Proposition 9 reduces to the following transformations based on Eqs. (25)–(28) and Corollary 1:

$$\left(\lim_{\tau \to \infty} \tau \left((I + \tau L)^{-1} - \bar{J} \right) + \bar{J} \right) (L + \bar{J})$$

$$= \lim_{\tau \to \infty} \tau \left((I + \tau L)^{-1} L + (I + \tau L)^{-1} \bar{J} - \bar{J} L - \bar{J}^2 \right) + \bar{J} L + \bar{J}^2$$

$$= \lim_{\tau \to \infty} \tau (I + \tau L)^{-1} L + \bar{J} = \lim_{\tau \to \infty} (I + \tau L)^{-1} (I + \tau L - I) + \bar{J}$$

$$= I - \lim_{\tau \to \infty} (I + \tau L)^{-1} + \bar{J} = I.$$

It now remains to apply Proposition 8.

Proof of Theorem 3. For $j \notin V_i$, the statement follows from Theorem 2, Proposition 9, and the definition of \bar{J} . For $j \in V_i$, using the same and Lemma 1, we have

$$\ell_{ij}^{+} = \lim_{\tau \to \infty} \tau \left(\frac{\sum_{k=0}^{n-v} \tau^{k} \varepsilon(\mathcal{F}_{k}^{ij})}{\sum_{k=0}^{n-v} \tau^{k} \varepsilon(\mathcal{F}_{k})} - \bar{J}_{ij} \right) = \lim_{\tau \to \infty} \frac{\sum_{k=0}^{n-v} \tau^{k+1} \left(\varepsilon(\mathcal{F}_{k}^{ij}) - \frac{1}{|V_{i}|} \varepsilon(\mathcal{F}_{k}) \right)}{\sum_{k=0}^{n-v} \tau^{k} \varepsilon(\mathcal{F}_{k})}$$

$$= \lim_{\tau \to \infty} \frac{\sum_{k=0}^{n-v-1} \tau^{k+1} \left(\varepsilon(\mathcal{F}_{k}^{ij}) - \frac{1}{|V_{i}|} \varepsilon(\mathcal{F}_{k}) \right)}{\sum_{k=0}^{n-v} \tau^{k} \varepsilon(\mathcal{F}_{k})} = \frac{\varepsilon(\mathcal{F}_{n-v-1}^{ij}) - \frac{1}{|V_{i}|} \varepsilon(\mathcal{F}_{n-v-1})}{\varepsilon(\mathcal{F}_{n-v})}.$$

Proof of Proposition 10. Symmetry, nonnegativity, and disconnection condition follow from (23).

Let us prove diagonal maximality. The matrix \bar{J} possesses this property in the nonstrict version $p_{ii} \geq p_{ij}$; therefore, by virtue of (23), it suffices to prove it for Q_{n-v-1} . By definition, for all $i, j = 1, \dots, n, \ q_{n-v-1,ij} = \varepsilon(\mathcal{F}_{n-v-1}^{ij})$ holds, where \mathcal{F}_{n-v-1}^{ij} is the set of all spanning rooted forests in G that contain n-v-1 edges and have i and j in the same tree rooted at i. Obviously, $\mathcal{F}_{n-v-1}^{ij} \subseteq \mathcal{F}_{n-v-1}^{ii}$. Show that $\mathcal{F}_{n-v-1}^{ii} \setminus \mathcal{F}_{n-v-1}^{ij} \neq \emptyset$. Consider an arbitrary $F \in \mathcal{F}_{n-v}^{ij}$, remove from F any edge that belongs to the path from i to j, and arbitrarily choose the root in the newly formed component containing j. The resulting subgraph belongs to $\mathcal{F}_{n-v-1}^{ii} \setminus \mathcal{F}_{n-v-1}^{ij}$. By the assumption of positivity of the edge weights, we have $\varepsilon(\mathcal{F}_{n-v-1}^{ii}) > \varepsilon(\mathcal{F}_{n-v-1}^{ij})$, whence $q_{n-v-1,ii} > q_{n-v-1,ij}$, and the property is proved. Note that diagonal maximality can be similarly proved for Q_1, \dots, Q_{n-v-2} ; for Q_0 it is obvious, whereas for $Q_{n-v} = \varepsilon(\mathcal{F}_{n-v})$ \bar{J} it is valid in a nonstrict version.

Prove the triangle inequality for proximities. The strict statement (for j=k and $i\neq j$) follows from the diagonal maximality. Prove that $p_{ij}+p_{ik}-p_{jk}\leq p_{ii}$. For i=j or i=k, we have the identity. Suppose that $i\neq j$ and $i\neq k$. Obviously, $\mathcal{F}_{n-v-1}^{ij}\cup\mathcal{F}_{n-v-1}^{ik}\subseteq\mathcal{F}_{n-v-1}^{ii}$. Hence,

$$\varepsilon(\mathcal{F}_{n-v-1}^{ij}) + \varepsilon(\mathcal{F}_{n-v-1}^{ik}) - \varepsilon(\mathcal{F}_{n-v-1}^{ij} \cap \mathcal{F}_{n-v-1}^{ik}) = \varepsilon(\mathcal{F}_{n-v-1}^{ij} \cup \mathcal{F}_{n-v-1}^{ik}) \le \varepsilon(\mathcal{F}_{n-v-1}^{ii}). \tag{31}$$

Define $\mathcal{F}_{n-v-1}^{ijk}$ as $\mathcal{F}_{n-v-1}^{ij} \cap \mathcal{F}_{n-v-1}^{ik}$ and note that $\mathcal{F}_{n-v-1}^{ijk}$ differs from $\mathcal{F}_{n-v-1}^{jik} = \mathcal{F}_{n-v-1}^{ji} \cap \mathcal{F}_{n-v-1}^{jk}$ only by the roots of the trees that contain i, j, and k simultaneously. Therefore,

$$\varepsilon(\mathcal{F}_{n-v-1}^{ij} \cap \mathcal{F}_{n-v-1}^{ik}) = \varepsilon(\mathcal{F}_{n-v-1}^{ijk}) = \varepsilon(\mathcal{F}_{n-v-1}^{jik}) \le \varepsilon(\mathcal{F}_{n-v-1}^{jk}). \tag{32}$$

Summing up the extreme left and extreme right parts of (31) and (32), we obtain

$$\varepsilon(\mathcal{F}_{n-v-1}^{ij}) + \varepsilon(\mathcal{F}_{n-v-1}^{ik}) \leq \varepsilon(\mathcal{F}_{n-v-1}^{ii}) + \varepsilon(\mathcal{F}_{n-v-1}^{jk}),$$

which, by the definitions of Q_{n-v-1} and \bar{J} and (23), implies the triangle inequality for proximities.

Prove transit property. The required inequality is valid for the matrix \bar{J} in a nonstrict form, so by virtue of (23), it remains to prove it for Q_{n-v-1} . Obviously, $\mathcal{F}_{n-v-1}^{it} \subseteq \mathcal{F}_{n-v-1}^{ik}$. To prove that $\mathcal{F}_{n-v-1}^{ik} \setminus \mathcal{F}_{n-v-1}^{it} \neq \emptyset$, consider an arbitrary $F \in \mathcal{F}_{n-v}^{it}$. Remove from F any edge that belongs to the path from k to t and arbitrarily choose the root in the newly formed component containing t. The resulting subgraph belongs to $\mathcal{F}_{n-v-1}^{ik} \setminus \mathcal{F}_{n-v-1}^{it}$. By the assumption of positivity of the edge weights, we conclude that $\varepsilon(\mathcal{F}_{n-v-1}^{ik}) > \varepsilon(\mathcal{F}_{n-v-1}^{it})$, and the property is proved.

To demonstrate the violation of *monotonicity*, it is sufficient to consider the graph G with the vertex set $V(G) = \{1, 2, 3\}$ and one edge (1, 2) whose weight is unity. Let an edge (1, 3) with weight unity be added to G.

Here, the accessibility via dense forests provides (for any $\alpha \neq 0$) $\Delta p_{13} = -1/9 < 5/36 = \Delta p_{12}$ (which violates item 1 of monotonicity) and $\Delta p_{23} = -4/9 < 5/36 = \Delta p_{21}$ (which violates item 2). With the same example, item 3 is also trivially violated, as $\Delta p_{22} = 11/36 > 0$. By adding an appropriate number of isolated vertices, similar examples can be generated for all n.

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