A Robust Method for Inferring Network Structures

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Inferring the network structure from limited observable data is significant in molecular biology, communication and many other areas. It is challenging, primarily because the observable data are sparse, finite and noisy. The development of machine learning and network structure study provides a great chance to solve the problem. In this paper, we propose an iterative smoothing algorithm with structure sparsity (ISSS) method. The elastic penalty in the model is introduced for the sparse solution, identifying group features and avoiding over-fitting, and the total variation (TV) penalty in the model can effectively utilize the structure information to identify the neighborhood of the vertices. Due to the non-smoothness of the elastic and structural TV penalties, an efficient algorithm with the Nesterov’s smoothing optimization technique is proposed to solve the non-smooth problem. The experimental results on both synthetic and real-world networks show that the proposed model is robust against insufficient data and high noise. In addition, we investigate many factors that play important roles in identifying the performance of ISSS.

Almost everything in our daily life can be modeled as complex networks, such as the social network¹,², transportation network³, protein-to-protein network⁴ and knowledge graph⁵. The interactions in these networks play an important role in identifying the networks’ structure, functionality and dynamics. Hence, many researchers utilize the detailed interaction information to do a lot of interesting research works, such as the centrality measures⁶,⁷, community detection⁸, robustness analysis⁹–¹¹, controllability¹² and network game¹³–¹⁵. However, the link information of networks is often invisible in many cases. Hence, it’s very important to propose a robust method in inferring the network structure from very few observed values (measurements) with noise, which are indirectly generated from the network.

Many researchers have made great efforts in solving the network inference problem. For instance, Han and Di et al.¹⁶ proposed the state-of-art method i.e., Lasso (Least Absolute Shrinkage and Selection Operator)¹⁷, which provides an estimation of a network with limited connectivity and low model prediction error. Hempe¹⁸ proposed an inference algorithm based on inner composition alignment to identify the network structure¹⁹,²⁰ on the time series data²¹. Timme²² and Domenico Napoletani et al.²³ inferred the complete connectivity of a network from its stable response dynamics. Daniel Marbach et al.²⁴ summarized many robust gene network inference methods and compared their performances. Soheil Feizi et al.²⁵ proposed network deconvolution as a general method to distinguish direct dependencies in gene expression regulatory networks.

Though many researchers have made great efforts in solving the network inference problem, it is still very challenging mainly on the following reasons. Firstly, the interactions in the network are very sparse. For most of the vertices of the network, they have few interactions with their neighbors, which are only a small portion of vertices compared with the network size, i.e. the total number of vertices. It leads to the sparseness of interactions for each vertex, which makes it hard to infer the local structure. Secondly, the inference of the inaccessible original network is mainly based on the observations, i.e. measurements generated from the network. However, almost all of measurements and outputs have noises. The noisy data present great challenges in the error control, and it creates great difficulties to identify the real network. Thirdly, the observations are always insufficient i.e., have missing terms. In many real world applications, it’s hard or costly to get all the measurements of the network from the beginning to the end. For many real world cases, we have only 5–20% observations¹⁶ on the whole network, which makes it an impossible task to infer the detailed network structure.
In this paper, we propose an iterative smoothing algorithm with structure sparsity (ISSS) method to infer the network structure. The elastic penalty is the combination of \(L_1\) and \(L_2\) penalties. The special \(L_1\) penalty can successfully model the sparseness of network information. The \(L_2\) penalty can prevent over-fitting of the model. The TV\(^*\) penalty of the method can treat the neighbors of each vertex as a continuous signal, which makes the model tend to infer the local information of the network, i.e. community structure. The three structural penalties lead to the non-smoothness of the loss function, which makes it hard to solve the optimization problem. By introducing the Nesterov’s smoothing technique\(^27\), the optimization problem can be successfully solved. Moreover, the existence of three penalties and the smoothing technique makes the inference method more robust, even when the network has an insufficient observation with noise. We apply the model on synthetic networks to infer the dynamics of these networks, such as Erdős Rényi (ER)\(^38\), Barabási Albert (BA)\(^29\) and Watts Strogatz (WS)\(^30\) networks. Furthermore, we also apply the model on many real world networks, such as the Karate\(^31\) and Netscience\(^32\) networks. The experimental results show the effectiveness of the ISSS model.

Problem Definition
Let’s take the ultimatum game (UG) on networks\(^33\) as an example. The vertices in the network represent players. If two people play the ultimatum game, there is an edge between them. Everyone in the game will play two times with his neighbors using strategy \((p, q)\), both as a proposer and a responder. \(p_j \in [0, 1]\) is the amount proposed by player \(i\) to offer his neighbor \(j\), while \(q_j\) is the minimum amount that \(i\) responds to his neighbor \(j\). For instance, player \(i\) has a strategy \([0.8, 0.65]\), and one of his neighbors \(j\) has a strategy \([0.6, 0.5]\). Since \(i\) proposes to offer \(p_i = 0.8\) to \(j\), which is larger than the minimum acceptance amount of \(j\), i.e., \(q_j = 0.5\), then player \(i\) will get a \(1 - 0.8 = 0.2\) payoff. At the same time, \(j\) offers \(i\) with \(p_j = 0.6\), which is lower than the minimum amount of \(i\) accepts, i.e., \(q_i = 0.65\), then player \(j\) rejects \(i’s\) offer, and both of them get nothing. The game lasts for \(M\) rounds. For round \(\mu \in [1, M]\) with time stamp \(t_\mu\), the corresponding strategy of player \(i\) is denoted as \((p_i(t_\mu), q_i(t_\mu))\). The payoff of player \(i\) with player \(j\) at round \(\mu\) can be summarized as follows:

\[
\phi_j(t_\mu) = \begin{cases} 
  p_j(t_\mu) + 1 - p_j(t_\mu) & p_j(t_\mu) \geq q_j(t_\mu) \
  1 - p_j(t_\mu) & p_j(t_\mu) < q_j(t_\mu) 
\end{cases}
\]

Hence, the overall payoff of player \(i\) with all its neighbors is defined as \(\gamma_i(t_\mu) = \sum_{j \in E(i)} \phi_j(t_\mu)\), where \(E(i)\) is the neighbors of player \(i\). The strategy \((p(t_{\mu+1}), q(t_{\mu+1}))\) changes from time to time with a random number \(\delta \in [-\varepsilon, \varepsilon]\). \(\varepsilon\) is set to 0.05 and the strategy \(p\) and \(q\) are set to range \([0, 1]\). The reconstruction problem is formulated as \(Y_\mu = \Phi_\mu \times X_\mu\) as shown in Fig. 1, where \(Y_\mu \in \mathbb{R}^{M \times 1}\) is given by the output of the network system for vertex \(i\). \(\Phi_\mu \in \mathbb{R}^{M \times N}\) is the observation, i.e. measurements which is constructed by Equation (1). \(X_\mu \in \mathbb{R}^{N \times 1}\) denotes the neighboring vector of vertex \(i\), which is the network structure we want to infer. \(t_\mu \in [1, M]\) is the accessible time instance in time series. Our task is to infer all the neighbors of vertex \(i\), i.e., \(X_i\) given noisy, sparse and incomplete \(Y_\mu\) and \(\Phi_\mu\) in Equation (2).

\[
\gamma_i(t) = \begin{bmatrix} \gamma_1(t) \\ \gamma_2(t) \\ \vdots \\ \gamma_N(t) \end{bmatrix} = \begin{bmatrix} \phi_{11}(t_1) & \phi_{12}(t_1) & \cdots & \phi_{1N}(t_1) \\ \phi_{21}(t_2) & \phi_{22}(t_2) & \cdots & \phi_{2N}(t_2) \\ \vdots & \vdots & \ddots & \vdots \\ \phi_{N1}(t_M) & \phi_{N2}(t_M) & \cdots & \phi_{NN}(t_M) \end{bmatrix} \begin{bmatrix} x_{11} \\ x_{12} \\ \vdots \\ x_{NN} \end{bmatrix}
\]

Here the UG on networks is just an example. There are also many other applications, such as the evolutionary games, transportation, communication processes, sociology and biology in papers\(^{16,34,35}\). For instance, the construction of biological interaction networks with the goal of uncovering causal relationships between genotype and phenotype constitutes a major research topic in systems biology\(^35\). With the increased availability of DNA microarray time-series data, it is possible to infer gene regulatory networks (GRNs) from gene expression data to understand dynamic GRNs\(^36\). The information-geometric network inference to use a real radio emulation testbed to infer the end-to-end rate distributions of stochastic network flows from link rate measurements\(^37\). G Zahoranszky-Kohalmi\(^38\) employs network inference method in investigating the drug-target and target-target interactions in order to design new drugs.

In these real world applications, the observations from the network, i.e., \(\Phi\), and \(Y\), have noises, and \(\Phi\) is generally sparse and incomplete, which are key factors in identifying the performance of the network inference method. In fact, the essence of the inferring network structure (network reconstruction) problem can be formulated by Equation (2). The performance of the model is determined by the network structure and the expressing ability of model itself. Thus if the networks are built using ER network model with the same parameters, then the performance of any methods should be very similar. In the next section, we will discuss the advantages of ISSS and the key factors in identifying the performance of the ISSS and Lasso models.

Results
In this section, we apply our model on many different types of synthetic and real world networks. Then we compare the experimental results of our model with the state-of-art method Lasso\(^16\) on ER, BA and WS networks. The experimental results show the effectiveness of our model, and it outperforms the baseline method significantly. In addition, we also investigate the key factors in identifying the performance of the model, such as the variance.
of the elements in measurement $\Phi_i$ and the properties of many real world networks. Finally, we compare the clustering coefficients of the network derived from the Lasso and ISSS model, respectively. And we also analyze the effectiveness of three penalties in the model.

**Experiments on three typical networks.** We take the network inference as a binary classification task, i.e. the edge exists or not. Hence, Area under the Receiver Operating Characteristic (AUROC) is employed to evaluate the performance of the models. The Area under the Receiver Operating Characteristic is a common summary statistic for the goodness of a predictor in a binary classification task. It is equal to the probability that a predictor will rank a randomly chosen positive instance higher than a randomly chosen negative one.

| Type | Method | Data 0.05 | 0.1 | 0.15 | 0.2 | 0.4 |
|------|--------|-----------|-----|------|-----|-----|
| ER   | Lasso  | 0.51      | 0.55| 0.59 | 0.64| 0.95|
|      | ISSS   | 0.63      | 0.71| 0.76 | 0.80| 0.95|
| BA   | Lasso  | 0.53      | 0.63| 0.81 | 0.92| 0.99|
|      | ISSS   | 0.73      | 0.79| 0.86 | 0.92| 1.00|
| WS   | Lasso  | 0.53      | 0.60| 0.71 | 0.87| 1.00|
|      | ISSS   | 0.71      | 0.79| 0.86 | 0.93| 1.00|

Table 1. Comparison between ISSS and Lasso. We use AUROC (Area under the Receiver Operating Characteristic) index to depict the performance of the inference task. Area is the area under the curve. It is a common summary statistic for the goodness of a predictor in a binary classification task. It is equal to the probability that a predictor will rank a randomly chosen positive instance higher than a randomly chosen negative one.
data, i.e. Data = 0.4, both ISSS and Lasso can successfully identify the network structure. As shown in Table 1, when the training data size is very small, the performance of ISSS is much better than Lasso. Take Data = 0.05 as an example, the AUCROC of ISSS is at least 0.1 larger than that of Lasso. It indicates that the ISSS improves the performance significantly with very few training data.

It is worth mentioning that variance of measurement $\Phi$'s elements in Equation (2) play an important role in inferring the network structure. The $\Phi$'s elements $\Phi_{ij} \in [0, 1]$ on ER, BA and WS in Table 1 has default variance $= 10^{-1}$. Here we will analyze the situation that $\Phi$ has many other variances, s.t. variance $= 10^{-2}, 10^{-3}$ and $10^{-4}$ in Fig. 2. We plot the performance of ISSS and Lasso with different variances of $\Phi$'s elements on ER, BA and WS networks.

On the networks with variance $= 10^{-4}$ in Fig. 2(a,d,g), i.e. the network structure is hard to reconstruct, Lasso fails to infer the network structure. The performance of Lasso is equal to random guess, i.e., the blue line in Fig. 2(a,d,g). With very large variance, the inference or reconstruction task is much easier. To show the whole curves, the upper bound of the y axis is set to 1.2 for all the figures in this paper.

In Figure 2. The performance of ISSS and Lasso on the data with variance $= 10^{-2}, 10^{-3}$ and $10^{-4}$. With very small variance $= 10^{-4}$, the performance of Lasso is equal to random guess, i.e., the blue line in Fig. 2(a,d,g). With very large variance, the inference or reconstruction task is much easier. To show the whole curves, the upper bound of the y axis is set to 1.2 for all the figures in this paper.
model. For instance, to infer a small network, the training time with \( \text{variance} = 10^{-3} \) is 10% shorter than that with \( \text{variance} = 10^{-1} \). That’s the reason that many systems prefer low variance measurements and outputs. In summary, the ISSS model performs well with low variance measurements and few training data.

To further investigate the relation between variance and training data size, as shown in Fig. 3(a,b,c), we fix the training data size, i.e., \( \text{Data} = 0.1, 0.5 \) and 1, then find out the performance of ISSS and Lasso as variance scale goes up from \((0, 1]\) with step 0.1. The experimental results on ER, BA and WS network are similar. Hence, we take ER network as an example in the figure. When \( \text{Data} = 1 \) and 0.5, ISSS can successfully infer the network structure with very small variance scale. With \( \text{Data} = 0.1 \), the AUROC keeps its value as the variance goes up. The performance of Lasso is just a little better than the random guess. However, the AUROC value of ISSS is larger than 0.70. It indicates that training data size is an important factor in identifying the upper bound of the performance.

To test the robustness of the ISSS against the noise, we add some Gaussian noises \( \mathcal{N}(\mu, \delta^2) \) to the output \( Y \) and measurement \( \Phi \). Then we apply the ISSS and Lasso model on the noisy data. The results are shown in Fig. 3(d,e,f). For low noise with \( \delta^2 = 10^{-3} \), the ISSS outperforms the Lasso, especially when the elements of \( \Phi \) have very small variance. For very high noise that follows the normal distribution with \( \delta^2 = 10^{-1} \), the performance of ISSS and Lasso are similar. For the noise with \( \delta^2 = 10^{-2} \), the performance of ISSS is better than Lasso for all variance scales.

**Experiments on real world networks.** We apply the ISSS and Lasso on many real world networks to evaluate the performance. Table 2 denotes the minimum data for achieving at least 0.95 AUROC in combination with several real networks. CC stands for clustering coefficient.

| Network       | Vertices | Edges | CC   | Average path | Centralization | Heterogeneity | Density | Lasso | ISSS |
|---------------|----------|-------|------|--------------|----------------|---------------|---------|-------|------|
| Karate        | 34       | 78    | 0.571| 2.408        | 0.4            | 0.833         | 0.139   | N/A   | 0.2  |
| Dolphins      | 62       | 159   | 0.259| 3.357        | 0.116          | 0.572         | 0.084   | N/A   | 0.5  |
| Netscience    | 1589     | 2743  | 0.638| 5.823        | 0.019          | 1.005         | 0.002   | N/A   | 0.8  |
| Adjnoun       | 113      | 435   | 0.173| 2.536        | 0.38           | 0.903         | 0.068   | N/A   | 0.6  |
| Football      | 115      | 613   | 0.403| 2.508        | 0.012          | 0.083         | 0.094   | N/A   | 1    |
| Les Miserables| 77       | 254   | 0.573| 2.641        | 0.397          | 0.91          | 0.087   | N/A   | 0.4  |

**Figure 3.** Insufficient data vs variance scale. In most cases, the AUROC of ISSS and Lasso rises, as the variance increases. With small variance, ISSS performs much better than the Lasso. With Data = 0.1, the performance cannot be improved with any variance. It indicates that insufficient data plays an important role in the inference task. Extremely insufficient data leads to the failure of all the methods. The experimental results with other Data \( \in [0.2, 1] \) values are similar. In this section, we take Data = 0.4 as a representative. As shown in this figure, with small noise, ISSS outperforms Lasso. With great noise, the performance of ISSS and Lasso reach the upper bound of the model. Hence the performance of the two methods are the same.
infer the network structure with higher centralization index with very few training data. The network with both higher heterogeneity and density can also be easily inferred. To evaluate the performance of ISSS and Lasso on large networks, we do some experiments on the power grid (4941 vertices, 6594 edges), roget (1022 vertices, 5075 edges), Gnutella peer-to-peer file sharing network (6301 vertices, 20777 edges) and collaboration network in computational geometry (7343 vertices, 11898 edges). As shown in Fig. 4, ISSS outperforms the Lasso on all the networks. The Gnutella peer-to-peer network is hard to infer. Both ISSS and Lasso require more training data to infer the Gnutella peer-to-peer network structure.

We compare the clustering coefficient of the network inferred by ISSS and Lasso with different training data sizes in this part. In Fig. 5, the horizontal axis represents the training data size, and the vertical axis is the clustering coefficient of the network inferred by ISSS and Lasso. The red solid line lies above the blue line all the time. It indicates that the ISSS model is inclined to infer the networks with stronger community structures than that of Lasso. As the training data size increases in Fig. 5, the clustering coefficient of the network inferred by ISSS approaches the ground truth, i.e., the yellow line. These results show that the TV penalty in ISSS model works well. Here is an example to demonstrate why the TV penalty works. For instance, a network has 50 vertices. As shown in Fig. 6, the horizontal axis represents all the 50 vertices in the network. If vertex $i$ is a neighbor of vertex $j$, it is 1, otherwise it is 0 in the figure. Lasso tends to predict the neighbors of vertex $i$ discretely as shown in Fig. 6(a), while the ISSS is opt to infer the network structure in a continuous way, as shown in Fig. 6(b). The reason for choosing TV penalty is that almost all of the vertices in many networks have similar natural number. Take the karate network as an example. Almost all the vertices' labels that are less than 20 are in the same community. For the dolphin network, the vertices' labels under 30 are connected with each other. For the networks don't have natural number labels or the vertices don't have continuous labels as shown in Fig. 6(a). We can remove the TV penalty from the model. The experimental results are shown in Table 3. The experiment is done on a BA network with continuous natural number labels. Without TV penalty, the ISSS model also works well. However, the ISSS with all the three penalties is still the best.

As we mentioned above, TV penalty is a factor in inferring the network structure. Hence, how to choose the value of parameter $\gamma$ is important as shown in Equation (4). In this part, we investigate the relationship between the most common used hyper parameter coefficients $\gamma$ and the training data size, i.e., $Data$. According to the results in Table 4, $\gamma = 10^{-3}$ and $10^{-4}$ have the best performance on almost all training data. Given $Data = 0.1$, $\gamma = 10^{-4}$ is the best choice. The hyper parameter $\beta, \lambda$ of $L_1, L_2$ are empirically set as 0.001 and 0.0001, respectively.

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**Figure 4.** The performance of ISSS and Lasso on power grid, roget, Gnutella peer-to-peer file sharing network and collaboration network in computational geometry. The performance of ISSS and Lasso ON Gnutella network are not good enough. The reason is that we need more training data to infer the network, i.e., $Data = M/N = 2$, where $M$ is the time instances and $N$ is the number of vertices in the network.
In this paper, we propose the robust ISSS model in solving the network reconstruction problem. Compared with the state-of-art Lasso, the ISSS model is more robust, which can successfully infer the network structure with insufficient training data against noise. The sparse regularization term $L_1, L_2$ and the structural TV penalties make

**Figure 5.** The clustering coefficient of the reconstructed network by ISSS and Lasso. The yellow line represents the real clustering coefficient of the network. The red line represents the clustering coefficient of the reconstructed network by ISSS.

**Figure 6.** The reconstruction of vertex $i$’s neighbors. Suppose there are 50 vertices in all. If vertex $i$ is connected with vertex $j$, the corresponding item in histogram is 1, otherwise it is 0. Lasso is good at predicting the neighbors in a discrete style, while the ISSS is inclined to predict continuous neighbors. The continuous neighbors are probably the way to construct the community structure of the network.

**Discussion**
In this paper, we propose the robust ISSS model in solving the network reconstruction problem. Compared with the state-of-art Lasso, the ISSS model is more robust, which can successfully infer the network structure with insufficient training data against noise. The sparse regularization term $L_1, L_2$ and the structural TV penalties make
the ISSS model reconstruct the network with strong community structure. The experiments on the WS, ER and BA networks show that the ISSS outperforms Lasso even when the network system has very few observations with great noises. We also do some experiments to analyze the factors in identifying the performance of the ISSS, i.e. the variance of $\Phi$, training data size and the clustering coefficient of the network.

In the future, on the one hand, we will continue to find out all the factors in identifying the upper and lower bound of ISSS's performance, and prove that from both theory and experiment perspectives. On the other hand, the community structure of a network defines the characteristic of a network, which identifies its functionality and should be preserved during the inferring process. Though ISSS model can identify the network with community structure, there could be room for improvement. For instance, the group Lasso and the tree group Lasso are the promising directions in network reconstruction task. Furthermore, we will optimize ISSS and apply the network inference method to solve the drug prediction and breast cancer prediction problems.

At present, it is still very challenging to infer many large-scale networks. Hence, it is a future trend with promising application field. And the evaluation criteria on directed and undirected networks are the same. As the development of network inference and compressed sensing research, more reasonable evaluation methods will be proposed to evaluate the experimental results on undirected networks.

**Methods**

The main goal of complex network reconstruction is to recover the connection $X_i$ by the payoff information $y_i$ and virtual-payoff matrix $\Phi_i$ of vertex $i$ from the time series of strategies. Note that the number of the neighbors of vertex $i$ is often much less than the total number of vertices in the entire complex network, i.e., $X_i$ is sparse. Han et al.\textsuperscript{40} adopted to use Lasso model to identify the neighbors of vertex $i$.

By using Lasso model, the problem of network reconstruction is formulated as

$$\min_{X_i} \| Y_i - \Phi_i X_i \|_2^2 + \lambda \| X_i \|_1,$$

where $\lambda$ is a non-negative regularization parameter. All nonzero elements of the reconstructed $X_i$ correspond to the neighbors of $i$ vertex. However, the Lasso-based model (3) only considers the sparse information.

In practice, to estimate a true signal in noise, the most frequently used methods are based on the total variation (TV) norm and the $\ell_1$ norm. TV penalty forces sparsity on the spatial derivative of the weight map. TV norms are essential $\ell_1$ norms of derivatives, hence $\ell_1$ estimation procedures are more appropriate for the subject of TV estimation. The space of functions of bounded total variation plays an important role when accurate estimation of discontinuities in solutions is required.\textsuperscript{26} By contrast, total variation is remarkably effective at simultaneously preserving edges whilst smoothing away noise in flat regions for image denoising. Therefore, we consider to use ridge regression model with the TV regularization to preserve the structural information of networks and enhance the robustness performance of network reconstruction. After imposed the TV regularization, the objective of our method is formulated as

$$\min_{X_i} F(X_i) \overset{\Delta}{=} \| Y_i - \Phi_i X_i \|_2^2 + \frac{\beta}{2} \| X_i \|_2^2 + \lambda \| X_i \|_1 + \gamma TV(X_i),$$

where

| TV coefficient | Data | 0.1 | 0.3 | 0.5 | 0.8 | 1 |
|----------------|------|-----|-----|-----|-----|---|
| 1.00E-06       | 0.8000 | 0.9700 | 0.9988 | 1.0000 | 1.0000 |
| 1.00E-05       | 0.8037 | 0.9750 | 0.9990 | 1.0000 | 1.0000 |
| 1.00E-04       | 0.7790 | 0.9815 | 0.9994 | 1.0000 | 1.0000 |
| 1.00E-03       | 0.7078 | 0.9830 | 0.9993 | 1.0000 | 1.0000 |
| 1.00E-02       | 0.7785 | 0.9538 | 0.9909 | 0.9996 | 0.9999 |
| 1.00E-01       | 0.7090 | 0.7832 | 0.8029 | 0.8363 | 0.8619 |
| 1.00E-00       | 0.4825 | 0.6137 | 0.6225 | 0.6406 | 0.6385 |

Table 4. Sensitivity analysis of TV penalty coefficient $\gamma$ in Equation (4).
where $TV(\cdot)$ represents the TV regularization, which is defined as $TV(X_i) = \sum_{j=1}^{N} |X_j(i) + 1 - X_j(i)|$. It is worth noting that the Lasso-based model \(^{40}\) is a special case of our model. When $\beta = 0$ and $\gamma = 0$, our model will reduce to the Lasso-based model \(^{40}\) for complex network reconstruction.

Compared to the model in ref. \(^{40}\), our model in (4) is able to utilize the structural information to help recover the connection of network. However, the TV regularization is a complex and non-smoothed sparsity-inducing penalties, and its proximal operator is unknown and difficultly computed. The traditional convex optimization methods, such as iterative soft-thresholding algorithm (ISTA \(^{43}\), fast or accelerated ISTA (FISTA) \(^{42}\) and second-order methods \(^{44-46}\), require only one non-smoothed term alone or access to the unknown proximal operator of the non-smooth part of the objective function. In general, the proximal operator of the sum of two non-smooth functions, i.e. $\ell_1$ and TV, is unknown and computing expensive. Thus, we can not use them solve this problem \(^{(4)}\) directly. Motivated by Nesterov’s smoothing technique \(^{27}\), we first smooth the TV penalty with the unknown proximal operator, while keeping the exact $\ell_1$ constraint and then use accelerated proximal gradient descent to minimize the whole function as shown in Algorithm 1.

Time-complexity of iterative convex optimization is kind of tricky to analyze, as it depends on a convergence criterion. Here we give a brief estimation of the time complexity. Suppose we have $N$ players, and $M$ time instances, as shown in Equation 2. The optimization procedure of the ISSSS is shown in Algorithm 1. The first 3 sets are the most time-consuming, which costs $O(T(M*N + N^2))$, in which $T$ is the number of iterations. For all $N$ vertices, the time complexity of the ISSSS is $O(T(M*N^2 + N^3))$. Lasso is implemented using LARS algorithm. \(1\) For $N < M$, $N^0 < N^0 * M$ and the computational complexity of Lasso is $O(N^2*M)$. \(2\) For $N \geq M$, $N^0 \geq N^0 * M$ and the complexity of Lasso is $O(N^3)$. With limited $T$ iterations, the time complexity of ISSSS is slightly higher than that of Lasso.

**Nesterov’s smoothing technique for TV penalty.** Denote $TV(X_i) = \sum_{j=1}^{N} |X_j(i) + 1 - X_j(i)|$. Using the duality concept \(^{47}\), we can establish the dual form of $TV(X_i)$, then for all $J$ is a vector of auxiliary variables associated with $X_j$. It is worth noting that the Lasso-based model \(^{40}\) is a special case of our model. When $\beta = 0$ and $\gamma = 0$, our model will reduce to the Lasso-based model \(^{40}\) for complex network reconstruction.

\[
TV(X_i) = \sum_{j \in G} ||A_{ij} X_j|| = \sum_{j \in G} \max_{\gamma \in \overline{G}} \langle z_{ij}, A_{ij} X_j \rangle = \max_{z} \langle z, A^T X \rangle,
\]

where $z \in \mathbb{R}^{|G|}$ is a vector of auxiliary variables associated with $A_{ij}$ and $z \in \mathcal{K} = \left\{ z = [z_{G_1}, \ldots, z_{G_{|G|}}], \|z\|_2 \leq 1, \forall G \in G \right\}$. The $A$ is the vertical concatenation of all the $A_{ij}$ matrices, that is

\[
A = \begin{bmatrix}
-1 & 1 & 0 & \ldots & 0 \\
-1 & 1 & 0 & \ldots & 0 \\
-1 & 1 & 0 & \ldots & 0 \\
-1 & 1 & 0 & \ldots & 0 \\
\end{bmatrix}
\]

\(\text{Algorithm 1.} \) The main procedures of solving the problem \(\text{(4)}\)

**Output:** the output $\Phi_i$ of network system for vertex $i$ and its observation $\Phi_i$, parameters $\mu$, $\alpha$, $\beta$ and $\gamma$, a Lipschitz constant $L_{f_x}$ and stopping criterion $\epsilon$.

**Input:** the output $\Phi_i$ of network system for vertex $i$ and its observation $\Phi_i$, parameters $\mu$, $\alpha$, $\beta$ and $\gamma$, a Lipschitz constant $L_{f_x}$ and stopping criterion $\epsilon$.

**Output:** the Optimal neighboring vector $X_j$.

Let $k = 1$. Initialize $X_j = X_j^0 \in \mathbb{R}^N$ randomly, $n_1 = t_0 = 1$;

**while** not converge (\(\|F(X_j^{k-1}) - F(X_j^k)\| \leq \epsilon\)) **do**

1. Compute $t_{k+1} = \left(1 + \sqrt{1 + 4t_k^2}\right)/2$;
2. Compute $v_k + \frac{\mu}{t_{k+1}} (X_j^{k-1} - X_j^k)$;
3. Calculate the gradient $\nabla f(v_k^{k+1}) = \Phi^T (\Phi v_k^{k+1} - Y_j) + \beta v_k^{k+1} + \gamma \nabla s_{\mu} (v_k^{k+1})$;
4. Compute $X_j^{k+1} = p_{L_{f_x}} (v_k^{k+1} = \text{sign} \left( v_k^{k+1} - \frac{1}{L_{f_x}} \nabla f(v_k^{k+1}) \right) (v_k^{k+1} - \frac{1}{L_{f_x}} \nabla f(v_k^{k+1}))$;
5. $k = k + 1$.

**end while**

The set $\mathcal{K}$ is the Cartesian product of unit balls in Euclidean space, therefore, a compact convex set. Before smoothing the TV penalty, we introduce the following important Lemma.

**Lemma 1** Let $s_{\mu}(X_j)$ be Nesterov’s smooth transform of $TV(X_j)$. If $M = \max_{z \in \mathcal{K}} \|z\|^2/2$, then for all $X_j \in \mathbb{R}^p$,

\[
s_{\mu}(X_j) \leq TV(X_j) \leq s_{\mu}(X_j) + \mu M.
\]

By using Nesterov’s smoothing technique, the smoothed TV penalty is formulated as

\[
s_{\mu}(X_j) = \max_{z \in \mathcal{K}} \left\{ \langle z, A^T X \rangle - \frac{\mu}{2} \|z\|^2 \right\} = \left\langle z^*(X_j), A^T X \right\rangle - \frac{\mu}{2} \|z^*(X_j)\|^2,
\]

where $\mu$ is a positive smoothing parameter and...
\[ z^*_\mu(X_i) = \arg \max_{z \in K} \left\{ \langle z, AX_i \rangle - \frac{\mu}{2} \| z \|_E^2 \right\}. \] (8)

**Theorem 1** (Nesterov’s Theorem). Let the function \( s_\mu \) be Nesterov’s smooth transform of a convex function TV penalty. We can obtain the following results:

1. \( s_\mu \) is convex and differentiable with gradient \( \nabla s_\mu(X_i) = \mathcal{A}^T z^*_\mu(X_i) \) and \( \nabla s_\mu(X_i) \) is Lipschitz continuous with constant \( L_{s_\mu} = \| \mathcal{A}^T \|_F / \mu \), where \( \| \mathcal{A}^T \|_F = \lambda_{\text{max}}(\mathcal{A}^T \mathcal{A}) \) is the largest eigenvalue of \( \mathcal{A}^T \mathcal{A} \).

2. For all \( X_i \in \mathbb{R}^d \), we have \( \lim_{\mu \to 0} s_\mu(X_i) = TV(X_i) \).

The proof of Theorem 1 is obtained according to Lemma 1. According to the projection theorem, we know that \( z^*_\mu(X_i) \) is the projection of \( \mathcal{A}X_i \) onto the compact and convex space \( K \), that is

\[ z^*_\mu(X_i) = P_K \left( \frac{1}{\mu} AX_i \right) = \prod_{G \in \mathcal{G}} P_{K_G} \left( \frac{1}{\mu} A_G X_i \right), \] (9)

where \( \Pi \) is the Cartesian product of a set and \( P_{K_G}(\cdot) \) is the projection onto each compact set \( K_G \) defined as

\[ P_{K_G}(x) = \frac{x}{\max(\| x \|_1, 1)} = \frac{x}{\| x \|_1}, \quad \text{if } \| x \|_1 \leq 1, \quad \text{otherwise}. \]

**Optimization.** After smoothing by Nesterov’s technique, the proximal operator of \( s_\mu \) becomes easily computed. We obtain a new optimization problem by using \( s_\mu(X_i) \) to replace the TV penalty of the problem (4):

\[ \min_{X_i} F_\mu(X_i) \triangleq f_\mu(X_i) + \lambda \| X_i \|_1 = \frac{1}{2} \| \mathcal{A} X_i - \Phi Y_i \|_F^2 + \frac{\beta}{2} \| X_i \|_1^2 + \lambda \| X_i \|_1 + \gamma s_\mu(X_i), \] (10)

where \( f_\mu(X_i) = \| \mathcal{A} X_i - \Phi Y_i \|_F^2 + \frac{\beta}{2} \| X_i \|_1^2 + \gamma s_\mu(X_i) \) is a smooth convex function, i.e., continuously differentiable with Lipschitz continuous gradient constant \( L_{f_\mu} \)

\[ \| \nabla f_\mu(u) - \nabla f_\mu(v) \| \leq L_{f_\mu} \| u - v \|, \quad \forall u, v \in \mathbb{R}^d, \]

and \( s_\mu(X_i) \) is Nesterov’s smoothing function of \( TV(X_i) \) and defined as Equation (7). Motivated by the idea of FISTA, we adopt the following quadratic model as the approximation of \( F_\mu(X_i) \) at a given point \( v \)

\[ Q_{L_{f_\mu}}(X_i, v) = f_\mu(v) + \langle X_i - v, \nabla f_\mu(v) \rangle + \frac{L_{f_\mu}}{2} \| X_i - v \|^2 + \lambda \| X_i \|_1, \] (11)

which admits a unique minimizer

\[ p_{L_{f_\mu}}(v) = \arg \min_{X_i} Q_{L_{f_\mu}}(X_i, v) = \arg \min_{X_i} \left\{ \lambda \| X_i \|_1 + \frac{1}{2} L_{f_\mu} \| X_i - v \|^2 \right\}, \] (12)

where \( \nabla f(v) = \Phi^T (\Phi v - Y_i) + \beta v + \gamma \nabla s_\mu(v) \). Note that \( p_{L_{f_\mu}}(v) \) is the well known component-wise soft thresholding operator

\[ \left[ p_{L_{f_\mu}}(v) \right]_j = \text{sign}(u_j)(|u_j| - \lambda)_+, \]

where \( \mu = v - \frac{1}{L_{f_\mu}} \nabla f(v) \) and \( (.)_+ = \max(., 0) \).

The main procedure of our method is described in Algorithm 1. Denote \( t_0 = 0 \), as FISTA, we generate two vectors \( (v^{k+1}, X_i^{k+1}) \) to minimize the smoothed model in (10) at \( k+1 \) iteration:

\[ v^{k+1} = X_i^k + \frac{t_k - 1}{t_{k+1}} (X_i^k - X_i^{k-1}) \quad \text{and} \quad X_i^{k+1} = p_{L_{f_\mu}}(v^{k+1}), \] (13)

where \( t_{k+1} = (1 + \sqrt{1 + 4t_k^2})/2 \). By using this iterative method to minimize the smoothed model in (10), it will converge to \( X_i^* \), which is the minimum of \( F_\mu(X_i) \). Moreover, \( \| X_i \|_1 \) is a strong convex function, the convergence rate is guaranteed by
\[ F_\mu(X^k) - F(X^*) \leq \frac{2L_f \|X^0 - X^*_f\|^2}{(k + 1)^2}, \]

(14)

where \( k \) is the number of iterations. Meanwhile, by the duality gap theory and theoretical results in refs 27, 42, 48, we can obtain the following important result:

\[ \lim_{k \to \infty} F_\mu(X^k) = F(X^*_f), \]

(15)

and the number of iterations is upper bounded by

\[ \sqrt{8 \|A\| M^2 \varepsilon^2} + \sqrt{\frac{2L_f \varepsilon}{\varepsilon}} \|X^0 - X^*_f\|, \]

(16)

provided that \( F_\mu(X^k) - F(X^*) < \varepsilon \). The more details of proof are referred to refs 27, 42 and 48.

Data Availability. All original data are available from the website FigShare https://figshare.com/articles/adjnoun_gml/4883708.

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**Acknowledgements**

We thank Wenbo Du for useful discussions. We also thank Mark Newman and Xiao Han for providing the point of presence data. This work was supported by the National Natural Science Foundation of China (Grand Nos 61370126, 61672081, U1636211), National High Technology Research and Development Program of China (No. 2015AA016004), Beijing Advanced Innovation Center for Imaging Technology (No. BAICIT-2016001), the Fund of the State Key Laboratory of Software Development Environment (No. SKLSDE-2015ZX-16).

**Author Contributions**

Y.Y. and Z.J.L. developed the study concept and design. Y.Y. collected the data. Y.Y. and T.J.L. analyzed the data. Y.Y. and X.M.Z. interpreted the data, and Y.Y., T.J.L and P.S.Y. drafted the manuscript. All authors provided critical revisions and approved the final version. The first two authors contribute equal contributions to this paper.

**Additional Information**

**Competing Interests:** The authors declare that they have no competing interests.

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