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Effective and Efficient Similarity Index for Link Prediction of Complex Networks

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Predictions of missing links of incomplete networks like protein-protein interaction networks or very likely but not yet existent links in evolutionary networks like friendship networks in web society can be considered as a guideline for further experiments or valuable information for web users. In this paper, we introduce a local path index to estimate the likelihood of the existence of a link between two nodes. We propose a network model with controllable density and noise strength in generating links, as well as collect data of six real networks. Extensive numerical simulations on both modeled networks and real networks demonstrated the high effectiveness and efficiency of the local path index compared with two well-known and widely used indices, the *common neighbors* and the *Katz index*. Indeed, the local path index provides competitively accurate predictions as the Katz index while requires much less CPU time and memory space, which is therefore a strong candidate for potential practical applications in data mining of huge-size networks.

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I. INTRODUCTION

Many complex systems can be well described by networks where nodes present individuals or agents, and links denote the relations or interactions between nodes. Complex network is therefore becoming an useful tool in analyzing a wide range of complex systems. Recently, the understanding of structure, evolution and function of networks has attracted much attention from physics community [1, 2, 3, 4, 5]. Another important scientific issue relevant to network analysis, namely the *Information Retrieval* [6, 7], however, received less attention. Originally, Information Retrieval aims at finding material of an unstructured nature that satisfies an information need from large collections [8]. It can be also viewed as dealing with prediction of links between words and documents, and is now further extended to standing for a number of problems on link mining [9]. Actually, link prediction problem is a long-standing challenge in modern information science, and a lot of algorithms have been proposed based on Markov chains and machine learning processes by computer science community [10, 11, 12, 13, 14]. However, their works have not caught up the current progress of the study of complex networks, especially they lack serious consideration of the structural characteristics of networks which may indeed provide useful information and insights for link prediction.

The problem of link prediction aims at estimating the likelihood of the existence of a link between two nodes, based on observed links and the attributes of nodes. It can be categorized into two classes: One is the prediction of missing links in sampling networks, such as the food webs and the world wide webs; the other is the prediction of links that may exist in the future of evolving networks, like the on-line social networks. In addition, the link pre-

diction algorithms (or other algorithms based on similar techniques) can also be applied to solve the link classification problem in partially labeled networks [15, 16], such as the prediction of protein functions [15] and to distinguish the research areas of scientific publications [16].

Up to now, most of the algorithms are designed according to the definition of node similarity. Node similarity can be defined just using the essential attributes of nodes, namely two nodes are considered to be similar if they have many common features [17]. Another group of similarity indices is based solely on the network structure, which is called structural similarity and can be further classified as node-dependent, path-dependent and mixed methods. An introduction and comparison of some similarity indices is presented in Ref. [18] in which the *Common Neighbors* [19], *Jaccard coefficient* [20], *Adamic-Adar Index* [21] and *Preferential Attachment* [22] are classified to be the node-dependent indices, while *Katz Index* [23], *Hitting Time* [24], *Commute Time* [25], *Rooted PageRank* [26], *SimRank* [27] and *Blondel Index* [28] are classified to be the path-dependent indices. Besides, Leicht, Holme and Newman proposed a measure to quantify the node similarity based on the assumption that two nodes are similar if their immediate neighbors in the network are themselves similar [29]. This leads to a self-consistent matrix formulation of similarity that can be evaluated iteratively using the adjacency matrix. This similarity index can also be considered as a candidate for accurate link prediction.

Besides the similarity-based prediction algorithms, some more complicated methods are proposed recently. Clauset, Moore and Newman proposed an algorithm based on the hierarchical network structure [30, 31]. Firstly, they use a hierarchical random graph to statistically fit the real network data. Then the dependence of the lateral-connection probability on the depth of the nodes in the hierarchy can be inferred. Finally, one can predict the missing links of the network according to the

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lateral-connecting probability by ranking them in the descending order. Furthermore, many efforts have been done for designing the recommender systems [32]. Actually, the process of recommending items to a user can be considered as the prediction of missing links in the user-item bipartite network [33]. Especially, physicists have recently proposed some information recommendation algorithms based on physical processes, such as energy diffusion [34, 35, 36] and heat conduction [37]. Although the relevant issue has not been fully explored, it highlights a possibility to improve the accuracy and efficiency of link prediction algorithms by applying classical physics dynamics.

There are many difficulties for the studies of link prediction. One is the sparsity of the target networks [38, 39, 40], which leads to a serious problem that the prior probability of a link is typically quite small, resulting in large difficulties in building statistical models. The other problem is the huge size of real systems that requires highly efficient algorithms. However, the complexity of computational time and memory, being a crucial factor in real applications, has not been systematically investigated. Generally speaking, the accuracy of an algorithm and its computational complexity have positive correlation, namely higher accuracy usually implies higher complexity. Note that, any highly accurate algorithm will become meaningless if the consuming time or memory is unacceptable. Therefore, designing an accurate and fast algorithm is a big challenge, especially for sparse and huge networks.

In this paper, we introduce a so-called *local path index* to characterize the node similarity. Extensive numerical simulations on both modeled networks and real networks demonstrate that this similarity index is simultaneously highly effective (its prediction accuracy is much higher than the *common neighbors*, and competitive with the Katz index) and highly efficient (the time and space required to compute it are much less than those for the Katz index). Especially, when the network is huge, the local path index shows great advantage compared with the Katz index since computing the latter asks for a CPU time scaling as cube of the network size while computing the former requires a linear CPU time as the network size. We therefore think this local path index is a strong candidate for potential practical applications in data mining of huge-size complex networks.

II. METHOD

Considering an unweighted undirected simple network $G(V, E)$, where V is the set of nodes and E is the set of links. The multiple links and self-connections are not allowed. For each pair of nodes, $x, y \in V$, we assign a score, s_{xy}. Since G is undirected, the score is supposed to be symmetry, say $s_{xy} = s_{yx}$. All the nonexistent links are sorted in decreasing order according to their scores, and the links in the top are most likely to exist. In this
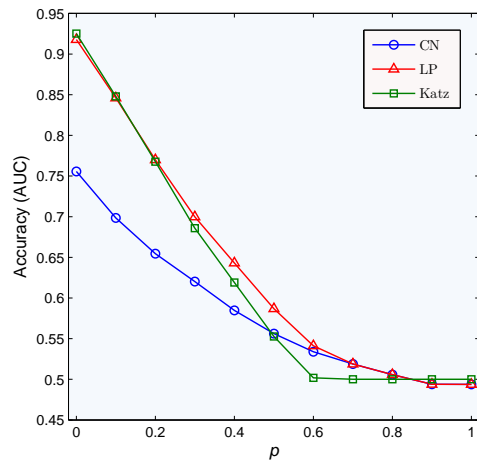

FIG. 1: (Color online) Prediction accuracy vs. the strength of randomness for three similarity indices: CN (circles), LP (triangles) and Katz index (squares). The network size, $N = 1000$, and the degree, $k = 10$, are fixed. Each data point is obtained by averaging over 10 independent realizations. When approaching the purely random case, $p = 1$, the accuracies of CN and LP go below 0.5, which is an artifact of the specific constrain on identical degree. That is, in the purely random case, two unconnected nodes with higher degrees in the training set are of less probability to be connected in the probe set since the total degree is identical for every node, however, they generally have more common neighbors and thus higher similarity.

paper, we adopt the simplest framework, that is, to directly set the similarity as the score, so the higher score means the higher similarity, and vice versa. In some link prediction algorithms, the scores may be not directly related to a certain similarity measurement, but describe the existence likelihood of links [10, 11, 12, 13, 14, 30], and in some other algorithms, scores may be generated by an integration of some similarities of node pairs in the neighborhood of the target links, such as the collaborative filtering method [41].

In this paper, we compare the prediction accuracies and computational complexity of three similarity indices: *Common Neighbors* (CN), *Katz Index* and a newly proposed similarity index, namely *Local Path Index* (LP index or LP for short). Their definitions and relevant motivations are introduced as follows:

(i) *Common Neighbors*, which is also called *structural equivalence* in Ref. [19]. In common sense, two nodes, x and y, are more likely to form a link in the future if they have many common neighbors. For a node x, let $\Gamma(x)$ denote the set of neighbors of x. The simplest measure of the neighborhood overlap is the directed count:

$$s_{xy} = |\Gamma(x) \cap \Gamma(y)|, \qquad (1)$$

where $|Q|$ is the cardinality of the set Q. It is obvious that $s_{xy} = (A^2)_{xy}$, where A is the adjacency matrix, in which $A_{xy} = 1$ if x and y are directly connected and
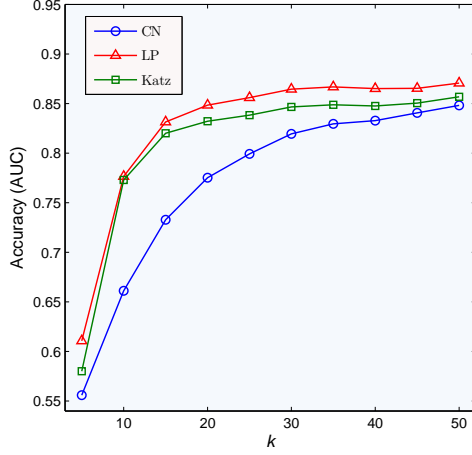
FIG. 2: (Color online) Prediction accuracy vs. network density for three similarity indices: CN (circles), LP (triangles) and Katz index (squares). Since in this model, every node has the same degree, we therefore directly use degree to denote the network density. The network size, $N = 1000$, and the strength of randomness, $p = 0.2$, are fixed. Each data point is obtained by averaging over 10 independent realizations.
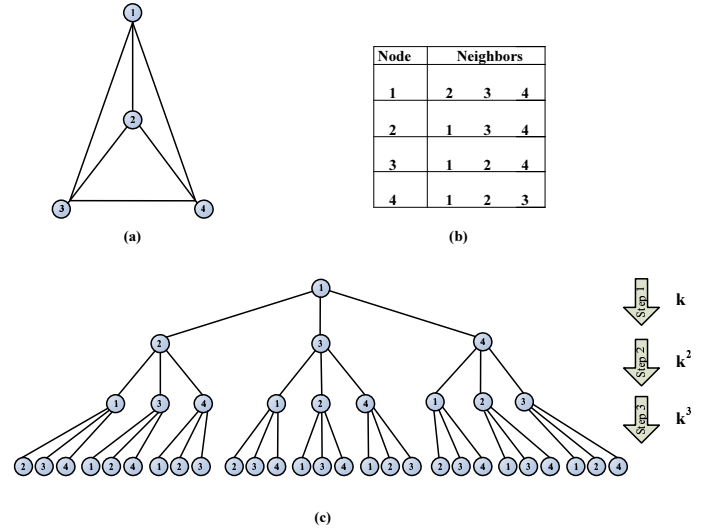

FIG. 3: (Color online) An illustration of time complexity in calculating CN and LP indices. (a) A fully connected network with four nodes as the example. (b) Lists of the neighborhood of each node. (c) Process of how to determine all the similarities relevant to node 1.

$A_{xy} = 0$ otherwise. Note that, $(A^2)_{xy}$ is also the number of different paths with length 2 connecting x and y. Newman [42] used this quantity in the study of collaboration networks, showing the correlation between the number of common neighbors and the probability that two scientists will collaborate in the future. Some more complicated measures, such as *Salton Index* [6], *Jaccard Index* [20], *Sørensen Index* [43] and *Adamic-Adar Index* [21], can also be categorized into CN-based measures. However, recently, extensive empirical analysis has demonstrated that the simplest CN (i.e., Eq. (1)) performs even better than those complicated variants [18, 44]. Therefore, we here select CN as the representative of all CN-based measures. Although CN consumes little time and performs relatively good among many local indices, due to the insufficient information, its accuracy can't catch up with the measures based on global information. One typical example is the *Katz Index* [23].

(ii) *Katz Index.* This measure is based on the ensemble of all paths, which directly sums over the collection of paths and exponentially damped by length to give the short paths more weights. The mathematical expression reads

$$s_{xy} = \sum_{l=1}^{\infty} \beta^l \cdot |paths_{xy}^{<l>}|, \tag{2}$$

where $paths_{xy}^{<l>}$ is the set of all paths with length l connecting x and y, and β is a free parameter controlling the weights of the paths. Obviously, a very small β yields a measure close to CN, because the long paths contribute very little. The S matrix can be written as $(I - \beta A)^{-1} - I$. Note that, β must be lower than the reciprocal of the maximum of the eigenvalues of matrix A to ensure the convergence of Eq. (2).

(iii)*Local Path Index.* To provide a good tradeoff of accuracy and complexity, we here introduce an index that takes consideration of local paths, with wider horizon than CN. It is defined as

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

where S denotes the similarity matrix and ϵ is a free parameter. Clearly, this measure degenerates to CN when $\epsilon = 0$. And if x and y are not directly connected (this is the case we are interested in), $(A^3)_{xy}$ is equal to the number of different paths with length 3 connecting x and y. Although it needs more information than CN, it is still a local measure of relatively lower complexity than global ones.

Choosing these three indices for comparison is because they all can be classified to path-dependent similarities with unified form as $s_{xy} = \sum \beta^l \cdot |paths_{xy}^{<l>}|$, where for CN, $l = 2$; for LP, $l = 2, 3$; and for Katz, $l = 1, 2, 3, \cdots, \infty$. Since we are only interested in the indirectly connected node pairs, Katz Index can be treated as a measure considering $l = 2, 3, \cdots, \infty$. Note that, all these three indices are used to quantify the structural equivalence, with an latent assumption that the link itself indicated a similarity between two endpoints (see, for example, the Leicht-Holme-Newman index [29] and transferring similarity [45]). An issue worth future exploration is whether a certain similarity measure on *regular equivalence* (see Ref. [46] for the mathematical definition of regular equivalence and Ref. [15] for a recent application on the prediction of protein functions) can provide better predictions.

To test the algorithmic accuracy, the observed links, E, is randomly divided into two parts: the training set, E^T, is treated as known information, while the probe set, E^P, is used for testing and no information in the probe set is allowed to be used for prediction. Clearly, $E = E^T \cup E^P$ and $E^T \cap E^P = \varnothing$. In this paper, the training set always contains 90% of links, and the remaining 10% of links constitute the probe set. We use a standard metric, *area under the receiver operating characteristic* (ROC) curve [47], to quantify the accuracy of prediction algorithms. In the present case, this metric can be interpreted as the probability that a randomly chosen missing link (a link in E^P) is given a higher score than a randomly chosen nonexistent link (a link in $U \setminus E$, where U denotes the universal set). In the implementation, among n times of independent comparisons, if there are n' times the missing link having higher score and n'' times the missing link and nonexistent link having the same score, we define the *accuracy* as $\frac{n' + 0.5n''}{n}$. If all the scores are generated from an independent and identical distribution, the accuracy should be about 0.5. Therefore, the degree to which the accuracy exceeds 0.5 indicates how much better the algorithm performs than pure chance. Readers are encouraged to see the Refs. [48, 49] for more information about how to evaluate the accuracy of prediction algorithms.

III. MODEL

In this section, we compare the three similarity indices in modeled networks with controllable density and randomness. Although the real networks have complex structural properties [5], such as the community structure, the mixing pattern and the rich-club phenomenon, as a start point, we only consider a very simple model, and to eliminate the effect of degree heterogeneity, we assume that every node has an identical degree, k. In this model, each node is characterized by a 10-dimensional vector with each element a randomly selected real number in the interval $(-1, 1)$. This vector represents the node's intrinsic features, such as the attributes of an object and the profiles of a person. Two nodes are considered to be similar and thus of high probability to connect to each other if they share many close attributes. Therefore, we define the *intrinsic similarity* between two nodes as the scalar product of the corresponding vectors, namely

$$s_{xy}^I = \vec{f}_x \cdot \vec{f}_y = s_{yx}^I, \qquad (4)$$

where $\vec{f}_x$ is the vector of node x, and the superscript emphasizes that this similarity is intrinsic and can not be observed in the real systems.

Given the network size, N, and the degree of each node, k, this model starts with an empty network but N nodes, that is, each node is of degree zero. At each time step, a node with the smallest degree is randomly selected (generally, there are more than one node having
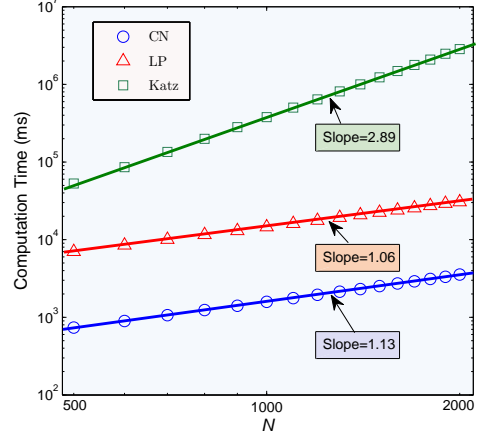

FIG. 4: (Color online) A log-log plot about how the computational time (in microsecond) depends on the network size for three indices, CN (circles), LP (triangles) and Katz (squares). The node degree, $k = 10$, and the strength of randomness, $p = 0.2$, are fixed. Each data point is obtained by averaging over 10 independent realizations. All computations were carried out in a desktop computer with a single Intel (R) Xeon (TM) processor (3.00 GHz) and 2GB EMS memory.

the smallest degree). Among all other nodes whose degrees are smaller than k, this selected node will connect to the most similar node with probability $1 - p$, while a randomly chosen one with probability p. This process will terminate when all nodes are of degree k. The parameter $p \in [0, 1]$ represents the strength of randomness in generating links, which can be understood as noise or irrationality that exists in almost every real system.

In Fig. 1 and Fig. 2, we report the comparison of algorithmic accuracy for those three similarity indices. Data points are corresponding to the optimal values of β (for Katz index) or ϵ (for LP index) subject to the highest accuracies. Clearly, both Katz index and LP index perform remarkable better than the simple CN index. As shown in Fig. 1, when the strength of randomness/noise is weak, LP index gives competitive result as Katz index, while for highly noisy cases, LP index performs even better. Whatever the similarity index, a link prediction algorithm is expected to give higher accuracy for a denser network, which is in accordance with what observed in Fig. 2. In the area with lacking information (i.e., small k) or rich information (i.e., large k), LP index performs slightly better than CN index, while in the middle with typical degree as the real networks, LP index can perform much better than the CN index.

The reason why the CN index performs remarkably poorer than LP index is that the probability that two node pairs are assigned the same similarity by CN is high. That is to say, CN index is less distinguishable, especially in the relatively sparse networks. For example, in the case $N = 1000$, $p = 0$ and $k = 10$, there are about 5×10^5 node pairs, 94.01% of which are as-
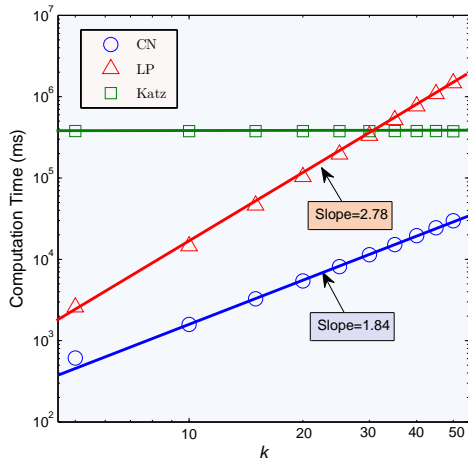
FIG. 5: (Color online) A log-log plot about how the computational time (in microsecond) depends on the node degree for three indices, CN (circles), LP (triangles) and Katz (squares). The network size, $N = 1000$, and the strength of randomness, $p = 0.2$, are fixed. Each data point is obtained by averaging over 10 independent realizations. The hardware environment is the same as what we stated in the caption of Figure 4.

signed zero score, and for all non-zero scores, 79.87% are 1. As shown later, the real cases may be even worse, for instance, in a router-level Internet with 5022 nodes, 99.59% of node pairs are assigned zero score by CN, while for all those non-zero scores, 91.11% of which are assigned score one. The additional information involving the next nearest neighbors introduced by LP index can make the similarities much more distinguishable, thus remarkably enhance the accuracy. Note that, if the maximal number of paths with length three connecting two arbitrary nodes is P_{max}, any ϵ in the interval $(0, \frac{1}{P_{max}})$ will give out exactly the same predictions. Therefore, the prediction accuracy for LP index is not sensitive to the parameter ϵ when ϵ is not so large. Indeed, setting ϵ as a small positive number like 0.01 one can obtain a near optimal accuracy, usually less than 1% smaller than the real optimum (see also Table II, where we compare the optimal AUC values with the values obtained by setting $\epsilon = 0.01$ for the six real networks). In finding the optimal value of β, one can first calculate the maximal eigenvalue of the adjacency matrix, and the optimal β is always smaller than its reciprocal. It is then easy to approach the optimal β. For example, the optimal values of β for relevant data points shown in Fig. 1 and Fig. 2 are all no larger than 0.03.

Next, we discuss the computational complexities of the three similarity indices. In calculating the CN index, for each node, denoted by x, we first search all x's neighbors (called the step 1), and then lay out the neighbors of each of x's neighbors, respectively (called the step 2). If a node y appears n times in the step 2, $s_{xy} = n$. Since the time complexity to traverse the neighborhood of a node

is simply k, the time complexity in calculating CN index is $\mathbb{O}(Nk^2)$. Analogously, for LP index, what we need to do is go one step further (called the step 3) to check all neighbors of each of x's second-order neighbors, respectively. If a node y appears n times in x's second-order neighborhood and m times in x's third-order neighborhood, $s_{xy} = n + \epsilon m$. Therefore, the time complexity in calculating the LP index is $\mathbb{O}(Nk^3)$. An detailed illustration for an example network consisted of four nodes is shown in Fig. 3. For the Katz index, the time complexity is mainly determined by the matrix inversion operator, which is $\mathbb{O}(N^3)$ [50]. In Fig. 4 and Fig. 5, we report the numerical results about computational complexity of the three similarity indices, which are well in accordance with the analysis. Beside the time complexity, memory space is another limitation for algorithmic implementation for huge-size networks. In calculating CN and LP indices, the memory required are of the order $\mathbb{O}(Nk)$, while for the Katz index, it is of the order $\mathbb{O}(N^2)$. In a word, compared with the widely applied CN index and Katz index, the LP index is not only highly effective (i.e., accurate), but also highly efficient (i.e., required relatively less memory and CPU time).

IV. EMPIRICAL ANALYSIS

In this paper, we consider six representative networks drawn from disparate fields: (i) PPI.— A protein-protein interaction network containing 2617 proteins and 11855 interactions [51]. Although this network is not connected (it contains 92 components), most of nodes belong to the giant component, whose size is 2375. (ii) NS.— A network of coauthorships between scientists who are themselves publishing on the topic of networks [52]. This network contains 1589 scientists, and 128 of which are isolated. Here we do not consider those isolated nodes. The connectivity of NS is not good. It is consisted of 268 connected components, and the size of the largest connected component is only 379. (iii) Grid.— An electrical power grid of western US [53], with nodes representing generators, transformers and substations, and links corresponding to the high voltage transmission lines between them. This network contains 4941 nodes and is well connected. (iv) PB.— A network of the US political blogs [54]. The original links are directed, here we treat them as undirected ones. PB has 1224 nodes and the giant component contains 1222 nodes. (v) INT.— The router-level topology of the Internet, which is collected by the *Rocketfuel Project* [55]. INT has 5022 nodes and is well connected, while it is an extremely sparse network with average degree being only 2.49. (vi) USAir.— the network of US air transportation system, which contains 332 airports and 2126 airlines [56]. Note that, all the similarity indices considered here, as well as those well-known indices (except the preferential attachment index) reported in Refs. [18, 44], will give zero score to a pair of nodes located in two disconnected components. Therefore, here we only

TABLE I: The basic topological features of the giant components of the six example networks. N and M are the total numbers of nodes and links, respectively. $\langle k \rangle$ is the average degree of the network. $\langle d \rangle$ is the average shortest distance between node pairs. C and r are clustering coefficient [53] and assortative coefficient [57], respectively. Nodes with degree 1 are excluded from the calculation of clustering coefficient. H is the degree heterogeneity, defined as $H = \frac{\langle k^2 \rangle}{\langle k \rangle^2}$, where $\langle k \rangle$ denotes the average degree.

Networks	N	M	$\langle k \rangle$	$\langle d \rangle$	C	r	H
PPI	2375	11693	9.847	4.59	0.388	0.454	3.476
NS	379	941	4.823	4.93	0.798	-0.082	1.663
Grid	4941	6594	2.669	15.87	0.107	0.003	1.450
PB	1222	16717	27.360	2.51	0.360	-0.221	2.970
INT	5022	6258	2.492	5.99	0.033	-0.138	5.503
USAir	332	2126	12.807	2.46	0.749	-0.208	3.464

consider the giant component, and when preparing the probe set, we also make sure that the remain training set representing a connected network. Actually, each time before removing of a link to the probe set, we first check if this removal will make the training network disconnected. Table 1 summarizes the basic topological features of the giant component of those networks. Brief definitions of the monitored topological measures can be found in the table caption, for more details, please see the review articles [1, 2, 3, 4, 5].

We apply the link prediction algorithm on the six real networks, and the accuracies is shown in Table 2, with those entries corresponding to the highest accuracies being emphasized by black. Clearly, the LP index always performs better than the CN index, especially, for INT, the AUC is sharply improved from 0.653 to 0.943. Except Grid, the LP index gives competitively accurate predictions as the Katz index. Grid is a strongly localized network with most of links being of short geographical lengths, and thus the average topological distance of Grid, $\langle d \rangle = 15.87$, is much larger than the other five example networks. Although Grid is geographically localized, the clustering coefficient is relatively small and it lacks short loops since such loops are redundant and of lower efficiency in the engineering viewpoint. Actually, in Grid, when a link is removed, it is usually hard to find a very short path (like of length 2 or 3) connecting the two endpoints. Therefore, the CN and LP indices, considering only very short paths, fail to re-find the correlation between two directly connected nodes if the link is removed. In addition, we note that the optimal value of ϵ for USAir is negative. In USAir, the large-degree nodes are densely connected and share many common neighbors. Even without the contribution of ϵA^3, the links among large-degree nodes are assigned very high scores, thus the additional item, ϵA^3, changes little of their relative positions. Considering two small local airports, x and y, which are connected to their local central airports,

TABLE II: Accuracies of the three similarity indices, measured by the area under the ROC curve (AUC). Each number is obtained by averaging over 10 independent realizations. The entries corresponding to the highest accuracies are emphasized by black. For LP and Katz indices, the AUC values are corresponding to the optimal parameter. LP* denotes the LP index with a fixed parameter $\epsilon = 0.01$. The very small difference between the optimal case and the case with $\epsilon = 0.01$ suggests that in the real application, one can directly set ϵ as a very small number, instead of finding out its optimum that may cost much time.

Nets	PPI	NS	Grid	PB	INT	USAir
CN	0.915	0.983	0.627	0.924	0.653	0.958
LP	0.970	**0.988**	0.697	**0.941**	0.943	**0.960**^{a}
Katz	**0.972**	**0.988**	**0.952**	0.936	**0.975**	0.956
LP*	0.970	0.988	0.697	0.939	0.941	0.959^b

^{a}For USAir, the optimal value of ϵ is negative. See the explanation in text.
^{b}For USAir, we set $\epsilon = -0.01$.

x' and y'. Of course, many hubs are common neighbors of x' and y', and x' and y' may be directly connected. If the link (x, x') is removed, the similarities between x and other nodes are all zero. Otherwise, the similarities $s_{xy'}$ (by x-x'-hub-y'), s_{xy} (by x-x'-y'-y), and s_{xh} where h represents a hub node (by x-x'-hub-h or x-x'-y'-h) are positive due to the contributions of paths with length 3. There are many links connecting small local airports and local centers, some of which are removed, and the others are kept in the testing set. According to the above discussion, the removed links have lower score than the nonexistent links due to the additional item ϵA^3. In a word, the very specific structure of USAir (the hierarchical organization consisted of hubs, local centers and small local airports) makes the LP index with positive ϵ worse than the simple CN corresponding to $\epsilon = 0$, which is also the reason why negative ϵ performs even better.

Table 3 presents the computation time of the link prediction algorithm on the three similarity indices. Clearly, CN costs the least. Note that, the computational complexity in calculating the LP index is very sensitive to the average degree, while the one in calculating the Katz index is very sensitive to the network size. Therefore, the algorithm using LP index has great superiority for the huge-size and sparse networks compared with the one adopting the Katz index. Take INT as an example, the algorithm using the Katz index runs about one day while the one using the LP index takes less than half minute. Since the real challenge on computational complexity is always relevant to the huge-size real networks, which are mostly very sparse [1], the LP index is much more practical than the Katz index. As a final remark, one may concern that whether to employ higher-order paths is worthwhile in practice, like to define a similarity

TABLE III: Computation time (in microsecond) of the link prediction algorithm on the three similarity indices of the six example networks. The hardware environment is the same as what we stated in the caption of Figure 4.

Nets	PPI	NS	Grid	PB	INT	USAir
CN	10690	253	5161	31112	6711	2208
LP	543589	1638	11344	2873403	27641	93892
Katz	8073316	27479	69961063	1051528	72550935	17603

TABLE IV: Comparison of the accuracies of the original local path index ($n = 3$, see Eq. (3)) and the higher-order local path index ($n = 4$, see Eq. (5)), measured by the area under the ROC curve (AUC). Each number is obtained by averaging over 10 independent realizations. The AUC values reported here are corresponding to the optimal parameter. The average shortest distance and the improvement (%) by considering higher-order paths are also laid out in this Table, and all the six real networks are ordered by their shortest average distances.

Nets	USAir	PB	PPI	NS	INT	Grid
$\langle d \rangle$	2.46	2.51	4.59	4.93	5.99	15.87
$n = 3$	0.960	0.941	0.970	0.988	0.943	0.697
$n = 4$	0.959	0.937	0.973	0.989	0.959	0.759
Improvement	-0.104	-0.425	0.309	0.101	1.70	8.90

index in the form

$$S = A^2 + \epsilon A^3 + \epsilon^2 A^4. \tag{5}$$

We give a brief discussion on this issue in *Appendix A*.

V. CONCLUSION AND DISCUSSION

In this paper, we introduced a local path index to estimate the likelihood of the existence of a link between two nodes. We propose a network model with controllable density and noise strength in generating links. The LP index provides slightly more accurate predictions than the Katz index, especially in the highly noisy cases. We further use six representative real networks to test the three similarity indices, showing that the LP index can provide competitively accurate predictions as the Katz index. Compared with the Katz index, the LP index requires much less CPU time and memory space, and is therefore more practical. Ignored the degree-degree correlation, the time complexities in calculating LP index and Katz index are $\mathbb{O}(N\langle k \rangle^3)$ and $\mathbb{O}(N^3)$, respectively. Hence for the huge (i.e., very large N) and sparse (i.e., very small average degree $\langle k \rangle$) networks, the advantage of the LP index is striking.

Highly accurate predictions are significant in practice. For example, many biological networks, such as protein-protein interaction networks, metabolic networks and food webs, the discovery of links/interactions costs much in the laboratory or the field. Instead of blindly checking all possible interactions, to predict in advance based on the interactions known already and focus on those links most likely to exist can sharply reduce the experimental costs if the predictions are accurate enough [30, 31]. For some others like the friendship networks in web society, very likely but not yet existent links can be suggested to the relevant users as recommendations of promising friendships. These recommendations can help users finding new friends and thus enhance their loyalties to the web sites. Besides the practical significance, it is worthwhile to emphasize that the study of link prediction can also provide some theoretical insights about the structural organization. For example, in this paper, the unexpected results on Grid and USAir give evidence to some specific structural properties that are not straightforwardly notable. Another example is that the preferential attachment index usually gives poor predictions, and when it works relatively good, it implies that the testing network has strong rich-club phenomenon [41, 44]. Although the focus of this paper is not to investigate the relations between suitable similarity indices and network structures, we believe it is an interesting issue worth further studies.

In this paper, we only considered the link prediction problem in static networks. However, many real networks are evolving all the time, and the links created in different times should be assigned different weights in principle. This time-involved link prediction problem is rarely investigated and of course worths a serious study in the future [58]. Most of previous studies in relevant direction only test the algorithmic accuracy in real networks. Here we argue that the modeled networks should be used, because one can control some meaningful parameters in a model, which can not be directly observed in the real networks (e.g., the strength of noise or irrationality). We hope the proposed model could become a prototype in testing the accuracy of link prediction algorithms, however, it is currently too simple and to make it closer to the real networks, such as introducing controllable degree heterogeneity and degree-degree correlation, is very helpful.

This paper concerns only the simple networks, however, the local path index can be easily extended to more complicated cases. For example, we can handle the directed networks by replacing the original adjacency matrix, A, by an asymmetry one, the weighted networks by replacing A by a weighted matrix, and the networks with self connections by assigning nonzero diagonal elements. Actually, Murate and Moriyasu [59] have already investigated the link prediction problem in weighted networks, however, the credibility of their work is recently challenged by the empirical evidence that the weak ties may play a more important role in link prediction than the strong ties [60].

Acknowledgments

APPENDIX A: SIMILARITY INDEX INVOLVING HIGHER-ORDER PATHS

A straightforward method to extend the local path index is to consider the higher-order paths. Such a similarity index is of the form

$$S = A^2 + \epsilon A^3 + \epsilon^2 A^4 + \cdots + \epsilon^{n-2} A^n, \quad (A1)$$

where $n > 2$ is the maximal order. As shown in Fig. 3, the computational complexity in an uncorrelated network is $\mathbb{O}(N \langle k \rangle^n)$, which grows fast with the increasing of n and will exceed the complexity for calculating the Katz index for large n. We therefore concentrate on the case of $n = 4$, equivalent to the one shown in Eq. (5).

As shown in Table IV, the improvements of accuracy are not much except for the power grid. Sometimes, to introduce higher-order relations will even decrease the accuracy, like for USAir and PB. The results are very sensitive to the average shortest distances of networks. If $\langle d \rangle$ is very short, to consider paths with length three seems enough, and the addition item, $\epsilon^2 A^4$, will make little effort (e.g., PPI, NS and INT) or even negative effort (e.g., USAir and PB). Only when the network is of long average shortest distance, to consider higher-order relations may be cost-effective. Since most real networks exhibit strongly small-world effect [1, 2, 3, 4, 5], a local path index taking into account paths with length no more than three may be practically sufficient.

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