Università di Perugia
Dipartimento di Matematica e Informatica

Numerical Approximation

A survey about Link Prediction

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Chapter 1

Introduction

1.1 Link Prediction 🔍

Definition 🔑: Link prediction finds missing links (in static networks) or predicts the likelihood of future links (in dynamic networks).

There exists a wide range of link prediction techniques like similarity-based indices, probabilistic methods, dimensionality reduction approaches, etc.

1.2 Background

A **social network** (a more general term is a complex network) is a standard approach to model communication in a group or community of persons. Such networks can be represented as a graphical model in which a node maps to a person or social entity, and a link corresponds to an association or collaboration between corresponding persons or social entities. When links can be deleted or added, during time, the network is called **dynamic**. Lots of issues arise when we study a social network, some of which are changing association patterns over time, factors that drive those associations, and the effects of those associations to other nodes. Here, we address a specific problem termed as link prediction.

Problem Characterization. Consider a simple undirected network $G(V, E)$ (Refer to the Figure 1), where V characterizes a vertex-set and E, the link-set.

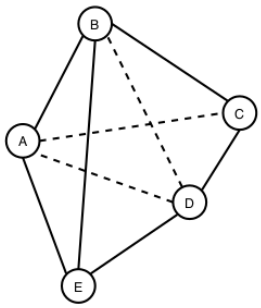


Figure 1.1: Network representation as a graph

We use (`vertex` ≡ `node`), (`link` ≡ `edge`) and (`graph` ≡ `network`) interchangeably. In the graph, a universal set U contains a total of $\frac{n(n-1)}{2}$ links (total node-pairs), where $n = |V|$ represents the number of total vertices of the graph. (|U| - |E|) number of links are termed as the *non-existing links*, and some of these links may appear in the near future when we talk about dynamic network. ***Finding such missing links (i.e., AC, BD, and AD) is the aim of link prediction***.

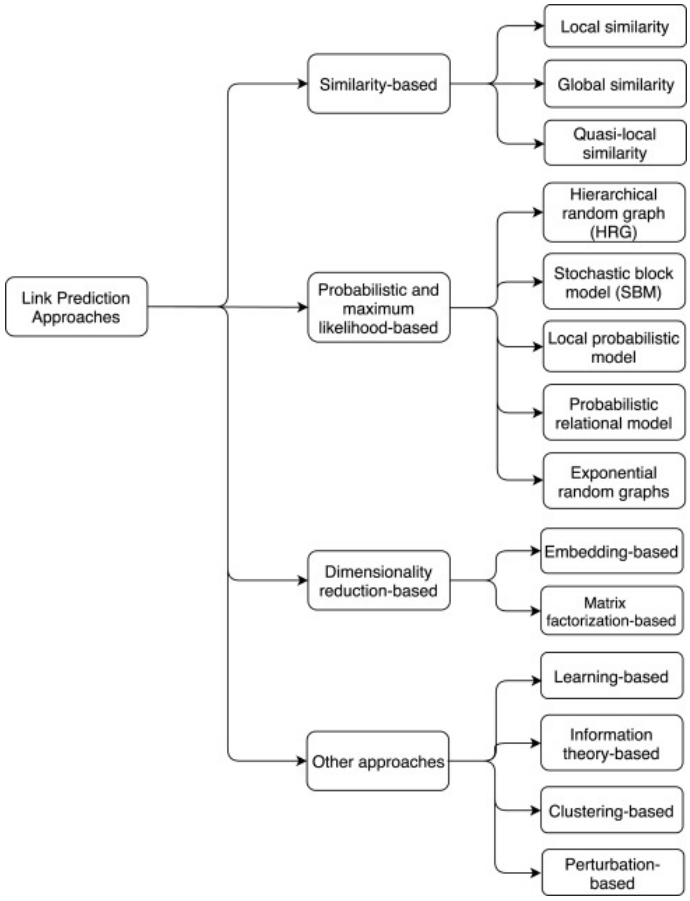
The link prediction problem can be defined as follow: *Suppose a graph* $G_{t_0-t_1}(V, E)$ *represents a snapshot of a network during time interval* $[t_0, t_1]$ *and* $E_{t_0-t_1}$*, a set of links present in that snapshot. The task of link prediction is to find set of links* $E_{t'_0-t'_1}$ *during the time interval* $[t'_0, t'_1]$ *where* $[t_0, t_1] \leq [t'_0, t'_1]$.

The link prediction idea is useful in several domains of application. Examples include automatic hyperlink creation, website hyper-link prediction in the Internet and web science domain, and friend recommendation on Facebook.

Chapter 2

Existing Methods

Recently, numerous methodologies of link prediction have been implemented. These methods can be grouped into several categories, like **similarity-based, probabilistic models, learning-based models**, etc.



2.1 Similarity-based Methods

Similarity-based metrics are the simplest one in link prediction, in which for each pair x and y, a similarity score $S(x, y)$ is calculated. The score $S(x, y)$ is based on the structural or node's properties of the considered pair. The non-observed links (i.e., $U - E^T$) are assigned scores according to their similarities. **The pair of nodes having a higher score represents the predicted link between them**. The similarity measures between every pair *can be calculated using several properties of the network*, one of which is structural property. Scores based on this property can be grouped in several categories like **local and global**, and so on.

2.1.1 Local similarity indices

Local indices are generally calculated using information about common neighbors and node degree. These indices **consider immediate neighbors of a node**. The following are some examples of local similarity indices with a description and method to calculate them:

- `Common Neighbors (CN)`: In a given network or graph, the size of common neighbors for a given pair of nodes x and y is calculated as the size of the intersection of the two nodes neighborhoods (Γ).

  $$S(x, y) = |\Gamma(x) \cap \Gamma(y)|$$

  The likelihood of the existence of a link between x and y increases with the number of common neighbors between them.

- `Jaccard Coefficient`: This metric is similar to the Common Neighbors. Additionally, it normalizes the above score, as given below:

  $$S(x, y) = \frac{|\Gamma(x) \cap \Gamma(y)|}{|\Gamma(x) \cup \Gamma(y)|}$$

  The Jaccard coefficient is defined as the probability of selection of common neighbors of pairwise vertices from all the neighbors of either vertex. The pairwise Jaccard score increases with the number of common neighbors between the two vertices considered. Some researcher (**Liben-Nowell et al.**) demonstrated that this similarity metric **performs worse** as compared to Common Neighbors.

- `Adamic/Adar Index (AA)`: Adamic and Adar presented a metric to calculate a similarity score between two web pages based on shared

features, which are further used in link prediction after some modification

$$S(x,y) = \sum_{z \in \Gamma(x) \cap \Gamma(y)} \frac{1}{log k_z}$$

where k_z is the degree of the node z. It is clear from the equation that more weights are assigned to the common neighbors having smaller degrees. This is also intuitive in the real-world scenario, for example, a person with more number of friends spend less time/resource with an individual friend as compared to the less number of friends.

- `Preferential Attachment (PA)`: The idea of preferential attachment is applied to generate a growing scale-free network. The term **growing** represents the incremental nature of nodes over time in the network. The likelihood incrementing new connection associated with a node x is proportional to k_x , the degree of the node. Preferential attachment score between two nodes x and y can be computed as:

  $$S(x,y) = k_x k_y$$

  This index shows the worst performance on most networks. The **simplicity** (as it requires the least information for the score calculation) and the **computational time** of this metric are the main advantages. PA shows better results if larger degree nodes are densely connected, and lower degree nodes are rarely connected. In the above equation, summation can also be used instead of multiplication as an aggregate function.

- `Resource Allocation Index (RA)`: Consider two non-adjacent vertices x and y. Suppose node x sends some resources to y through the common nodes of both x and y then the similarity between the two vertices is computed in terms of **resources sent** from x to y. This is expressed mathematically as:

  $$S(x,y) = \sum_{z \in \Gamma(x) \cap \Gamma(y)} \frac{1}{k_z}$$

  The difference between **RA** and **AA** is that the RA index heavily penalizes to higher degree nodes compared to the AA index. Prediction results of these indices become almost the same for smaller average degree networks. This index shows good performance on heterogeneous networks with a high clustering coefficient, especially on transportation networks.

- `Cosine similarity or Salton Index (SI)`: This similarity index between two records (documents) is measured by calculating the Cosine of the angle between them. The metric is all about the orientation and not magnitude. The Cosine similarity can be computed as

$$S(x,y) = \frac{|\Gamma(x) \cap \Gamma(y)|}{\sqrt{(k_x k_y)}}$$

- `Sorensen Index`: It is very similar to the Jaccard index. **McCune et al.** show that it **is more robust than Jaccard against the outliers**.

$$S(x,y) = \frac{2|\Gamma(x) \cap \Gamma(y)|}{k_X + k_y}$$

- `CAR-based Common Neighbor Index (CAR)`: CAR-based indices are presented based on the assumption that the link existence between two nodes is more likely if their common neighbors are members of a local community (local-community-paradigm (LCP) theory). In other words, the likelihood existence increases with the number of links among the common neighbors (local community links (LCLs)) of the seed node pair as described in the following figure.

$$S(x,y) = CN(x,y) \text{ x } LCL(x,y) = CN(x,y) \text{ x } \sum_{z \in \Gamma(x) \cap \Gamma(y)} \frac{|\gamma(z)|}{2}$$

where $CN(x,y) = |\Gamma(x)\Gamma(y)|$ is number of common neighbors. $LCL(x,y)$ refers to the number of local community links which are defined as the links among the common neighbors of seed nodes x and y. $\gamma(z)$ is the subset of neighbors of node z that are also common neighbors of x and y.

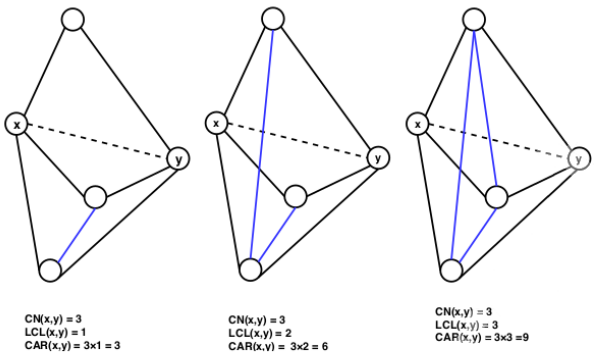


Figure 3: *CAR Index* = (*Number of CNs*) × (*Number of LCLs*)

- `CAR-based Adamic/Adar Index (CAA)`: If LCL is considered as an accuracy enhancer, then the CAA index is obtained by incorporating the LCL theory to the well known AA index and mathematically expressed by the equation given below.

$$S(x,y) = \sum_{z \in \Gamma(x) \cap \Gamma(y)} \frac{|\gamma(z)|}{\log_2(k_z)}$$

- `CAR-based Resource Allocation Index (CRA)`: Is a general application of the LCL theory to other indices and generate the CRA index by incorporating this concept into the existing RA index of the literature. Mathematically, the CRA can be expressed as

$$S(x,y) = \sum_{z \in \Gamma(x) \cap \Gamma(y)} \frac{|\gamma(z)|}{k_z}$$

- `CAR-based Preferential Attachment Index (CPA)`: This is the preferential attachment index based on the CAR index. CPA is obtained by incorporating the LCL theory to the original PA method and expressed mathematically by

$$S(x,y) = e_x e_y + e_x CAR(x,y) + e_y CAR(x,y) + CAR(x,y)^2$$

  where e_x is the number of neighbors of x not shared by y and $CAR(x,y)$ is the similarity score of the node pair x and y using CAR index. CAR-based methods listed above show the best performance on LCP networks. The LCP networks are related to dynamic and heterogeneous systems and facilitate network evolution of social and biological networks.

- `Hub Promoted Index (HPI)`: This similarity index promotes the formation of links between the sparsely connected nodes and hubs. It also tries to prevent links formation between the hub nodes. This similarity metric can be expressed mathematically as

$$S(x,y) = \frac{|\Gamma(x) \cap \Gamma(y)|}{min(k_x, k_y)}$$

- `Hub Depressed Index (HDI)`: This index is the same as the previous one but with the opposite goal as it avoids the formation of links between hubs and low degree nodes in the networks. The Hub depressed index promotes the links evolution between the hubs as well as the

low degree nodes. The mathematical expression for this index is given below.

$$S(x,y) = \frac{|\Gamma(x) \cap \Gamma(y)|}{max(k_x, k_y)}$$

- `Local Naive Bayes-based Common Neighbors (LNBCN)`: The above similarity indices are somehow based on common neighbors of the node pair where each of the which are equally weighted. This method is based on the Naive Bayes theory and arguments that different common neighbors play different role in the network and hence contributes differently to the score function computed for non-observed node pairs

$$S(x,y) = \sum_{z \in \Gamma(x) \cap \Gamma(y)} [log(\frac{C(z)}{1 - C(z)}) + log(\frac{1-\rho}{\rho})]$$

  where $C(z)$ is node clustering coefficient and ρ is the network density expressed as

$$\rho = \frac{|E|}{n(n-1)/2}$$

- `Leicht-Holme-Newman Local Index (LHNL)`: The logic below this index is that two vertices are similar to each other if their corresponding neighbors are self-similar to themselves. This score is defined by the ratio of the path of length two that exits between two vertices and the expected path of the same length between them.

$$S(x,y) = \frac{|\Gamma(x) \cap \Gamma(y)|}{k_x k_y}$$

- `Node Clustering Coefficient (CCLP)`: This index is also based on the clustering coefficient property of the network in which the clustering coefficients of all the common neighbors of a seed node pair are computed and summed to find the final similarity score of the pair. Mathematically

$$S(x,y) = \sum_{z \in \Gamma(x) \cap \Gamma(y)} C(z)$$

  where

$$C(z) = \frac{t(z)}{k_z(k_z - 1)}$$

  is clustering coefficient of the node z and $t(z)$ is the total triangles passing through the node z.

- `Node and Link Clustering coefficient (NLC)`: This similarity index is based on the basic topological feature of a network called "*Clustering Coefficient*". The clustering coefficients of both nodes and links are incorporated to compute the similarity score.

$$S(x,y) = \sum_{z \in \Gamma(x) \cap \Gamma(y)} \frac{|\Gamma(x) \cap \Gamma(z)|}{k_z - 1} \text{ x } C(z) + \frac{|\Gamma(y) \cap \Gamma(z)|}{k_z - 1} \text{ x } C(z)$$

2.1.2 Global similarity indices

Global indices are computed using entire topological information of a network. The computational complexities of such methods are higher and seem to be infeasible for large networks.

- `Katz Index`: This index can be considered as a variant of the shortest path metric. It directly aggregates over all the paths between x and y and dumps exponentially for longer paths to penalize them. It can be expressed mathematically as:

$$S(x,y) = \sum_{l=1}^{\infty} \beta^l |paths_{x,y}^{<l>}| = \sum_{l=1}^{\infty} \beta^l (A)_{x,y}^l$$

where, $paths_{x,y}^{<l>}$ is considered as the set of total l length paths between x and y, β is a damping factor that controls the path weights and A is the adjacency matrix. For the convergence of above equation,

$$\beta < \frac{1}{\lambda_1}$$

where λ_1 is the maximum eigenvalue of the matrix A. If 1 is added to each element of the diagonal of the resulting similarity matrix S, this expression can be written in matrix terms as

$$S = \beta AS + I$$

where I is the identity matrix of the proper dimension. The similarity between all pairs of nodes can be directly computed using the closed-form by rearranging for S in the previous expression and subtracting the previously added 1 to the elements in the diagonal. Katz score for each pair of nodes in the network is calculated by finding the similarity matrix as

$$S = (I - \beta A)^{-1} - I$$

The computational complexity of the given metric is high, and it can be roughly estimated to be cubic complexity which is not feasible for a large network.

- `Random Walk with Restart (RWR)`: Let α be a probability that a random walker iteratively moves to an arbitrary neighbor and returns to the same starting vertex with probability $(1 - \alpha)$. Consider q_{xy} to be the probability that a random walker who starts walking from vertex x and located at the vertex y in steady-state. Now, this probability of walker to reach the vertex y is expressed mathematically as

$$\overrightarrow{q_x} = \alpha P^T \overrightarrow{q_x} + (1 - \alpha)\overrightarrow{e_x}$$

  where $\overrightarrow{e_x}$ is the seed vector of length $|V|$ (i.e., the total number of vertices in the graph). This vector consists of zeros for all components except the elements x itself. The transition matrix P can be expressed as

$$\overrightarrow{q_x} = (1 - \alpha)(I - \alpha P^T)^{-1}\overrightarrow{e_x}$$

  Since this similarity is not symmetric, the final score between the node pair (x, y) can be computed as

$$S(x, y) = q_{xy} + q_{yx}$$

  It is clear from the above equation that matrix inversion is required to solve, which is quite expensive and prohibitive for large networks.

- `Shortest Path`: The inverse relation between the similarity and length of the shortest path is captured by the following mathematical equation given below.

$$S(x, y) = -|d(x, y)|$$

  where Dijkstra algorithm is applied to efficiently compute the shortest path d(x, y) between the node pair (x, y). The prediction accuracy of this index is low compared to most local indices.

- `Leicht-Holme-Newman Global Index (LHNG)`: This global index is based on the principle that two nodes are similar if either of them has an immediate neighbor, which is similar to the other node. This is a recursive definition of similarity where a termination condition is needed. The termination condition is introduced in terms of self-similarity, i.e., a node is similar to itself. Thus, the similarity score equation consists of two terms: first, the neighbor similarity, and the second, self-similarity, as given below.

$$S(x, y) = \phi \sum_z A_{x,z} S_{z,y} + \psi \delta_{x,y}$$

  Here, the first term is neighborhood similarity and the second term is self-similarity. ψ and ϕ are free parameters that make a balance

between these two terms. When the free parameter $\psi = 1$, this index resembles to the Katz index.

- `Cosine based on L+ (Cos+)`: Laplacian matrix is extensively used as an alternative representation of graphs in spectral graph theory. This matrix can be defined as $L = D - A$, where, D is the diagonal matrix consisting of the degrees of each node of the matrix and A is the adjacency matrix of the graph. The pseudo-inverse of the matrix defined by Moore-Penrose is represented as L^+ and each entry of this matrix is used to represent the similarity score between the two corresponding nodes. The most common way to compute this pseudo-inverse is by computing the **singular value decomposition (SVD)** of the Laplacian matrix [$(L = U\Sigma VT)$, where U and V are left and right singular vectors of SVD] as follows

  $$L^+ = V\Sigma^+ U^T$$

  Σ^+ is obtained by taking the inverse of each nonzero element of the Σ. Further, the similarity between two nodes x and y can be computed using any inner product measure such as Cosine similarity given as

  $$S(x, y) = \frac{L^+_{x,y}}{\sqrt{L^+_{x,x} L^+_{y,y}}}$$

- `Average Commute Time (ACT)`: This index is based on the random walk concept. A random walk is a Markov chain which describes the movements of a walker. It defined as the average number of movements/steps required by a random walker to reach the destination node y, and come back to the starting node x. If $m(x, y)$ be the number of steps required by the walker to reach y from x, then the following expression captures this concept.

  $$n(x, y) = |E|(l^+_{xx} + l^+_{yy} - 2l^+_{xy})$$

  where l^+_{xy} denotes the (x, y) entry of the matrix L^+ . Pseudo-inverse of the Laplacian, L^+ can be computed as

  $$L^+ = (L - \frac{ee^T}{n})^{-1} + \frac{ee^T}{n}$$

  where e is a column vector consisting of 1's. Smaller value of this equation will represent higher similarity. The final expression is the following

  $$S(x, y) = \frac{1}{l^+_{xx} + l^+_{yy} - 2l^+_{xy}}$$

- `Normalized Average Commute Time (NACT)`: This is a variant of ACT that takes into account node degrees. For a high degree node (hub) y, $m(x, y)$ is usually small regardless of x, the similarity measure is normalized with stationary distribution π of the Markov chain describing random walker on the graph. This normalized measure can be computed with the following equation

$$S(x, y) = \frac{1}{(m(x, y)\pi_y + m(y, x)\pi_x)}$$

- `Matrix Forest Index (MF)`: his index is based on the concept of spanning tree which is defined as the subgraph that spans total nodes without forming any cycle. The spanning tree may contain total or less number of links as compared to the original graph. Chebotarev and Shamis proposed a theorem called matrix-forest theorem which states that the number of spanning tree in a graph is equal to the co-factor of any entry of Laplacian matrix of the graph. Here, the term forest represents the union of all rooted disjoint spanning trees. The similarity between two nodes x and y can be computed with the equation given below

$$S = (I + L)^{-1}$$

  where $(I + L)\_(x, y)$ is the number of spanning rooted forests (x as root) consisting of both the nodes x and y. Moreover, this quantity is equal to the co-factor of $(I + L)_{(x,y)}$.

- `SimRank`: This is a measure of structural context similarity and shows object-to-object relationships. It is not domain-specific and recommends to apply in directed or mixed networks. The basic assumption of this measure is that two objects are similar if they are related to similar objects. SimRank computes how soon two random walkers meet each other, starting from two different positions. This measure can be represented in matrix form as

$$S(x, y) = \alpha W^T S W + (1 - \alpha) I$$

  where, $\alpha \in (0, 1)$ is a constant. W is the transformation matrix and computed by normalizing each column of adjacency matrix A as

$$W_{ij} = \frac{a_{ij}}{\sum_{k=1}^{n}}$$

  The computational complexity of this measure is high for a large network, and to reduce its time, the authors suggest pruning recursive branches.

- `Rooted Pagerank (RPR)`: The idea of PageRank was originally proposed to rank the web pages based on the importance of those pages. The algorithm is based on the assumption that a random walker randomly goes to a web page with probability α and follows hyper-link embedded in the page with probability $(1-\alpha)$. Chung et al. used this concept incorporated with a random walk in link prediction framework. The importance of web pages, in a random walk, can be replaced by stationary distribution. The similarity between two vertices x and y can be measured by the stationary probability of y from x in a random walk where the walker moves to an arbitrary neighboring vertex with probability α and returns to x with probability $(1-\alpha)$. Mathematically, this score can be computed for all pair of vertices as

  $$RPR = (1-\alpha)(I - \alpha\hat{N})^{-1}$$

  where $\hat{N} = D^{-1}A$ is the normalized adjacency matrix with the diagonal degree matrix $D[i,i] = \sum_j A[i,j]$.

2.1.3 Quasi-local indices

Quasi-local indices have been introduced as a trade-off between local and global approaches or performance and complexity. These metrics are as efficient to compute as local indices. Some of these indices extract the entire topological information of the network. The time complexities of these indices are still below compared to the global approaches.

- `Local Path Index (LP)`: This metric has the intent to furnish a good trade-off between accuracy and computational complexity. The metric is expressed mathematically as

  $$S^{LP} = A^2 + \epsilon A^3$$

  where ϵ represents a free parameter. Clearly, the measurement converges to common neighbor when $\epsilon = 0$. If there is no direct connection between x and y, $(A^3)_{xy}$ is equated to the total different paths of length 3 between x and y. The index can also be expanded to generalized form

  $$S^{LP} = A^2 + \epsilon A^3 + \epsilon^2 A^4 + ... + \epsilon^{(n2)} A^n$$

  where n is the maximal order. Computing this index becomes more complicated with the increasing value of n. The LP index outperforms the proximity-based indices, such as RA, AA, and CN.

- `Path of Length 3 (L3)`: Georg Simmel, a German sociologist, first coined the concept "triadic closure" and made popular by Mark Granovetter in his work "*The Strength of Weak Ties*". The authors proposed a similarity index in protein-protein interaction (PPI) network, called ***path of length 3 (or L3)*** published in the Nature Communication. They experimentally show that the triadic closure principle (TCP) does not work well with PPI networks. They showed the paradoxical behavior of the TCP (i.e., the path of length 2), which does not follow the structural and evolutionary mechanism that governs protein interaction. The TCP predicts well to the interaction of self-interaction proteins (SIPs), which are very small (4%) in PPI networks and fails in prediction between SIP and non SIP that amounts to 96%. They showed that the L3 index performs well in such conditions and give mathematical expression to compute this index as

$$S(x,y) = \sum \frac{a_{x,u}a_{u,v}a_{v,y}}{k_u k_v}$$

- `Similarity based on Local Random Walk and Superposed Random Walk (LRW and SRW)`: This metric propose a new similarity measures by exploiting the random walk concept on graphs with limited walk steps. They defined node similarity based on random walks of lower computational complexity compared to the other random walk based methods. Given a random walker, starting from the node x, the probability of reaching the random walker to the node y in t steps is

$$\overrightarrow{\pi}\_x(t) = P^T \overrightarrow{\pi}\_x(t-1)$$

  where $\overrightarrow{\pi}\_x(0)$ is a column vector with x^{th} element as 1 while others are 0's and P^T is the transpose of the transition probability matrix P. P_{xy} entry of this matrix defines the probability of a random walker at node x will move to the next node y. It is expressed as $P_{xy} = \frac{a_{kx}}{k_x}$, where a_{xy} is 1 when there is a link between x and y and 0, otherwise. The authors computed the similarity score (LRW) between two nodes based on the above concept as

$$S^{LRW}(x,y) = \frac{k_x}{2|E|}\pi_{xy}(t) + \frac{k_y}{2|E|}\pi_{xy}(t)$$

  This similarity measure focus on only few steps covered by the random walker (hence quasi-local) and not the stationary state compared to other approaches. Random walk based methods suffer from the situation where a random walker moves far away with a certain probability

from the target node whether the target node is closer or not. This is an obvious problem in social networks that show a high clustering index i.e., clustering property of the social networks. This degrades the similarity score between the two nodes and results in low prediction accuracy. One way to counter this problem is that continuously release the walkers at the starting point, which results in a higher similarity between the target node and the nearby nodes. By superposing the contribution of each walker (walkers move independently), SRW is expressed as

$$S^{SRW}(x, y)(t) = \sum_{l=1}^{t} S^{LRW}(l)$$

2.1.4 Some Remarks

Similarity-based approaches mostly focus on the structural properties of the networks to compute the similarity score. ***Local approaches*** consider, in general, neighborhood information (direct neighbors or neighbors of neighbor), which take less time for computation. This is the property that makes the local approaches feasible for massive real-world network datasets. ***Global approaches*** consider the entire structural information of the network; that is why time required to capture this information is more than local and quasi-local approaches. Also, sometimes, entire topological information may not be available at the time of computation, especially in a decentralized environment. So, parallelization over the global approaches may not possible or very complex compared to the local and quasi-local approaches. The performance or prediction accuracy of these approaches (i.e., global approaches) is better compared to local and quasi-local. ***Quasi-local approaches*** extract more structural information than local and somehow less information compared to the global.