Link prediction via matrix completion

Ratha Pech¹, Dong Hao¹,²(a), Liming Pan¹, Hong Cheng³ and Tao Zhou¹,²(b)

¹ CompleX Lab, University of Electronic Science and Technology of China - Chengdu 611731, PRC
² Big Data Research Center, University of Electronic Science and Technology of China - Chengdu 611731, PRC
³ Center for Robotics, University of Electronic Science and Technology of China - Chengdu 611731, PRC

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Abstract – Inspired by the practical importance of social networks, economic networks, biological networks and so on, studies on large and complex networks have attracted a surge of attention in the recent years. Link prediction is a fundamental issue to understand the mechanisms by which new links are added to the networks. We introduce the method of robust principal component analysis (robust PCA) into link prediction, and estimate the missing entries of the adjacency matrix. On the one hand, our algorithm is based on the sparse and low-rank property of the matrix, while, on the other hand, it also performs very well when the network is dense. This is because a relatively dense real network is also sparse in comparison to the complete graph. According to extensive experiments on real networks from disparate fields, when the target network is connected and sufficiently dense, whether it is weighted or unweighted, our method is demonstrated to be very effective and with prediction accuracy being considerably improved compared to many state-of-the-art algorithms.

Introduction. – In the past decade, the rapid expansion of studies on complex networks has brought together different disciplines including physics, mathematics, computer science, sociology, economics, biology and so on [1,2]. The theory of complex networks provides us with novel insights for understanding the real-world linking patterns. The real-world linked datasets are usually dynamically changing and subjected to unobservability. On the one hand, the datasets are growing and changing over time through the increment of new links [3]. On the other hand, the missing or unobservable entries extensively exist in the datasets [4]. Therefore, predicting missing links is of great importance for studying the newly appeared and unobserved relations between data entries.

The link prediction problem essentially concerns the knowledge discovery and topology remodeling for large volumes of dynamic and noisy datasets [5], which also aims at uncovering to what extent the evolution of networks can be modeled and analyzed according to the intrinsic features and structures of the network itself [6]. So far it has been generally accepted as a fundamental paradigm not only in physics but also in bioinformatics, sociology, statistics and computer science.

Great effort has been made to solve the link prediction problem [7–15] and most of the algorithms are based on the similarity between vertex pairs since these algorithms are designed according to the fact that similar vertices are more likely to connect to each other. These algorithms are called similarity-based algorithms. Roughly, the similarity indices can be classified into three categories [8], i.e., local [16,17], global [18,19] and quasi-local [20,21] indices. The most popular methods are the local ones because they are simple and applicable for very large-scale networks. Although they are computational efficient, the local similarity-based link prediction algorithms are sometimes less accurate.

The global topological information can be exploited through the adjacency matrix, where the nonzero entries denote the connections between vertices, while missing links and nonexisting links are both denoted by zero entries. In most cases, a very small fraction of zero entries (called hidden nonzero entries or hidden entries) represent the missing links and the rest (called null entries) represent the nonexisting links. Essentially speaking, a link prediction algorithm aims at recovering the hidden
nonzero entries from the real null entries according to all the nonzero entries in the adjacency matrix. However, for a real-world network, the adjacency matrix is usually very sparse (i.e., most of its entries are zeros), providing highly limited information. How to precisely predict the missing links based on the sparse information is a challenging issue.

In this work, we introduce the robust principal component analysis (robust PCA) [22] method, namely low rank (LR), into link prediction and design a novel global information-based prediction algorithm based upon the low-rank and sparse property of the adjacency matrix. Then, by minimizing the nuclear norm of the matrix which fits the training data, we reconstruct a network that is close to the original network and accordingly identify the missing links. It is shown that when the target network is connected and sufficiently dense, we can find out the missing links with much higher accuracy compared to some of the state-of-the-art algorithms.

**Method.** – An undirected network consists of a set of vertices \(V\) and a set of links \(E\). We do not consider multiple links and self-connections. Suppose we have an observed network represented by the adjacency matrix \(A \in \mathbb{R}^{n \times n}\), which is a snapshot or a subset of an original network \(G^*\). The sets of links in \(A\) and \(G^*\) are denoted by \(E^T\) and \(E\), respectively. Denote the rest of the links in \(E\) as \(E^P\), namely \(E = E^T \cup E^P\) and \(E^T \cap E^P = \emptyset\). Then \(E^T\) is the training set for learning and prediction and \(E^P\) is the probe set for verifying the prediction accuracy. Without loss of generality, in the experiment we dynamically take 80%, 85%, 90%, and 95% of all the links in \(G^*\) as the training set and the rest as the probe set, respectively.

The objective of the link prediction is to find out the missing links of the original network \(G^*\), or equivalently, to recover a network \(G\) which is sufficiently close to \(G^*\), based on the observed entries of \(A\) (it is worth noting that it is generally intractable to recover exactly \(G^*\)). Assume that i) \(X^* \in \mathbb{R}^{n \times n}\) conveys the pattern as to how the network evolves (how predicted links are added and some existing links are eliminated) and we call \(X^*\) the backbone network; ii) \(X\) is the subset of \(X^*\) containing only the predicted links, which can be obtained by resorting the values of elements corresponding to nonzero entries in \(A\) to be zero, \(X^*\) and \(X\) have real number values. Identifying network \(X^*\) is the crucial intermediate step for recovering the original network and predicting the missing links accordingly. The observed network \(A\) is the only information we can utilize. \(X^*\) can be represented by subtracting an error/noise matrix \(E \in \mathbb{R}^{n \times n}\) from \(A\) and this noise matrix should be much sparser than either \(A\) or \(X^*\). Therefore, \(X^*\) can be written as

\[
X^* = A - E, \tag{1}
\]

where \(E\) is the noise matrix in which positive entries are the spurious links and negative entries represent the missing links that appear in \(X^*\). The relationship among \(G, A, X, X^*\) and \(E\) is illustrated in fig. 1. The recovered network \(G\) is obtained as

\[
G = X + A. \tag{2}
\]

The principal component analysis (PCA) can be utilized to obtain \(X^*\) and \(E\) simultaneously by converting the observed network \(A\) into a set of linearly uncorrelated variables called principal components, which captures the backbone network \(X^*\). When the data is slightly corrupted PCA can perform well, however, it cannot perform well with the grossly corrupted data. Therefore, a more robust matrix completion approach against high-dimensional noise \(E\) is required for link prediction in real complex networks. Hence, we apply the robust principal component analysis (robust PCA) in the matrix completion for link prediction.

Mathematically, according to the theory of robust PCA, recovering matrix \(X^*\) can be transformed into the following optimization problem:

\[
\min \text{rank}(X^*) + \gamma ||E||_0 \text{ subject to } X^* = A - E, \tag{4}
\]

where \(\text{rank}(X^*)\) denotes the rank of matrix \(X^*\), the operator \(||.||_0\) is the \(l_0\)-norm (i.e., the number of nonzero entries of a matrix), and \(\gamma\) is the parameter balancing these two terms. Normally, a precise solution of \(X^*\) guarantees that \(G = G^*\), which means that the precise solution of \(X^*\) can be used to perfectly recover the original network. Finding
the precise solution of $X^*$ in eq. (4) is a highly nonconvex optimization problem and its complexity is nondeterministic polynomial. However, some approximate solutions with exponential time complexity can be obtained based on robust PCA [23]. Firstly, since a matrix with rank $r$ has exactly $r$ nonzero singular values, $\text{rank}(X^*)$ is just the number of nonzero singular values of the matrix $X^*$. Secondly, according to the pioneering works [24, 25], the solution of the $l_1$-norm is also a sparse solution of the $l_0$-norm. Hence, the tightest relaxation of $\text{rank}(X^*)$ can be written as

$$\min_{X^*} ||X^*||_1 + \lambda ||E||_1 \quad \text{subject to} \quad X^* = A - E, \quad (5)$$

where $||.||_1$ denotes the nuclear norm (i.e., the sum of singular values) of the matrix, $||.||_1$ is the $l_1$-norm (i.e., the sum of the absolute values of the matrix entries), $E$ is a sparse matrix (i.e., most of its entries are zeros) and $\lambda$ is the positive weighting parameter balancing the low-rank property and sparsity.

On the one hand, the backbone network $X^*$ contains the predicted links not in $A$; on the other hand, it also eliminates some possible links in $A$. After obtaining $X^*$, we check only the newly appearing links and ignore the observed links in $A$, as shown in eq. (3), then we merge $X$ with $A$ to recover a matrix $G$ as illustrated in eq. (2). This matrix is recovered from the observed data $A$ through the above procedure, and it is supposed to be close to the original network $G^*$.

Each pair of vertices (e.g., $x$ and $y$) in $G$ is bundled with a score $S_{xy}$ corresponding to nonzero entries of $X$. The scores in $G$ or $X$ denote the likelihoods of missing or newly emerging links such that the higher they are, the more chances they have to be the missing or predicted links. It is worth noting that the above approach can also be applied to solve the link prediction problem in directed networks [29]. Finally, we sort the score of unobserved links in a descending order and select the top $L$ links. In this work, $L$ is the cardinality of the probe set. We check whether each of these $L$ links really appears in the probe set and record the number of appearing links as $L_r$. As we set the $L$ as the cardinality of the probe set, the precision value is also equal to the recall value at this point [8] as

$$Pr = L_r / L. \quad (6)$$

**Analysis.** – One crucial question is: to what extent can we predict the missing links by utilizing the above matrix completion method? In [26], the authors proved that when the $m$ observed entries of an $n \times n$ matrix with rank $r$ satisfy the following inequality,

$$m \geq Cn^{1.2}r \log(n), \quad (7)$$

where $C$ is a positive constant, one can perfectly recover all entries of the matrix with a very high probability through solving a simple convex optimization problem. However, for the real-world data, the adjacency matrix is very sparse where the order of the number of nonzero entries is normally much less than $n^{1.2}r \log(n)$. Fortunately, for the link prediction problem, it is not required to recover all the nonzero entries of the adjacency matrix, since only a small portion of these zero entries are the missing links and the rest of zero entries are the null links. Therefore, we are still able to estimate that the missing and likely existing links even with the nonzero entries are much less than what is required for eq. (7).

The time-consuming part of the proposed algorithm (LR) is to compute the singular value decomposition (SVD) of the adjacency matrix. By utilizing PROPACK [30] the complexity of each iteration of the algorithm reduces from $O(n^3)$ to $O(kn^2)$, where $k$ is the estimated rank of the matrix. This is due to the low-rank property as $k \ll n$ which makes the LR scalable for large networks. For instance, LR takes only about 141.986 seconds to work with a router network containing 5022 nodes and 6258 links on normal Intel(R) Core (TM) i7-6700 PC with 8 GB of RAM.

The LR method contains a parameter $\lambda$ which plays the role to balance the low-rank property of the recovered matrix and sparsity of the noise or spurious link matrix. The optimal value of $\lambda$ can be obtained from the empirical simulation as it varies according to the sparsity and structure of the networks. The optimal $\lambda$ of LR for each network in this study as well as the optimal parameters for other global methods are illustrated.

As LR and other global similarity-based algorithms prefer the global structures of the networks, we define a global structure of the adjacency matrix such that

$$g = \frac{D}{\tau \log(|V|)}, \quad (8)$$

where $D$ is the density of the network, $\tau$ is the ratio between the rank and the dimension value of the adjacency matrix, and $|V|$ is the cardinality of the node set, i.e., the number of nodes. If $D$ is large and $\tau$ is small, then the network is homogenous, i.e., its rank is much smaller than its dimension. The logarithmic function on $|V|$ is to normalize the scale of the network. Large networks have more global information for the network structures. Hence, the performances of the global method should have correlation with the global structure. The Pearson correlation coefficients between the precision and the global structure $g$ are displayed in table 3.

**Simulation.** – We implement LR, the local similarity-based algorithms, quasi-local, and global similarity-based algorithms on the 18 real networks including 16 unweighted and 4 weighted networks in which three of the weighted networks are the same as those in unweighted
networks. These networks are i) jazz [31] —jazz musician network, the link denotes the relationship between two persons if they used to play together in the same band at least once; ii) yeast [32] —the network of protein-protein interaction; iii) political blogs (PB) [33] —the network of hyperlinks between weblogs on US politics; iv) hamster [34] —the friendship network of users of the web site hamsterer.com; v) router [35] —the router-level topology of the Internet; vi) FWF [36] —the network of predator-prey interactions in Florida Bay in the dry season; vii) world trade (WT) [37] —the network of miscellaneous manufactures of metal among 80 countries in 1994; viii) contact [38] —a contact network between people measured by carried wireless devices; ix) metabolic [39] —the metabolic network of the nematode worm *C. elegans*; x) *C. elegans* [39] —the neural network of worms; xi) FWM [40] —the food web in Mangrove Estuary during the wet season; xii) macaca [41] —cortical networks of the macaque monkey; xiii) karate [42] —the network of relationship among the members in the karate club; xiv) football [43] —the network of American football games consisting of Division IA colleges during the regular season, Fall in 2000. xv) dolphin [44] —network of bottlenose dolphins living in Doubtful Sound (New Zealand); xvi) email [45] —the network of email interchanges between the members of the University of Rovira I Virgili; xvii) USAir [46] —the air transportation network of airports; xviii) FWE [47] —the network of the predator-prey interactions of Everglades Graminoids in the wet season. The topology statistics of the eighteen networks are shown in table 1.

We conducted 100 times the simulations of LR for each network and only report the average values and standard error in this paper. We compare the precision values with six popular unweighted local similarity-based algorithms, e.g., common neighbor (CN) [16], Adamic-Adar (AA) [48], resource allocation (RA) [17], local community paradigm, e.g., Cannistraci-Alanis-Ravasi (CAR), Cannistraci-Adamic-Adar (CAA), and Cannistraci-resource-allocation (CRA) [49]. In addition, we compare LR with the local path (LP) index [20] which is the quasi-local method and three global methods including Katz [18], SPM [7], and LOOP [50]. The detailed results from the ten unweighted-based algorithms and LR are shown in table 2. We can see that LOOP outperforms the rest. The second best global method is SPM, while LR stands as the third. Although LOOP performs better than the others, it is not applicable to large-scale networks. On the other hand, the structure perturbation method (SPM) outperforms LR on 11 of 16 unweighted networks, however, SPM cannot deal with weighted networks. LR, in addition, is better than the hierarchical structure model (HSM) [51] and the stochastic block model (SBM) [4] in terms of computational efficiency. Among the local parameter-free methods, CRA performs best followed by CAA and RA. In terms of mean ranking, CRA is better than LP and Katz, meanwhile LP and Katz are better than RA and other local methods. This is not a surprise since these results have also been reported in others works [52–54] such that they are some of the best mechanistic parameter-free local models.
The traditional algorithms do not perform well on yeast, the algorithms are very low as the network is very sparse. Networks. The precisions on the router network computed from all networks. The values in the brackets are the values of optimal parameters of the methods. The highest precisions in global and local methods are respectively shown in boldface.

| Networks | LR⁺ | SPM⁺ | LOOP⁺ | Katz⁺ | LP⁺ | RA | CRA | AA | CAA | CN | CAR |
|----------|-----|------|-------|------|-----|----|-----|----|-----|----|-----|
| Jazz     | 0.610(.13) | 0.674 | 0.692 | 0.492(.001) | 0.491(.01) | 0.541 | 0.556 | 0.528 | 0.531 | 0.507 | 0.518 |
| Yeast    | 0.526(.14) | 0.558 | N/A   | 0.246(.001) | 0.166(.10) | 0.259 | 0.162 | 0.163 | 0.145 | 0.146 | 0.141 |
| PB       | 0.195(.07) | 0.235 | N/A   | 0.175(.001) | 0.181(.10) | 0.146 | 0.174 | 0.169 | 0.173 | 0.171 | 0.172 |
| Hamster  | 0.440(.10) | 0.462 | 0.472 | 0.064(.010) | 0.070(.20) | 0.058 | 0.160 | 0.063 | 0.060 | 0.062 | 0.057 |
| Router   | 0.115(.10) | 0.159 | N/A   | 0.022(.010) | 0.101(.02) | 0.006 | 0.020 | 0.016 | 0.018 | 0.019 | 0.019 |
| FWF      | 0.565(.14) | 0.561 | 0.576 | 0.103(.001) | 0.307(.50) | 0.077 | 0.079 | 0.077 | 0.076 | 0.074 | 0.078 |
| WT       | 0.442(.12) | 0.489 | 0.452 | 0.419(.010) | 0.415(.20) | 0.438 | 0.417 | 0.423 | 0.397 | 0.396 | 0.384 |
| Contact  | 0.619(.10) | 0.595 | 0.580 | 0.569(.001) | 0.591(.50) | 0.562 | 0.562 | 0.562 | 0.560 | 0.561 | 0.559 |
| Metabolic| 0.215(.10) | 0.355 | 0.365 | 0.143(.010) | 0.153(.30) | 0.264 | 0.207 | 0.193 | 0.151 | 0.140 | 0.137 |
| C. elegans| 0.128(.10) | 0.167 | 0.200 | 0.101(.010) | 0.123(.30) | 0.106 | 0.119 | 0.103 | 0.096 | 0.095 | 0.088 |
| FWM      | 0.552(.14) | 0.542 | 0.566 | 0.151(.010) | 0.306(.30) | 0.128 | 0.134 | 0.125 | 0.130 | 0.124 | 0.126 |
| Macaca   | 0.751(.18) | 0.732 | 0.755 | 0.566(.010) | 0.630(.30) | 0.516 | 0.562 | 0.533 | 0.560 | 0.544 | 0.552 |
| Karate   | 0.114(.23) | 0.150 | 0.194 | 0.149(.001) | 0.153(.01) | 0.134 | 0.208 | 0.134 | 0.208 | 0.150 | 0.168 |
| Football | 0.213(.17) | 0.238 | 0.150 | 0.206(.100) | 0.185(.10) | 0.134 | 0.171 | 0.142 | 0.159 | 0.141 | 0.154 |
| Dolphin  | 0.069(.25) | 0.120 | 0.125 | 0.099(.100) | 0.133(.10) | 0.111 | 0.143 | 0.120 | 0.145 | 0.143 | 0.154 |
| Email    | 0.063(.16) | 0.151 | N/A   | 0.133(.001) | 0.133(.01) | 0.154 | 0.159 | 0.154 | 0.145 | 0.139 | 0.143 |

Table 3: The average predicting precision obtained by 100 independent runs on the four real weighted networks. The probe set contains 10% of total connections. The values in the brackets are the values of parameters of the methods.

| Networks | LR⁺ | rWRA | rWAA | rWCN | WRA | WAA | WCN | RA | AA | CAA | CN |
|----------|-----|------|------|------|-----|-----|-----|----|----|-----|----|
| USAir    | 0.408(.10) | 0.423 | 0.390 | 0.325 | 0.395 | 0.377 | 0.307 | 0.458 | 0.391 | 0.372 |
| C. elegans| 0.129(.10) | 0.109 | 0.112 | 0.108 | 0.109 | 0.119 | 0.116 | 0.104 | 0.105 | 0.098 |
| FWE      | 0.532(.10) | 0.158 | 0.156 | 0.149 | 0.158 | 0.213 | 0.206 | 0.171 | 0.162 | 0.151 |
| Football | 0.220(.19) | 0.058 | 0.050 | 0.042 | 0.058 | 0.058 | 0.025 | 0.083 | 0.100 | 0.117 |

Fig. 2: (Color online) The precision values on the 16 real unweighted networks for different sizes of the probe sets. The results are obtained by 100 independent runs and the short vertical lines represent standard deviations.

for link prediction in both mono-partite and bipartite networks.

The precisions on the router network computed from all the algorithms are very low as the network is very sparse. The traditional algorithms do not perform well on yeast, hamster, FWF, and FWM networks, while LR performs much better. LR performs well on dense networks. For sparse and small networks such as karate, and dolphin, LR fails to predict the missing links. Email is quite large, but it is very sparse and its rank is high, therefore, LR cannot
The precision values on the four real weighted networks for different sizes of probe sets.

Table 4: The average ranking of the different methods across all the 16 networks and Pearson correlation coefficients (CC) between precision and global structure ($g$), defined as in eq. (8), of the 16 unweighted networks.

| Method     | Average ranking | CC   |
|------------|-----------------|------|
| LOOP*      | 2.063           | 0.658|
| SPM*       | 3.313           | 0.713|
| LR         | 4.625           | 0.534|
| CRA        | 4.688           | 0.790|
| LP*        | 5.688           | 0.587|
| Katz*      | 6.688           | 0.576|
| CAA        | 6.938           | 0.486|
| RA         | 6.938           | 0.543|
| AA         | 7.250           | 0.578|
| CAR        | 7.875           | 0.570|
| CN         | N/A             | N/A  |

When the target network is sufficiently dense and connected, the proposed method performs better than the traditional algorithms. In other words, the local similarity-based methods do not perform well on the dense network. This indicates that the low-rank matrix recovery can well utilize the dense information in the adjacency matrix while the local similarity indices cannot. All of the networks we employ in this paper are undirected, however, the proposed method can be extended to deal with directed networks.

One disadvantage of the proposed method is the parameter $\lambda$. This parameter plays a very important role in the low rank and sparsity decomposition of the networks. In this work, we tune the parameter based on the empirical simulations to obtain the optimal values for each network. However, in the real-world problem we do not have the probe set to testify the parameter $\lambda$, but we can still divide the existing links into training set and probe set, and train the data to obtain a good value for this parameter.

Although, the trained optimal value of $\lambda$ from the training set may not be identical to the optimal value for the whole set of existing links, these two values should be close to each other if the data set is large.

Although LR can be used to predict the missing links in both weighted and unweighted networks, some networks, such as neural networks and signed opinion networks, should be treated as special cases. Those weights should be regularized to some positive values in advance. After prediction, one can adjust the weights in an inverse way. This kind of extension deserves further investigation, and currently we do not know how LR performs. We leave these problems to further work.

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| LOOP*      | 2.063           | 0.658|
| SPM*       | 3.313           | 0.713|
| LR         | 4.625           | 0.534|
| CRA        | 4.688           | 0.790|
| LP*        | 5.688           | 0.587|
| Katz*      | 6.688           | 0.576|
| CAA        | 6.938           | 0.486|
| RA         | 6.938           | 0.543|
| AA         | 7.250           | 0.578|
| CAR        | 7.875           | 0.570|
| CN         | N/A             | N/A  |
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