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Graph Theory and Pathfinder Primer

Graph theory is the mathematical study of structures consisting of *nodes* with *links* connecting some pairs of nodes (Carre, 1979; Christofides, 1975; Harary, 1969). Terminology in graph theory varies somewhat from one source to another. Our terms represent a distillation of various sources with adaptations to our purposes.

A *graph G* consists of *nodes* and *links*. The nodes are a finite set, e.g., $\{1, 2, ..., n\}$, and the links are a subset of the set of all node pairs. For example, the node pairs (1, 2), (4, 3), (7, 1), designate links between the first and the second node in each pair. The nodes connected by a link are known as *endpoints* of the link. A link is *incident* to a node if the node is an endpoint of the link. The *degree of a node* is the number of links incident to the node. A graph can be displayed by a diagram in which nodes are shown as points, and links are indicated by lines or arrows connecting appropriate pairs of points.

A graph may be either directed or undirected. A *directed graph* (sometimes referred to as a *digraph*) has directed links (or *arcs*). The order of the nodes in a pair designating an arc specifies a direction for the arc which is regarded as going *from* the first (or *initial*) node *to* the second (or *terminal*) node. In diagrams of directed graphs, arcs are represented as arrows extending from the initial node to the terminal node. An *undirected graph* has undirected links (or *edges*). The nodes in a pair designating an edge are regarded as unordered. In diagrams of undirected graphs, edges are represented as lines connecting appropriate nodes. In our usage, the terms *graph* and *link* refer to the general case which includes both directed and undirected graphs.

A *walk* is an alternating sequence of nodes and links such that each link in the sequence connects the nodes that precede and follow it in the sequence. For example, given nodes $\{1, 2, 3, 4\}$, the sequence, 3, (3,2), 2, (2,1), 1, (1,4), 4, specifies a walk, while the sequence, 3, (3,2), 2, (1,4), 4, (2,1), 1, does not. A walk can be specified by the sequence of nodes which it visits in which case the existence of the appropriate links is assumed. For the example walk specified above, the node sequence is 3,2,1,4. The *length of a walk* corresponds to the number of links in the walk. A walk is a *path* if all the nodes in the walk are distinct. A link is a path of length 1. A *cycle* is a closed path with all nodes distinct except the first and last nodes, which are identical.

A *connected graph* contains a path between any two nodes. A *tree* is a connected graph with no cycles. An undirected tree with n nodes has exactly $n-1$ edges, and it contains exactly one path between any two nodes. A *complete graph* has all possible links.

Links may have positive real numbers (weights, distances, or costs) associated with them in which case the graph is known as a *network*. The graph corresponding to a network is obtained by deleting the weights. The graph represents the structure of a network, and the weights associated with links in a network, provide quantitative information to accompany that structure. The *weight* of link (i,j) is designated by w_{ij}. A graph may be regarded as a network with all link weights equal to one (1). In a network, the *weight of a path* is the sum of the weights associated with the links in the path. A *geodesic* is a minimum weight path connecting two nodes. The *distance* between two nodes is the weight of a geodesic connecting the nodes. The *minimal spanning tree* (Kruskal, 1956) of an undirected network consists of a subset of the edges in the network such that the subgraph is a tree and the sum of the link weights is minimal over the set of all possible trees.

Various characteristics of graphs are conveniently represented by matrices. A graph G can be represented by the *adjacency matrix A*, the $n \times n$ matrix with $a_{ij} = 1$ if G contains the link (i,j) and $a_{ij} = 0$ otherwise. A network is similarly represented by the *network adjacency matrix* A with $a_{ii} = 0$, $a_{ij} = w_{ij}$, $i \neq j$ if the network contains the link (i, j), otherwise $a_{ij} = \infty$. The *reachability matrix* of G is the $n \times n$ matrix in which the ij^{th} entry is 1 if there is a path in G from node i to node j and is 0 otherwise. The *distance matrix D* of a network is the $n \times n$ matrix in which d_{ij} is the (minimum) distance from node i to node j in a network. If there is no path from node i to node j (a disconnected network), $d_{ij} = \infty$. The distance matrix of a graph contains the (minimum) number of links between pairs of nodes. The distance matrix is not necessarily symmetric, but it will be symmetric if the network consists of undirected links. A link in a network is *redundant* if the network obtained by removing the link yields the same distance matrix as the original network.

Pathfinder Networks

Pathfinder networks are derived from proximity data.[1] In defining Pathfinder networks (PFNETs), it is helpful to conceptualize proximity data as a complete network[2] with the weight on each link equal to the proximity between the entities connected by the link. Call this network the DATANET. The DATANET is a direct representation of the proximities, but because of the density of links in the network, it is not very informative. The essential idea underlying Pathfinder networks is that a link in a DATANET is a link (with the same weight) in a PFNET if and only if the link is a minimum weight path in the DATANET. Equivalently, we can say that the PFNET has the same distance matrix as the DATANET, but the PFNET has the minimum number of links needed to yield that distance matrix.

A variety of different PFNETs can be derived from a given set of proximity data. A particular PFNET is determined by the values of two parameters, r and q. These two parameters represent generalizations of the usual definition of distances in networks. The r parameter determines how the weight of a path is computed from the weights on links in the path. The q parameter limits the number of links allowed in paths.

The r Parameter

Usually, in graph theory, the weight of a path is the sum of the weights of the links in the path. When link weights are obtained from empirical data, it may not be justifiable to compute path weight in this way because that computation assumes ratio-scale measurement (cf. Stevens, 1951). For computing distances in DATANETs, we need a distance function that will permit computations of distances in networks with different assumptions about the level of measurement associated with the proximities. From the perspective of deriving networks from proximities, such a distance function should preserve ordinal relationships between link weights and path weights for all permissible transformations of the proximities with different assumptions about the level of measurement associated with the proximities. Then, ordinal comparisons of path weights and link weights could be used to determine link membership in PFNETs.

A distance function with the required qualities can be defined by adapting the Minkowski distance measure to computing distances over paths in networks. It can easily be shown that the Minkowski r distance satisfies the requirements of a path algebra for networks as defined by Carre (1979). The r distance function replaces the normal sum with the r distance so that $x + y$ is replaced by $(x^r + y^r)^{1/r}$, $x \geq 0$, $y \geq 0$, $r \geq 1$. Given a path P consisting of k links with weights $w_1, w_2, \ldots, w_k$, the weight of path P, $w(P)$ becomes:

$$w(P) = \left(\sum_{i=1}^{k} w_i^{\,r} \right)^{1/r} \quad \text{where } r \geq 1,\ w_i \geq 0 \text{ for all } i.$$

Note that with $r = 1$, the function corresponds to simple addition (the usual definition of distances in networks). With $r = \infty$, the function is the maximum function. In fact,

$$\lim_{r \to \infty} \left(w_i^{\,r} + w_j^{\,r} \right)^{1/r} = maximum\ (w_i, w_j).$$

Thus with $r = \infty$, computing network distances with the Minkowski r distance only requires maximum (as above) and minimum (for identifying geodesics or minimum weight paths) operations which are order preserving and, therefore, appropriate for ordinal scale measurement. In particular, the ordinal relationships of path weights will be preserved for any nondecreasing transformation of the link weights (proximities).

In summary, the r parameter for PFNETs is the value of r in the Minkowski r distance computation for the weight of a path as a function of the weights of links in the path.

The q Parameter

The distance matrix of a network is usually determined by finding the minimum weight paths regardless of the number of links in those paths. The q parameter is another generalization of this definition of network distance. This parameter places an upper limit on the number of links in paths used to determine the minimum distance between nodes in the DATANET. There are two reasons for using the q parameter, one psychological, and the other representational. From a psychological perspective, there may be some limit on the number of links that could meaningfully connect nodes in a particular domain. This amounts to a limit in the chain of relations that can be constructed relating any two concepts in the domain. This limit can be incorporated into the network generation procedure with the q parameter. The representational motivation for the q parameter is that it provides a method for systematically controlling the density of links in PFNETs. Users of PFNETs may have various reasons for preferring networks of varying density.

With the two parameters r and q, a particular PFNET is identified as PFNET(r, q). The properties of PFNETs and their relation to one another are discussed in detail in Chapter 1.

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[1] Similarity, relatedness, and psychological distance are closely related concepts indicating the degree to which things "belong together" psychologically. Proximity is a general term which represents these concepts as well as other measurements, both subjective and objective, of the relationship between pairs of entities. In this chapter, we use the term, proximity, to refer to such measurements. In the techniques we propose, the measurements have the direction of distances (or distance estimates) so that small values represent similarity, relatedness, or nearness, and large values represent dissimilarity, lack of relatedness, or distance.

[2] The proximity estimates will define a complete network when the set of proximities is complete. Missing data can be handled by using infinity for missing values. Pairs of entities with infinite proximities will never be linked in any PFNET. This fact can also be used to prevent the linking of any two nodes simply by using infinite proximities for the appropriate pairs. PFNETs are not necessarily connected when some of the proximities are infinite.

Glossary

adjacent - Two nodes are adjacent in a graph if and only if they are connected by a link.

adjacency matrix - The adjacency matrix of a graph with n nodes is the $n \times n$ matrix $\mathbf{A}$ with $\mathbf{A}_{ij} = 1$ if nodes i and j are adjacent in the graph, otherwise $\mathbf{A}_{ij} = 0$. The adjacency matrix of a network is the $n \times n$ matrix $\mathbf{A}$ with $\mathbf{A}_{ii} = 0$ and $\mathbf{A}_{ij} = w_{ij}$ (the weight of the link between nodes i and j) if the nodes i and j are adjacent, otherwise $\mathbf{A}_{ij} = \infty$.

arc - An arc is a directed link with a direction from the initial or originating node to the terminal node. In diagrams, arcs are usually shown as arrows pointing from the initial node to the terminal node.

center - A center of a graph or network is a node with minimum *eccentricity*.

clique - A clique is a maximal subgraph with three or more nodes in which every node in the subgraph is connected to every other node in the subgraph.

complement - The complement G´ of a graph G has the same nodes as G, but two nodes in G´ are connected by a link if and only if they are not connected by a link in G. G´ has the opposite set of links to those in G.

complete graph or complete network - A graph or network with all possible links, that is, a link for every pair of nodes.

connected graph - A graph is connected if there is a path between the nodes in every pair of nodes.

cutnode or cutpoint - If removing a node and its incident links results in a disconnected graph, that node is a cutpoint or a cutnode.

cycle - A cycle is a closed path with the same first and last nodes.

degree - The number of links incident to a node is the degree of that node.

density - The number of links in a graph divided by the number of possible links.

diameter - The diameter of a connected graph or network is the length of any longest geodesic.

distance - The distance between nodes in a network is the length of the geodesic connecting the nodes, or equivalently, the distance between two nodes is the length of the minimum-length path connecting the nodes. Distances in networks do not have the same limitations as distances in space. For example, network distances can be asymmetrical (d_{ij} may not be the same as d_{ji}), but network distances do obey the triangle inequality ($d_{ij} \leq d_{ik} + d_{kj}$). See also graph-theoretic distance.

eccentricity - The eccentricity of a node is the maximum distance between that node and all other nodes in a graph or network.

edge - An edge is an undirected link. In diagrams, edges are usually shown as lines drawn between the nodes connected by the edge.

geodesic - The path of minimum length between the nodes in a pair is the geodesic connecting the nodes.

graph - A graph is a finite set of nodes and a subset of pairs of nodes (the links).

graph-theoretic distance - The distance measured by the minimum number of links connecting two nodes in a graph is the graph-theoretic distance. This definition of distance is a special case of the general notion of distance in a network. For graph distance, consider the weight on each link to be 1 (one) and use $r = 1$ in the definition of the length of a path.

incident - All links connected to a node are incident to that node.

indegree - The number of arcs terminating on a node is the indegree of that node.

isomorphic - Two graphs are isomorphic if there exists a one-to-one correspondence between their nodes that results in the same set of links in the two graphs.

length (of a path) - In a graph, the length of a path is the number of links in the path. In a network, the length of a path consisting of k links with weights, $w_1, w_2, ...w_k$ is computed by: $(w_1^r + w_2^r + ... + w_k^r)^{1/r}$, where r is a parameter, $1 \le r \le \infty$. Note that $r = 1$ corresponds to simple addition of the link weights. With $r = \infty$, the length of a path can be computed using the maximum function, $\mathrm{Max}(L_1, L_2, ..., L_k)$, which is the limit of the general function as r approaches infinity.

link - A link is a connection between nodes. A particular link can be identified by the pair of nodes it connects (the endnodes of the link). Links can be directed (arcs) or undirected (edges).

loop - A loop is a link connecting a node to itself.

median - A median of a graph or network is a node with the smallest average distance to all other nodes in the graph.

minimum-cost network (MCN) - The Pathfinder network generated with $r = \infty$ and $q = n{-}1$, where n is the number of nodes.

minimal dominating node set - The minimal set of nodes from which every node in the graph can be reached over, at most, one link.

minimal spanning tree - A minimal spanning ree of a network consists of a subset of the links in the network such that the subset constitutes a tree, and the sum of the link weights in the subset are minimal over all possible subsets.

minimum cycle - A cycle with minimum distance.

network - A network is a graph with nonnegative real numbers (weights) associated with the links. Each link in a network has a weight.

node - Along with links, nodes are the basic units of graphs and networks. A graph is defined as a finite set of nodes with links connecting some pairs of the nodes.

ordinal level measurement - Measurement on a scale in which only the order of the values is thought to be meaningful. Thus, any values which have the same order as the original values constitute an equivalent scale. Operations on values from ordinal scales should only rely on the order of values (see *r* parameter).

outdegree - The number of arcs originating from a node is the outdegree of that node.

path - A sequence of distinct nodes and connecting links in a graph or network.

Pathfinder graph - The graph obtained by deleting the link weights from a Pathfinder Network.

Pathfinder network - The network obtained by deleting from the complete network corresponding to a proximity matrix every link whose weight is larger than the length of the geodesic connecting the endnodes of the link. The weights on the remaining links are the same as the weights on the corresponding links in the complete network.

PFNET(*r*, *q*) - A Pathfinder graph or network computed with particular values of the parameters r and q.

proximity - Proximity is a term used to refer to a measure of relationship between two entities. Measures of similarity, relatedness, dissimilarity, distance, conditional probability, or association are all instances of proximity measures. In the context of networks, proximity measures have the direction of distance with small values representing similarity, closeness, or high relatedness, and large values representing dissimilarity, farness, or low relatedness.

***q* parameter** - The q parameter specifies a limit on the number of links allowed in paths as path lengths are determined in deriving a Pathfinder network from proximity data. Only paths of q or fewer links are considered. For a network with n nodes, meaningful values of q range from 2 to $n{-}1$. With $q = n{-}1$, there is essentially no limit on the lengths of paths because the longest possible paths have $n{-}1$ links.

ratio-level measurement - Measurement on a scale with a true zero point and meaningful differences or intervals on the scale. Physical measurement is usually ratio level. A ratio scale is preserved by multiplying by a positive constant (a change of unit). All other transformations distort the ratio properties.

reachable - A node is reachable from another node in a graph if there is a path from the first node to the second in the graph.

***r* parameter** - The r parameter is the value used in the computation of the lengths of paths in determining a Pathfinder network. Meaningful values of r range from 1 through infinity. When $r = \infty$, link membership in Pathfinder networks is determined solely by the order of the proximity data values. Thus, infinite r is appropriate for ordinal-level measurement. Other values of r require ratio-level measurement.

subgraph - A subgraph is obtained by removing a subset of nodes and their incident links from a graph.

tree - A connected graph with no cycles.

triangle inequality - The triangle inequality is satisfied when a set of meaures, d_{ij}, on pairs of points i and j, $d_{ij} \le d_{ik} + d_{kj}$ for all i,j,k.

weight - The cost or distance associated with a link. A network is a graph with weighted links.

***z* parameter** - The z parameter determines the width of the interval used to make link membership decisions with the FUZZYPF algorithm (see Chapter 3).

Author Index

Numbers in italic indicate the pages on which the complete references can be found.

Subject Index