Node similarity distribution of complex networks and its application in link prediction

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Over the years, quantifying similarity of nodes has been a hot topic, yet distributions of node similarity for complex networks remain unknown. In this paper, we consider a typical measure called common neighbor based similarity (CNS), which literally characterizes similarity of nodes based on the number of common neighbors (CN) they share in the network. By means of the generating function, we propose a general framework to calculate the distributions of CNS for various complex networks, including the Erdős-Rényi (ER), regular ring lattice, small-world network model, scale-free network model, and real-world networks. In particular, we show that for the ER network, the CNS of node sets with an arbitrary size obeys the Poisson distribution. We also connect the node similarity distribution to the link prediction problem. An interesting finding is that the prediction performance depends solely on the CNS distributions of connected node pairs and unconnected ones. The farther these two CNS distributions are apart, the better the prediction performance is. With these two CNS distributions, we further derive theoretical solutions with respect to two key metrics of prediction performance: i) Precision and ii) area under the receiver operating characteristic curve (AUC), which significantly reduce the evaluation cost of link prediction.

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I. INTRODUCTION

Due to the increasingly available data from various complex systems and the advanced computing and inference techniques, great progress has been achieved in understanding the common properties of complex networks \(^1\)\(^2\). Empirical studies have demonstrated that plenty of real-world networks have properties such as high clustering \(^3\), ultra-short average path length \(^3\)\(^4\), and power-law node degree distribution \(^5\)\(^6\), spatiality \(^7\), temporality \(^8\)\(^9\), multilayer \(^10\), interdependency \(^11\), etc. The revealing of the underlying properties of complex networks enables us to have a glance at the evolutionary principles of complex systems and build elegant models of complex networks \(^2\).

Node similarity is one of those network properties affecting the evolution of complex networks \(^12\). It quantifies the degree of similarity or proximity among network nodes based on the intrinsic node properties or the network topology information \(^13\). The definition of node similarity based on node properties can vary among networks even in the same domain \(^14\). For instance, in social networks, node similarity can be defined based on any one or combination of many node properties that may include race, religion, sex, job, etc. Moreover, the availability and reliability of various node property data can usually not be guaranteed. Consequently, the graph-based definition of node similarity has become more and more popular in recent years, since it is not domain-specific and does not require node property information. One of the significant findings \(^15\) in this direction is that node similarity can be quantified based on the neighbors of nodes. If two nodes have many common neighbors, they are usually similar, whereas if they have few common neighbors, they are generally not similar, which has been observed in many types of networks \(^13\). Many other graph-based definitions further considered the neighbor of neighbor \(^16\), the paths between nodes \(^17\), the network community information \(^18\)\(^19\), etc. Note that the advantage of graph-based definition also lies in the relatively low computational complexity.

Node similarity has wide applications in many network-related problems. Link prediction \(^13\) is one of these problems, which is actually grounded in the empirical observation that similar entities are likely to interact with each other. The task of link prediction is to estimate the link formation probability, which is often proportional to the node similarity score, in order to make predictions on the missing or future links of the current network. To achieve good prediction accuracy, tools from the areas of complex networks \(^15\) and machine learning \(^20\) have been employed to design link prediction methods. The graph-based link prediction methods seem more appealing than the other methods, since they are more general and computational cost saving, while with competitive prediction accuracy.

Based on how much the network topological information is used, the graph-based link prediction methods can be divided into three categories: the local, global and quasi-local methods. The local methods include the indices such as Common Neighbor (CN) \(^15\), Adamic-Adar (AA) \(^21\), Resource Allocation (RA) \(^22\), Preferential Attachment (PA) \(^6\), and many derivatives \(^20\). These local methods use only the neighbor-based topological information, and show good enough accuracy with relatively low computational cost, which is significant for large and dynamic networks. The limitation of this type of methods is that they neglect the possibility of link for-
II. COMMON NEIGHBOR BASED SIMILARITY DISTRIBUTION

Let $G(V, E)$ be a graph, where $V$ is the node set and $E$ is the link set. The number of nodes in $V$ is $N = |V|$. Let $A$ be the adjacent matrix of $G$, in which $A_{ij} = 1$ if node $i$ and $j$ are connected with a link; otherwise, $A_{ij} = 0$. We have $\sum_{j \neq i} A_{ij} = N(k)$, where $(k)$ is the average node degree. Let $V_q = \{v_1, v_2, \ldots, v_q\}$ be a node set, where $v_i \in V$ and $q \in [1, N]$ is the size of $V_q$. Note that the node order is irrelevant in the node set. The CNS of $V_q$ can be calculated as

$$\Theta(V_q) = \sum_{t \in V - V_q} \delta(A_{v_1t} + A_{v_2t} + \cdots + A_{v_qt} - q),$$

where $\delta(x) = 1$ if $x = 0$; otherwise, $\delta(x) = 0$. Specially, we have $\Theta(\{v_i\}) = \kappa_{vi}$, where $\kappa_{vi}$ is the degree of node $v_i$, and $\Theta(V_N) = 0$. Given an arbitrary node pair $(i, j)$, the probability that the two nodes are connected is denoted by $\Gamma_{ij}$, where $\Gamma_{ij} = \Gamma_{ji}$. Then, the probability that all nodes in $V_q$ are connected with node $t$ is

$$\Gamma_{V_q \rightarrow t} = \prod_{v_i \in V_q} \Gamma_{v_it},$$

and thus the probability that not all the nodes in $V_q$ are connected with node $t$ is $\Gamma_{V_q \rightarrow t} = 1 - \Gamma_{V_q \rightarrow t}$. With these two probabilities, we further obtain the generating function \[^{[51]}\] of the probability distribution, $P[\Theta(V_q) = w]$, for the event that the node set $V_q$ has $w$ common neighbor nodes, which is

$$G_{\Theta(V_q)}(x) = \prod_{t \in V - V_q} (\Gamma_{V_q \rightarrow t} + \Gamma_{V_q \rightarrow t}x) = \prod_{t \in V - V_q} (1 - \prod_{v_i \in V_q} \Gamma_{v_it} + x \prod_{v_i \in V_q} \Gamma_{v_it}).$$

Then, according to the property of generating function, we have

$$P[\Theta(V_q) = w] = \frac{G_{\Theta(V_q)}(0)}{w!}.$$  \(^{(4)}\)

Furthermore, by definition of probability distribution, the CNS distribution of node sets of size $q \geq 1$ is given by

$$P(\Theta = w) = \frac{q! \sum_{V_q \subseteq V} P[\Theta(V_q) = w]}{N(N-1) \cdots (N-q+1)} = \frac{q! \sum_{V_q \subseteq V} G_{\Theta(V_q)}(0)}{w!N(N-1) \cdots (N-q+1)}. \quad \text{\((5)\)}$$

In the above, we present a general CNS distribution calculation framework for node sets of an arbitrary size. Note that the node degree is a special case of CNS, when the node set contains only one node, and the node degree distribution can be obtained through Eqs. \((2)-(5)\).

In the applications, we usually consider the CNS of the node sets with a specific size. For example, in the link prediction problem, the CNS of only two nodes are considered. We can set $q = 2$ in Eq. \((5)\) to obtain the corresponding CNS distribution of all the node sets containing two nodes, denoted as $P_a(\Theta^2 = w)$. We can also calculate the CNS of only connected node pairs $P_c(\Theta^2 = w)$, or disconnected node pairs $P_d(\Theta^2 = w)$. The three CNS distributions satisfy

$$\left\{ \begin{array}{l}
P_a(\Theta^2 = w) = P_c(\Theta^2 = w) \chi_c + P_d(\Theta^2 = w) \chi_d, \\
\chi_c = \frac{\chi(\theta)}{N(\theta)} = 1 - \chi_d.
\end{array} \right. \quad \text{\((6)\)}$$

In the following, we explore the CNS distributions of different types of complex networks, including various modeled networks and real-world networks.
all the nodes are located on a ring. Node
connected, (b) disconnected, and (c) all node pairs.

FIG. 1. CNS distributions of regular networks for (a) con-

II.1. Regular ring lattice

We consider a regular ring lattice (RRL) 1, in which
all the nodes are located on a ring. Node i (i = 1, 2, . . . , \(N\)) has m neighbors in each of the two sides. The average node degree \(<k>\) is 2m. For an arbitrary node pair (i, j) in the RRL, the connection probability is \(\Gamma_{ij} = \delta(|i - j| \leq m).\) Then, through Eqs. (2)-(5), we obtain the CNS distribution of regular networks.

Figure 1 shows the result of CNS distribution of node pairs (node sets of size \(q = 2\)) for regular networks with \(N = 1,000\) and \(m = 50\), from which we observe that the simulation and analytical results are well matched. In FIG. 1(a), for connected node pairs, CNS is bounded in \([m - 1, 2m - 2]\), and \(P_c(w) = 1/m.\) In FIG. 1(b), for disconnected node pairs, \(P_d(0) = \frac{N - 1 - 4m}{N - 1 - 2m} \approx 1\), while for a wide range of CNS, \(P_d(w) = 2/(N - 1 - 2m) \approx 0, w = 1, 2, \ldots, m.\) Since \(\chi_c = 2m/(N - 1) \approx 0,\) the CNS distribution of all node pairs is dominated by the disconnected node pairs as shown in FIG. 1(c).

II.2. The ER network model

We assume an Erdös-Rényi (ER) random network 32 of \(N\) nodes. The connection probability of any node pair in the ER network is \(p^E = \frac{2n}{N(N-1)},\) where \(n\) is the expected number of links. The average node degree is \(<k> = 2n/N \approx p^E N.\) According to the definition of ER model, we know that all the nodes are equivalent. For an arbitrary node pair (i, j), the connection probability

is \(\Gamma_{ij} = \frac{<k>}{N-1}.\) By substituting this into Eq. (3), we get

\[
G_{\Theta(V_q)}(x) = \prod_{t \in V - V_q} (1 - \prod_{v_i \in V_q} \prod_{v_j \in V_q} \Gamma_{v_i t})
\]

\[
= \left[ 1 - \frac{<k>^q}{(N-1)^q} + \frac{<k>^q x}{(N-1)^q} \right]^{N-q}.
\]

Combining Eq. (4) and Eq. (7), we have

\[
P(\Theta(V_q) = w) = G_{\Theta(V_q)}^{(w)}(0)
\]

\[
= \frac{w!}{(N - q)^w \left( \frac{<k>^q}{(N-1)^q} \right)^w}
\]

\[
\times \left( 1 - \frac{<k>^q}{(N-1)^q} \right)^{N-q-w}.
\]

Plugging Eq. (8) into Eq. (5) and also assuming \(N \to \infty,\) we obtain

\[
P(\Theta = w) = \left( \frac{N - q}{w} \right)^w \left( \frac{<k>^q}{(N-1)^q} \right)^w
\]

\[
\times \left( 1 - \frac{<k>^q}{(N-1)^q} \right)^{N-q-w} \approx e^{-\lambda \frac{w}{w!}},
\]

where \(\lambda = <k>^q N^{1-q}.\) Eq. 9 indicates that the CNS of node sets of size \(q\) follows the Poisson distribution in ER random networks, where the mean and variance are both \(<k>^q N^{1-q}.\) Thus, the CNS distribution becomes more uneven when the average node degree (network size or node set size) increases (decreases).

Figure 2 depicts the CNS distribution of ER networks with \(N = 10,000\) and \(<k> = 500\) for node pairs. The simulation results well match the analytical results. An alternative derivation leads to the same results, which are presented in the supplemental material 32.

II.3. The small-world network model

We derive the CNS distribution of the Watts and Strogatz (WS) model 3, which is one of the most typical
models that generate small-world networks. In the WS model, the initial network is a regular ring lattice of $N$ nodes. Each node is connected to its $2m$ nearest neighbors. Then, each link is randomly rewired with probability $p^{WS}$. Multiple links and self-connections are not allowed. Thus, the expected number of rewired links is $p^{WS}mN$. The average node degree equals $2m$, which is unchanged before and after the random rewiring process. Then, the connection probability of a node pair $(i, j)$ is

$$\Gamma_{ij} = \delta(|i-j| \leq m)(1-p^{WS}) + \frac{2p^{WS}mN\delta(|i-j| > m)}{N(N-1)-2mN}. \quad (10)$$

Substituting Eq. (10) to Eqs. (2)-(5), we obtain the CNS distribution for the WS model.

Figure 3 presents the CNS distribution of the WS small-world networks with $N = 1,000$, $m = 25$, and $p^{WS} = 0.4$ for node pairs, from which we observe that the simulation results are consistent with the analytical results. In Fig. 3(a), for the connected node pairs, the CNS shows a clear bimodal distribution. Shown differently in Fig. 3(b) and (c), for the disconnected node pairs and all the node pairs, the CNS distributions are close to the Possion distribution with a long tail. The result of the Newman and Watts (NW) small-world networks is given in the supplemental material.

II.4. The unified ring model

The RRL is a very basic model. By deleting, adding, and rewiring links among nodes with probability, this model can evolve into many other models, e.g., the WS, NW and ER models. Particularly, deleting each link from a RRL with probability $p^M$ yields a new model, called modified ring lattice (MRL). The generated network of the MRL model has $(1-p^M)mN$ links with average node degree $(k) = 2(1-p^M)m$. The connection probability between an arbitrary node pair $(i, j)$ in the MRL model is $\Gamma_{ij} = \delta(|i-j| \leq m)(1-p^M)$.

We further provide a general model, called unified ring model, to unify the above mentioned ring based models, which include the RRL, MRL, WS, NW, and ER models. In the unified model, there is initially an empty ring (without links) of $N$ nodes located with even interval. The nodes are labeled clockwise from 1 to $N$ with a designated starting node. Then, we connect each node pair with probability $\eta$ if the corresponding node label distance is no greater than $m$, otherwise with probability $\alpha$. The connection probability of a node pair $(i, j)$ in the unified ring model can be expressed as

$$\Gamma_{ij} = \delta(|i-j| \leq m)\eta + \delta(|i-j| > m)\alpha. \quad (11)$$

Substituting Eq. (11) to Eqs. (2)-(5), we obtain the CNS distribution of node sets of an arbitrary size for the unified ring model.

We specially consider a node set of two nodes, $V_2 = \{i, j\}$, in the unified ring model. For the node pair $(i, j)$, any other node $t$ should be in one of the three types depending on the label distance $|t-i|$ and $|t-j|$.

- The first type satisfies $|t-i| \leq m$ and $|t-j| \leq m$. We assume that the number of this type of nodes is $s_{ij}$, and we have:

$$s_{ij} = \begin{cases} 2m - 1 - |i-j|, & \text{if } 0 < |i-j| \leq m - 1 \\ 2m - |i-j|, & \text{if } m \leq |i-j| \leq 2m \\ 0, & \text{otherwise} \end{cases} \quad (12)$$

For any node $t$ of the first type, $\Gamma_{(i,j)\rightarrow t} = \eta^2$.

- The second type satisfies either of the following conditions: i) $|t-i| \leq m$ and $|t-j| > m$ and ii) $|t-i| > m$ and $|t-j| \leq m$ with $\Gamma_{(i,j)\rightarrow t} = \eta\alpha$, and the number of this type of nodes is $4m - 2s_{ij}$.

- The last type satisfies $|t-i| > m$ and $|t-j| > m$ with $\Gamma_{(i,j)\rightarrow t} = \alpha^2$, and the number of this type of nodes is $N - 2 - 4m + s_{ij}$.

Then, by Eq. (3) we obtain the generating function of the CNS distribution of node set $\{i, j\}$ for the unified model,

$$G_{ij}(x) = [1 - \eta^2 + \eta^2x]^{s_{ij}}(1 - \eta\alpha + \eta\alpha x)^{4m - 2s_{ij}} \times (1 - \alpha^2 + \alpha^2 x)^{N - 2 - 4m + s_{ij}}. \quad (13)$$

The ring based models, including the RRL, MRL, ER, WS, and NW models, are special cases of the unified ring model. The corresponding $\eta$, $\alpha$, and generating function for each of these models are summarized in Table 1, from which we can clearly see the relation among models. For example, for the WS model, if $(1 - \eta\alpha + \eta\alpha x)^{4m - 2s_{ij}} \rightarrow 1$, then $G_{ij}(x) \rightarrow (1 - \eta^2 + \eta^2x)^{s_{ij}}(1 - \alpha^2 + \alpha^2 x)^{N - 2 - 4m + s_{ij}}$, which in form is the product of the generating functions of the MRL and ER models. In other words, the CNS...
distribution of the WS model can be the convolution of the CNS distributions of the MRL and ER models with proper parameter settings,
\[ P_{ij}^{WS}(w) \approx P_{ij}^{MRL}(w) \ast P_{ij}^{ER}(w), \quad (14) \]
where \( \ast \) represents convolution. Note that for the ER model, we have \( P_{ij}^{ER}(w) = P_{ij}^{ER}(w) \). Similarly, for the NW model, if \( (1 - \alpha + \alpha x)^{4m-2s_{ij}} \rightarrow 1 \), then \( G_{ij}(x) \rightarrow x^{s_{ij}}(1 - \alpha^2 + \alpha^2 x)^N - s_{ij} - 4m \), which in form is the product of the generating functions of the RRL and ER models. In other words, the CNS distribution of the NW model can be the convolution of the CNS distributions of the RRL and ER models with proper parameter settings,
\[ P_{ij}^{NW}(w) \approx P_{ij}^{RRL}(w) \ast P_{ij}^{ER}(w). \quad (15) \]

II.5. The scale-free network model

We consider the Barabási-Albert (BA) model [2], which is one of the most typical models for generating scale-free networks. In the BA model, initially there are \( m_0 \) fully connected nodes labeled as 1, 2, \ldots, \( m_0 \). For each time a new node, labeled from \( m_0 + 1 \), is added into the network with \( m \leq m_0 \) links connecting the existing nodes until the total number of nodes reaches \( N \). The probability that a node is selected for each link is proportional to its degree. For instance, the probability that the new node \( i \) selects node \( j \in [1, i - 1] \) is \( p_j(i) = k_j(i) / \sum_{i=1}^{i-1} k_i(i) \), where \( k_j(i) \) is the degree of node \( j \) when node \( i \) is just added into the network. For the generated BA network, the average node degree is \( (k) = 2m \), and the node degree distribution obeys the power law with exponent three. When constructing the links of a new node, the overall times of node selection should be no less than \( m \) because of duplication. Assume that for node \( i \) the average node selection times in the link construction process is \( T_i \). Then, the overall connection probability of nodes \( i \) and \( j \) with \( j < i \) satisfies the following equations:
\[ \begin{align*}
\Gamma_{ij} &= 1 - (1 - p_j(i))^T_i, \\
\sum_{j < i} \Gamma_{ij} &= m.
\end{align*} \quad (16) \]
By Eq. (16) we obtain \( \Gamma_{ij} \) and thus \( \Gamma_{ji} \) (since they are equal). Then, we update the node degree with \( k_j(i+1) = k_j(i) + \Gamma_{ji} \). After obtaining the connection probabilities of all node pairs, we substitute them into Eqs. (2)-(5) to calculate the CNS distribution of the BA model.

Figure 4 shows the CNS distribution of the BA scale-free networks with \( N = 1,000 \), and \( (k) = 50 \) for node pairs, where the simulation results and analytical results are consistent with each other. Clearly, all the three CNS distributions, \( P_c \), \( P_d \), and \( P_a \), approximately follow the power-law distributions with long tails, the power-law parameters of which are given in the corresponding subfigures. The results of the static model (ST) [3] and the configuration model [31] are provided in the supplemental material [33].

II.6. Real-world networks

We also consider the real-world networks and select some typical network data downloaded from the Stanford Network Analysis Platform (SNAP) [35] and the Koblenz Network Collection (KONECT) [36]. All the network data are processed by ignoring the directions of the links and deleting the multiple and self connections. The CNS distributions of these real-world networks for all the connected node pairs are given in FIG. 5. From FIG. 5, we see that for most of the real-world networks
the CNS distributions of connected node pairs approximately follow the power law with various power-law parameters. Also, for some specific real-world networks, the CNS of connected node pairs follows the exponential law.

III. APPLICATION

Link prediction is a basic problem in both network science and information science with applications across many domains. The structural similarity-based link prediction methods become more and more popular because of their universality and relatively low computational cost. The idea behind this type of link prediction methods is that the connection probability of two nodes is highly correlated with the degree of their structural similarity. Usually, each unconnected node pair is assigned a similarity score according to the given similarity index, and then all the unconnected node pairs are ranked in decreasing order based on their similarity scores. The node pairs located more ahead in the ranking are supposed to have larger possibility to be presented in the set of missing or future links. Among all the structural similarity-based link prediction methods, the CN (Common Neighbor) index is the most fundamental one, which quantifies the similarity of a node pair as the number of common neighbors the node pair shares. The CN index is taken as a standard reference of many more advanced link prediction methods, which consider more topological information to better quantify the node similarity.

III.1. Prediction accuracy evaluation

To evaluate the prediction accuracy of a certain similarity index, we usually divide the network into a test set and a training set. The former consists of the randomly extracted links, which are usually 10 or 20 percent of all links, whereas the latter is made up of the remaining links. The network structure of the training set is the whole information that are used for link prediction. Based on this network structure, we calculate the similarity scores of all unconnected node pairs. With these similarity scores, we can further assess the given similarity index according to the mainstream metrics of prediction accuracy, such as the AUC and Precision.

Let us further split the unconnected node pairs in the network of the training set into two sets. The first set contains the node pairs whose links are moved into the test set. The second set consists of the node pairs that are not connected in the original network. Each time we compare the similarity scores of a randomly selected node pair from the first set and another randomly selected one from the second set. We do this comparison totally $n$ times, and if there are $n'$ times that the former is larger and $n''$ times that they are equal, we have

$$AUC = \frac{n' + 0.5n''}{n}.$$  \hspace{1cm} (17)

From this definition, we infer that a valid link prediction should obtain an AUC value larger than 0.5. Besides the AUC, another typical measurement of prediction accuracy is Precision. To calculate the Precision, we usually rank the unconnected node pairs (union of the first set and second set) with decreasing order of similarity scores. If $L'$ out of the top-$L$ node pairs belong to the first set, we have

$$\text{Precision} = \frac{L'}{L},$$  \hspace{1cm} (18)

where $L$ is usually set to be equal to the size of the test set.

III.2. Theoretical solutions of AUC and Precision

We show that the prediction accuracy of the CN index is determined by the CNS distributions of the connected and unconnected node pairs, i.e., $P_c$ and $P_d$, which can further be extended to the other similarity-based link prediction methods. Statistically, randomly removing a small percent of links does not significantly affect the CNS distribution of the network. Therefore, we assume that for the original network and the network of the training set, the CNS distributions of connected and unconnected node pairs are approximately the same, which is the key precondition of the following calculation. Assuming that the number of links in the test set is $\epsilon N(k)/2$, $0 < \epsilon < 1$. Then, the AUC can be calculated as

$$AUC = \sum_{x=0}^{N-2} P_c(w=x)[P_d(w<x) + \frac{P_d(w=x)}{2}].$$ \hspace{1cm} (19)
Moreover, we rank all the unconnected node pairs in the network of the training set (or in the union of the first set and second set defined in the above) with decreasing order of CNS scores, and then consider the top-$L$ node pairs. Let us denote the number of unconnected node pairs with CNS scores no less than $x$, which belong to the first set by $\Phi_c(x)$, the second set by $\Phi_d(x)$ and the whole training set by $\Phi(x)$. Then, we have

\[
\begin{align*}
\Phi_c(x) &= \sum_{w=x}^{N-2} \frac{N(k)}{N(N-1)(k)} P_c(w), \\
\Phi_d(x) &= \sum_{w=x}^{N-2} \frac{N(k)}{N(N-1)(k)} P_d(w), \\
\Phi(x) &= \Phi_c(x) + \Phi_d(x).
\end{align*}
\]

We obtain the CNS score of the $L$-th node pair, $x_L$, by solving the following inequation:

\[
\Phi(x + 1) \geq L > \Phi(x).
\]

Then, the Precision is calculated as

\[
\text{Precision} = \frac{\frac{N(k)}{N(N-1)(k)} P_c(x_L) | L - \Phi(x_L + 1)|}{\frac{N(k)}{N(N-1)(k)} P_d(x_L)}.
\]

Loosely, we have

\[
\text{Precision} \approx \frac{\Phi_c(x)}{\Phi(x)}
\]

Through the above calculation, we obtain the theoretical solutions of the AUC and Precision. The advantage of this calculation framework is that we do not need to consider the division of the training and test sets, and therefore avoid the related computational cost.

Here we only take the CN index as an example to present the theoretical calculation of the AUC and Precision. The calculation framework is also applicable to the other similarity-based link prediction methods. Note that for the other similarity indices, the CNS distribution should be replaced by the corresponding similarity distributions in the calculation.

### III.3. Simulation results

To further validate our theoretical solutions of AUC and Precision, we conduct the link prediction task in three real-world networks [67]. The self-connections and multiple links are deleted from the network data. Some typical similarity indices (see Appendix) are used as the examples including the local indices (CN, RA and AA), quasi-local index (LP) and global index (Katz). In the experiment, we do totally 100 times of test set and training set division according to the 10/90 rule. When calculating the AUC, the comparison times are $n = 10^4$. For the Precision, $L$ is equal to the size of the test set. The theoretical results are calculated by using Eqs. (19) and (22). For each index, we show both the experimental and theoretical results of AUC and Precision in Table 2, from which we observe that the experimental and theoretical results match well.

**FIG. 6.** CNS distributions of the connected (orange) and unconnected (green) node pairs in three real-world networks. $\xi_c$ and $\xi_d$ are the medians of the corresponding distributions.

In fact, we can even get some insight of the prediction accuracy from the similarity distributions of connected and unconnected node pairs without calculating the AUC and Precision. Let us again take the CN index as an example. In Fig. 6, for all the three real-world networks, the curves of $P_c$ are overall on the right of the curves of $P_d$. This confirms the common assumption of link prediction, that is, node pairs with more common neighbors are more prone to be connected. Furthermore, the prediction accuracy depends on the distance of the similarity distributions of connected and unconnected node pairs, which can be indicated by the distance of their medians shown in Fig. 6. The farther the two distributions are apart, the better the prediction performance will be. This conclusion is obtained by combining the results of Table 2 and Fig. 6, and can also be inferred from Eq. (19).

### IV. CONCLUSION

In summary, we discuss the node similarity distribution of complex networks with applications to the link prediction problem. Specifically, by utilizing the generating function, we develop a general framework to calculate the distribution of common neighbor based similarity (CNS) for node sets with an arbitrary cardinality. Then, we explore the CNS distributions of various complex network models and real-world networks. We propose an unified ring model to unify the RRL, WS, NW, and ER models. Through the unified model, we can obtain the relationship among these models in terms of CNS distribution.

Particularly, we discover that for the ER random networks the CNS of node sets of an arbitrary size follows the Poisson distribution. For the small-world network models, the CNS of connected node pairs follows the bi-modal distribution, while the CNS of the disconnected or all node pairs approximately follows the Poisson distribution with a long tail. For the scale-free network models, the CNS distributions of connected, disconnected and all node pairs approximate a power law with a long tail. We also find through empirical experiments that for most real-world networks, the CNS of connected node pairs approximately follows the power-law distribution, whereas for some specific real-world networks, it nearly obeys the exponential distribution.

In the application aspect, we find that the performance of similarity-based link prediction is essentially deter-
Table II. Link prediction performance of three real-world networks.

|                  | Jazz (nodes: 198, links: 5484) |                        |                        |                        |                  |
|------------------|--------------------------------|------------------------|------------------------|------------------------|------------------|
|                  | CN                             | RA                     | AA                     | LP                     | Katz             |
| Performance      |                                 |                        |                        |                        |                  |
| Experimental AUC | 0.954                          | 0.973                  | 0.963                  | 0.948                  | 0.940            |
| Theoretical AUC  | 0.958                          | 0.974                  | 0.965                  | 0.950                  | 0.947            |
| Experimental Precision | 0.508                  | 0.555                  | 0.520                  | 0.501                  | 0.443            |
| Theoretical Precision | 0.523                  | 0.551                  | 0.536                  | 0.478                  | 0.464            |

|                  | Usair (nodes: 1532, links: 2126) |                        |                        |                        |                  |
| Performance      |                                 |                        |                        |                        |                  |
| Experimental AUC | 0.934                          | 0.954                  | 0.945                  | 0.931                  | 0.919            |
| Theoretical AUC  | 0.941                          | 0.960                  | 0.953                  | 0.955                  | 0.951            |
| Experimental Precision | 0.359                  | 0.459                  | 0.397                  | 0.382                  | 0.350            |
| Theoretical Precision | 0.371                  | 0.474                  | 0.393                  | 0.385                  | 0.376            |

|                  | Political blogs (nodes: 1222, links: 19021) |                        |                        |                        |                  |
| Performance      |                                 |                        |                        |                        |                  |
| Experimental AUC | 0.918                          | 0.923                  | 0.923                  | 0.927                  | 0.924            |
| Theoretical AUC  | 0.923                          | 0.928                  | 0.926                  | 0.953                  | 0.938            |
| Experimental Precision | 0.170                  | 0.147                  | 0.169                  | 0.173                  | 0.172            |
| Theoretical Precision | 0.175                  | 0.153                  | 0.173                  | 0.199                  | 0.183            |

mined by the similarity distributions of connected and unconnected node pairs. The farther the two distributions are apart, the better prediction accuracy will be obtained. More importantly, we derive the theoretical solutions of AUC and Precision based on the node similarity distributions, and thus present an effective way to avoid the experimental performance evaluation in link prediction and the associated large computational cost.

Note that we only focus on CNS distribution of node sets of size two in various complex networks except for the ER random network, which is completely solved for node sets of any size. The CNS distribution of larger node sets in complex networks needs to be further explored, since it has potential applications in high-order link prediction problems. When the number of sampled node sets are huge, we can classify those node sets based on their isomorphism types, which are the interconnection patterns of the nodes in the node set, and then focus on the CNS distributions of the desired isomorphism types. Moreover, the application of node similarity in the other network-related problems, e.g., epidemic spreading, control, game, etc., is also worth exploration.

Acknowledgments

Here we present the definitions of some typical similarity indices of link prediction that are used in the main text, including CN, RA, AA, LP, and Katz. We denote the similarity score of node pair \((a, b)\) by \(S_{ab}\) and the corresponding similarity matrix by \(S\). \(\Omega_{ab}\) is the set of common neighbors of node pair \((a, b)\). \(k_z\) is the degree of node \(z\). Also, \(A^l\) represents the \(l\)-th power of the adjacency matrix \(A\), and \((A^l)_{ab}\) equals the number of paths of length \(l\) between node \(a\) and \(b\).

(1) Common neighbors (CN) index \[13\]. This index quantifies the similarity of a pair of nodes as the number of common neighbors they share,

\[ S_{ab} = |\Omega_{ab}|. \]  

(2) Resource Allocation (RA) index \[22\]. This index is enlightened by the resource allocation problem. Each neighbor of node \(a\) gets a unit of resource from node \(a\) and then equally distributes it to all its neighbors. The amount of resource obtained by node \(b\) can be taken as the similarity of nodes \(a\) and \(b\),

\[ S_{ab} = \sum_{z \in \Omega_{ab}} \frac{1}{k_z}. \]

(3) Adamic-Adar (AA) Index \[21\]. This index is also dependent on the common neighbors, similar to the CN and RA, while each common neighbor is penalized by the inverse logarithm of its degree,

\[ S_{ab} = \sum_{z \in \Omega_{ab}} \frac{1}{\log(k_z)}. \]

(4) Local Path (LP) Index \[16\]. The above three indices consider only the contribution of common neighbors (paths of length 2) in link prediction. The paths of larger length between two nodes can also reflect, to some extent, their similarity, especially when there are no common neighbors. Besides the common neighbors, the LP index further considers the paths of length 3, which is defined as

\[ S_{ab} = (A^2)_{ab} + \varphi(A^3)_{ab}, \]

where \(\varphi\) is a free parameter controlling the weight of paths of length 3 in the measurement of node similarity.
In the experiment, we set empirically $\varphi = 0.02$, which is a proper value for the three real-world networks considered in the main text.

(5) Katz index $^{17}$. This index considers all the paths between two nodes,

$$S_{ab} = \sum_{l=1}^\infty \varphi^l (A^l)_{ab},$$

where the free parameter $\varphi$ controls the weight of paths, and is set to be 0.01 empirically. We often directly calculate the node similarity matrix, $S = (I - \varphi \cdot A)^{-1} - I$, where $I$ is the identity matrix.

Through the definition of the Katz index, we see that the paths of length one (links) are included, which even have the largest weight among the paths of various lengths. Thus, the similarity score of a connected node pair significantly changes when the link of the node pair is moved to the test set, which is undesirable in link prediction and disturbs the theoretical calculation of AUC and Precision. An approach for effective remediation is removing the first item in the definition of Katz to ignore the paths of length one, or simply replacing $P_c(w)$ with $P_c(w + \varphi)$ in the theoretical calculation of AUC and Precision.

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