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Topology identification of complex networks from noisy time series using ROC curve analysis

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Abstract As it is known, there is various unknown information in most real world networks, such as uncertain topological structure and node dynamics. Thus how to identify network topology from dynamical behaviors is an important inverse problem for physics, biology, engineering, and other science disciplines. Recently, with the help of noise, a method to predict network topology has been proposed from the dynamical correlation matrix, which is based on a general, one-to-one correspondence between the correlation matrix and the connection matrix. However, the success rate of this prediction method depends on the threshold, which is related to the coupling strength and noise intensity. Different coupling strength and noise intensity result in different success rate of prediction. To deal with this problem, we select a desirable threshold to improve the success rate of prediction by using Receiver Operating Characteristic (ROC) curve analysis. By the technique of ROC curve analysis, we find that the accuracy and efficiency of topology identification is mainly determined by coupling strengths. The success rate of estimation will be reduced if the coupling is too weak or too strong. The presence of noise facilitates topology identification, but the noise intensity is not always crucial to the effectiveness of topology identification.

Keywords Complex networks · Topology identification · Noise · ROC curves

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1 Introduction

Nowadays, complex networks have been playing an increasing role in the study of natural or man-made systems. Examples of such networks include transportation, phone call networks, the World Wide Web, Internet, electrical power grids, food webs, and so on [1, 2]. Over the past decades, the main research focus has been on the impact of topological structures or the statistical properties on the dynamics of complex networks [3–7]. However, significant research interests have been shifted to a challenging issue, which can be described as an inverse problem, i.e. how to estimate the topological structures from dynamical behaviors of complex networks. Some methods have been proposed to address this inverse problem, one of which is the so-called adaptive synchronization technique [8–16]. However, for the technique based on adaptive control, the key to successful estimation of network topology is the linear independence condition, which requires sufficient information and is difficult to verify in real life. Besides, numerous adaptive controllers leads to huge computation, making the scheme impractical in large-scale networks.

Quite surprisingly, the new technique based on the noise-induced relationship between dynamical correlation and network topology does not confront these problems [17]. Theoretical and numerical explorations have shown that there exists a one-to-one correspondence between the dynamical correlation matrix and the connection matrix. The reason lies in the fact that noise enables an accurate prediction of network topology from time series. In Ref. [17], a network coupled by N nonidentical oscillators under noise is considered, which can be expressed as follows:

$$\dot{x}_i = F_i(x_i) - c\sum_{j=1}^{N} L_{ij}H(x_j) + \eta_i, \tag{1}$$

where x_i denotes the d-dimensional state variable of the ith oscillator, c is the coupling strength, the function $F_i(\cdot)$ is the corresponding nonlinear vector function, $H(\cdot)$ is the output function of the individual oscillators, and η_i is the noise term. In addition, $L = (L_{ij})_{N\times N}$ describes the coupling topology of the network, in which $L_{ij} = -1$ if j connects to i (otherwise 0) for $i \neq j$ and $L_{ii} = -\sum_{j=1,j\neq i}^{N} L_{ij}$.

Since L contains full information about the network topology, identifying a network topology, as given in (1), becomes a problem of estimating all elements of the matrix L. To solve this problem, Ref. [17] constructed a dynamical correlation matrix C as mentioned above,

$$C_{ij} = \langle [x_{ik}(t) - \bar{x}(t)] \cdot [x_{jk}(t) - \bar{x}(t)] \rangle, \tag{2}$$

where $\bar{x}(t) = (1/N)\sum_{i=1}^{N} x_{ik}(t)$, and x_{ik} is some component with noise of the ith oscillators. Furthermore, consider linear coupling such that $DH = I$ with Gaussian white noise and ignore the intrinsic dynamics DF is the Jacobian matrix of the coupling function H. Then for an undirected network with symmetric coupling matrix, L can be estimated by

$$L = [\sigma^2/(2c)]C^+, \tag{3}$$

where C^+ denotes the pseudo-inverse of the dynamical correlation matrix C, and σ^2 is the noise intensity. Set l is twice the total number of links. We can calculate l through $l = (S\sigma^2 + \sqrt{S^2\sigma^4 + 8cNS\sigma^2})/4c$ and keep its integral part, where $S = \sum_{i=1}^{N} 1/C_{ii}$. One then ranks all non-diagonal elements of the matrix L in an ascending order, and sets the threshold as the value of the lth item in the ascending-ordered matrix elements. Then the connection matrix can be obtained by setting all elements in L with values above the threshold to be zero and others to be -1, the latter corresponding to existent links.

As a matter of fact, some existent links might always fail to identify in real application if the threshold are determined through the above method. The aim of this paper is not only to provide an appropriate method to determine the threshold, but also to discuss the influence of coupling strength and noise intensity on topology identification. Based on ROC curve analysis, it is shown that too large or too small coupling strength cuts down the success rate of prediction. However, changing the noise intensity cannot greatly improve accuracy and efficiency of topology identification.

The rest of the paper is organized as follows. In Sect. 2 we give three examples which may cause the possible failures of topology identification. In Sect. 3, ROC curve analysis is applied to determine the threshold and analyze the role of coupling strength and noise intensity. Finally, the paper is closed with some concluding remarks.

2 Examples showing failure of topology identification

In this section, three examples are concretely presented to show occurrence of failed topology identification.

First, let us consider consensus dynamics:

$$\dot{x}_i = c\sum_{j=1}^{N} P_{ij}(x_j - x_i) + \eta_i, \tag{4}$$

where $P = (P_{ij})_{N\times N}$ is the adjacency matrix with $P_{ij} = 1$ if node j connects to i (otherwise 0) and $P_{ii} = 0$. Then each non-diagonal element of the matrix $L = P - K$ ($K = (K_{ij})$ is the diagonal matrix of all node degrees) is a parameter to be identified.

In particular, when the network topology is chosen as a friendship network of karate club [18], through Eq. (2) with the coupling strength $c = 0.1$ and the noise intensity $\sigma^2 = 2$, the matrix $[\sigma^2/(2c)]C^+$ could be easily obtained. Figure 1 shows the distribution of non-diagonal elements of $[\sigma^2/(2c)]C^+$. A bimodal distribution can be observed: one peak centered at -1

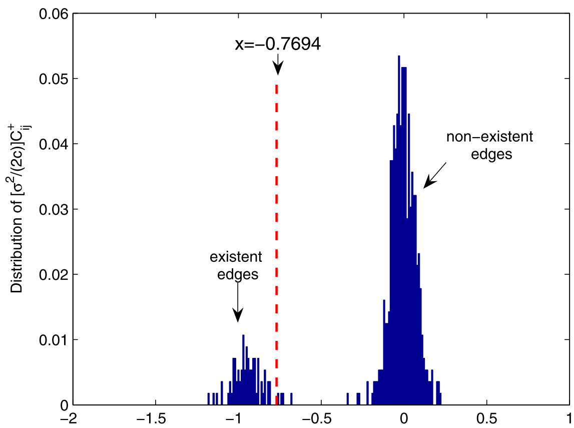

Fig. 1 Distribution of the values of the non-diagonal elements of $[\sigma^2/(2c)]C^+_{ij}$. Here, consensus dynamics with $c = 0.1$, $\sigma^2 = 2$ is used for a friendship network of karate club. The threshold is marked by *red dashed lines* (Color figure online)

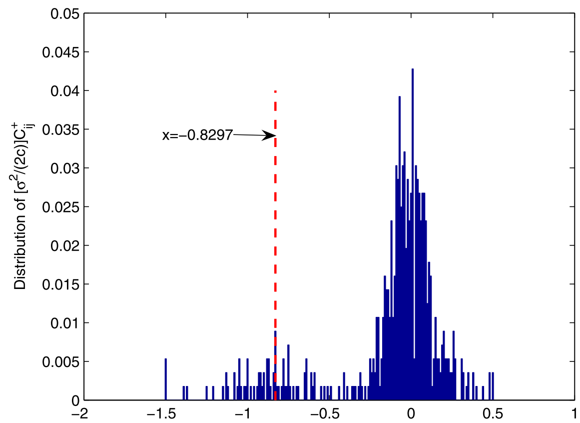

Fig. 3 Distribution of the values of the non-diagonal elements of $[\sigma^2/(2c)]C^+_{ij}$. Here, consensus dynamics $c = 0.1$, $\sigma^2 = 0.00001$ is used for a friendship network of karate club. The threshold is marked by *red dashed lines* (Color figure online)

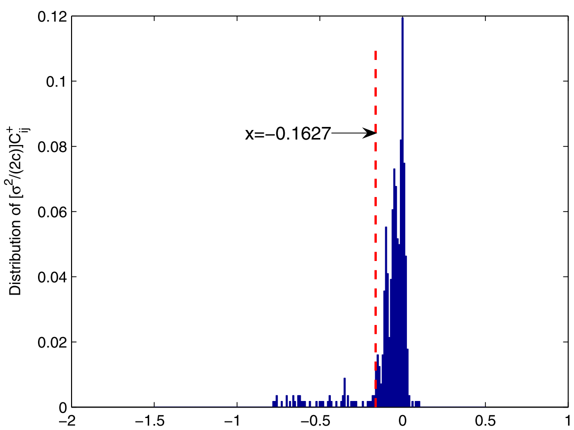

Fig. 2 Distribution of the values of the non-diagonal elements of $[\sigma^2/(2c)]C^+_{ij}$. Here, consensus dynamics $c = 1$, $\sigma^2 = 2$ is used for a friendship network of karate club. The threshold is marked by *red dashed lines* (Color figure online)

corresponds to existent edges and the other peak centered at zero corresponds to zero elements in L. As shown in Fig. 1, one obtains the threshold separating two peaks is -0.7694, which leads to success rates of existent links and of non-existent links are 0.9615 and 1, respectively. Namely, some edges fail to be identified; they are misunderstood for non-existent. In fact, the largest gap between two peaks can perfectly identify the network topology. For example, if the threshold is intuitively determined as -0.5, the success rates of existent links and of non-existent links in both cases are 1. That is to say, all existent and non-existent links are successfully identified.

However, in some cases, two peaks are not separated by large gap. Usually, we cannot obtain two clear peaks when the coupling strength and noise intensity are improper. Here we fix the noise intensity $\sigma^2 = 2$, and change the coupling strength $c = 1$. The distribution of non-diagonal elements of $[\sigma^2/(2c)]C^+$ is shown in Fig. 2. It can be seen from Fig. 2 that there exists only one peak centered at zero and the threshold is -0.1627. Therefore the success rate of existent links and of non-existent links is 0.5641 and 0.9814, respectively. Obviously, it is contrary to expectation that quite a few existent and non-existent links fail to be identified.

Analogously, we fix the coupling strength $c = 0.1$ and choose the noise intensity $\sigma^2 = 0.00001$. Figure 3 shows the distribution of non-diagonal elements of $[\sigma^2/(2c)]C^+$. From Fig. 3 we find that there exists no clear peak centered at -1 and the distribution of the elements is quite in confusion. Therefore the success rates of existent links and of non-existent links are 0.5385 and 0.9917, respectively, under the threshold of -0.8297. This example, as well as the second one, reinforces the fact that failure of topology identification does occur when the coupling strength and the noise intensity are chosen inappropriately.

Three concrete examples have shown that unknown topology identification might be failed when the threshold is selected as mentioned, because the threshold is determined based on the hypothesis that $L = [\sigma^2/(2c)]C^+$ holds accurately. However, in real numerical computation, it is unavoidable that the Laplacian matrix L produced by the dynamical correlation matrix may not be completely consistent with the true topological structure. In particular, when the coupling strength or the noise intensity is improper, the dynamical correlation matrix C cannot contain all information of the true topology of a network, which would result in a failure of topology identification.

3 Topology identification by ROC analysis

In the previous section it was shown that selecting an appropriate threshold is of vital importance for a successful topology identification. In order to select a sound threshold, we, in what follows, adopt ROC curve analysis, a method that has a long history but is unappreciated in topology identification of complex networks.

3.1 ROC curves construction

Receiver Operating Characteristic (ROC) curves analysis was first used during World War II for the analysis of radar signals contaminated by noise [19–21]. More recently it has become remarkably useful in medicine to determine a cut-off value for a clinical test [22]. Here we apply ROC curves analysis to evaluate the impact of the coupling strength and noise intensity on the network topology identification.

For the results of topology identification of a network, one can divide all the possible links into two groups. One group is classified as the existent link (positive), the other group as the non-existent link (negative), according to whether the corresponding estimation value is less or greater than a chosen cut-off value. Associated with any cut-off value is the true positive rate and the true negative rate. It is known from the previous section that the identification will find some, but not all, existent or non-existent links. The success rate of existent links (SREL), i.e., the ratio of the existent links found by the identification to the total number of existent links in a network is the true positive rate (also known as sensitivity). The success rate of non-existent links (SRNL), i.e., the ratio of the non-existent links found by the identification to the total number of non-existent links is the true negative rate (also known as specificity). The schematic outcomes are represented and the statistics are defined in Table 1.

Table 1 Schematic outcomes

Identification	Actual value		Total
	Existent	Non-existent	
Positive	a (true positive)	b (false positive)	$a+b$
Negative	c (false negative)	d (frue negative)	$c+d$
Total	$a+c$	$b+d$	$a+b+c+d$

Sensitivity = True Positive Rate = SREL = $a/(a+c)$
Specificity = True Negative Rate = SRNL = $d/(b+d)$
False Positive Rate = $b/(b+d) = 1 -$ Specificity

The goal is that the ROC curve analysis could find a cut-off value that will minimize the number of false positives and false negatives. In a ROC curve the true positive rate (sensitivity) is plotted as a function of the false positive rate (1-specificity) for all possible values of the cut-off points [23]. Each point on the ROC curve represents a sensitivity/specificity (SREL/SRNL) pair corresponding to a particular decision threshold. Note that all ROC curves start at the point $(0, 0)$, representing a threshold at which they all are classified as non-existent links, and end at $(1, 1)$, meaning a threshold at which all are classified as existent links, as shown in Figs. 4, 5, 6, 7. The ROC curve of an identification with perfect discrimination (no overlap in the two distributions) will pass through the upper left corner $(0, 1)$ with 100 % sensitivity (SREL) and 100 % specificity (SRNL). Therefore the closer the ROC curve is to the upper left corner, the higher the overall accuracy of the identification.

An important measure of the effectiveness of topology identification is the area under the ROC curve (AUC). If this area is equal to 1.0, then the ROC curve consists of two straight lines, one vertical from the point $(0, 0)$ to the point $(0, 1)$ and the next horizontal from $(0, 1)$ to $(1, 1)$. This means 100 % accuracy because both the SREL and SRNL are 1.0 with no false positives and no false negatives. In fact, AUC, with values close to 1.0 indicates high identification effectiveness. We will compare the impact of coupling strength and noise intensity on the effectiveness of topology identification by statistically comparing the AUC for each estimation.

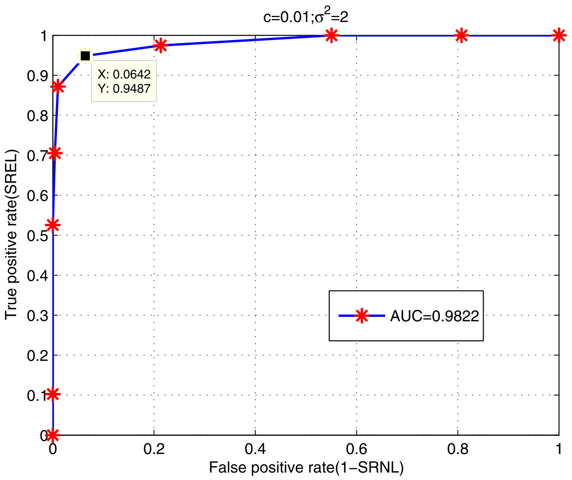

Fig. 4 ROC curve for topology identification. Here, consensus dynamics $c = 0.01$, $\sigma^2 = 2$ is used for a friendship network of karate club

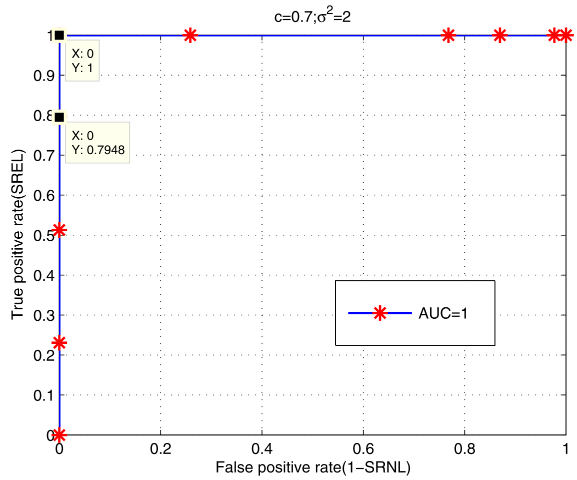

Fig. 6 ROC curve for topology identification. Here, consensus dynamics $c = 0.7$, $\sigma^2 = 2$ is used for a friendship network of karate club

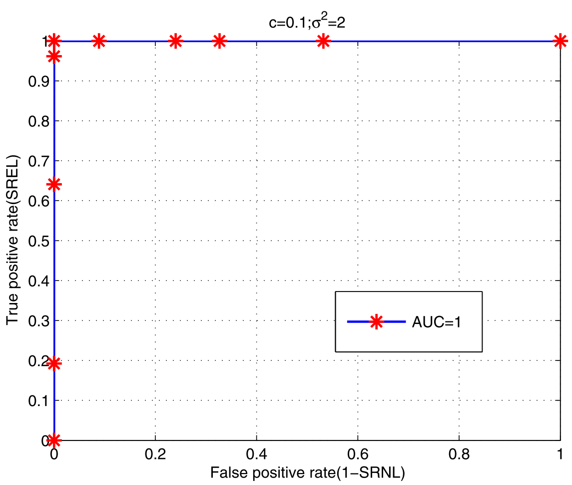

Fig. 5 ROC curve for topology identification. Here, consensus dynamics $c = 0.1$, $\sigma^2 = 2$ is used for friendship network of karate club

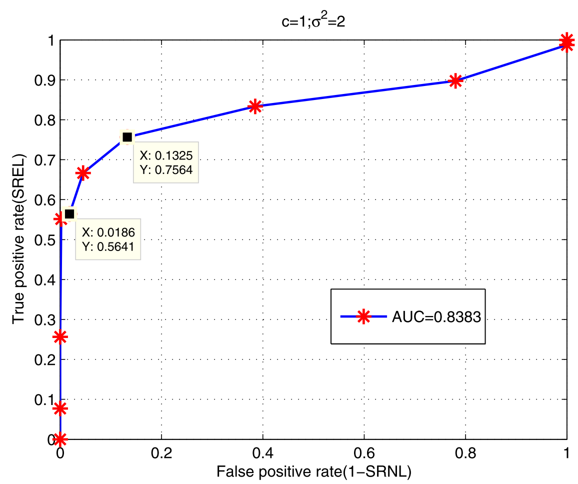

Fig. 7 ROC curve for topology identification. Here, consensus dynamics $c = 1$, $\sigma^2 = 2$ is used for a friendship network of karate club

3.2 Threshold selection in ROC curves

The fundamental trade-off between true positives and false positives is inherent when one estimates the network topology by using noise-induced dynamical correlation matrix. To identify the network topology with high SREL and SRNL, we use here the information presented in a ROC curve to choose the most desirable threshold.

In the case of consensus dynamics with $c = 0.1$ and $\sigma^2 = 2$ for a friendship network of karate club, for example, one obtains SREL $= 0.9615$ and SRNL $=$ 1 with the threshold $= -0.7694$, as mentioned in Sect. 2. We know that some existent links are not found. Therefore, we plot a ROC curve to show the trade-off between the existent links found (true positives) and the non-existent ones which are mistakenly taken for existent links (false positives) at every possible thresholds. Since the values of the non-diagonal elements of $[\sigma^2/(2c)]C^+$ are in the range of -1.2 to 0.25, which can be seen from Fig. 1, we set the values of the cut-off as $[-1.2, -1, -0.9, -0.7694,$

Table 2 Sensitivity and specificity results for different cut-off values with $c = 0.1, \sigma^2 = 2$

Cut-off values	Sensitivity (SREL)	Specificity (SRNL)	False positive rate (1 − SRNL)
−1.2	0	1	0
−1	0.1923	1	0
−0.9	0.641	1	0
−0.769	0.9615	1	0
−0.7	***1***	***1***	***0***
−0.1	1	0.911	0.089
−0.05	1	0.7598	0.2402
−0.03	1	0.6729	0.3271
0	1	0.468	0.532
0.25	1	0	1
			AUC = 1

$-0.7, -0.1, -0.05, -0.03, 0, 0.25]$, and compute the true positive rates (SREL) and the false positive rates (1−SRNL) over these different cut-off values. The results are shown in Table 2. This yields the ROC curve as shown in Fig. 5, which presents the trade-off and the area under the ROC curve for topology identification in this case.

From Fig. 5 and Table 2 one see that the ROC curve passes the upper left corner (0, 1) with AUC = 1, which implies that setting the optimal threshold as −0.7 can discriminate perfectly the existent links from the non-existent links, with 100 % SREL and 100 % SRNL. This obtained SREL is obviously improved compared with the result at the threshold = −0.7694.

For the case of $c = 0.7, \sigma^2 = 2$, as shown in Fig. 6, we can obtain the optimal threshold = −0.2 based on the ROC curve analysis, which results in SREL = 1 and SRNL = 1. This is far more accurate than the results with SREL = 0.7681 and SRNL = 1 at the threshold of = −0.3633 based on the theoretical determination in [17]. However, for most cases, topology identification should not be expected to perform perfectly, and thus the ROC curves cannot pass the upper left corner (0, 1), such as shown in Figs. 4 and 7. Hence, one can choose the point on the curve closest to the upper corner. We see that the corresponding threshold is optimal, since it maximizes the separation between existent (positive cases) and non-existent links (negative cases).

3.3 Comparison with coupling strengths

Presented visually, ROC curves allow inspection of a fundamental trade-off between true positives and false positives for a fixed coupling strength. When comparing the impacts of two coupling strengths, AUC can be used as a measure of which coupling strength is better overall. ROC curves make it clear that the curve with larger AUC represents the coupling strength that will perform better. Here, we fix the noise intensity at $\sigma^2 = 2$.

From Figs. 4–7 it is found that AUC first increases, then trends toward the constant 1.0, and finally decreases as the coupling strength increases. This implicates that too small or too large coupling strength leads to a failure in topology identification. Only when the coupling strength is in a bounded domain, the network topology will be perfectly estimated.

Therefore, it poses one question: "Why does the coupling strength cause so huge differences in topology identification?" The key to the answer lies in the dynamical correlation matrix, which might have a close link with the connections between nodes. When the coupling strength is very small, dynamical correlation matrix cannot contain all the information about the network topology, since the dynamical relation between every two nodes is very weak. When the coupling strength is increased to some value, nodes in the network approximatively synchronize. That is to say,

$$x_i(t) \to \hat{x}(t) = \frac{1}{N}\sum_{i=1}^{N} x_i(t), \quad t \to \infty, \ \forall 1 \le i \le N.$$

Namely, the dynamical correlation $C_{ij} = \langle [x_i(t) - \hat{x}(t)] \cdot [x_j(t) - \hat{x}(t)] \rangle$ between node i and node j will trends toward zero, as shown in Fig. 8. Thus nodes in the network have a close resemblance in the dynamical correlation, which gives rise to a singular dynamical correlation matrix, and a failure to identify the network topological structure.

3.4 Comparison with noise intensity

Noise, as a bridge between dynamical correlation and topology, cannot be neglected in practice. So in this subsection we will study the impact of the noise intensity on topology identification.

First, we fix the coupling strength $c = 0.001$ and change the value of the noise intensity σ^2. We find

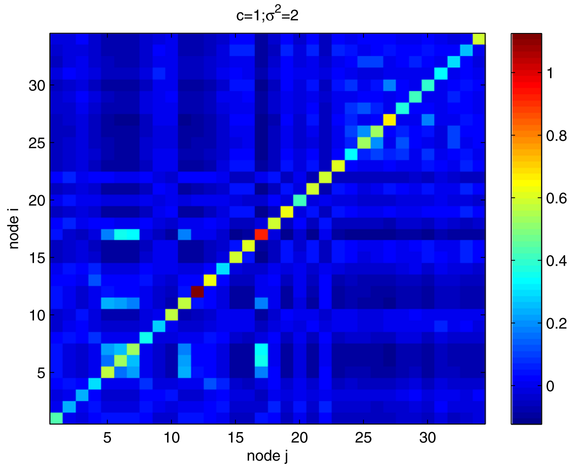

Fig. 8 Dynamical correlation between node i and node j. Here, consensus dynamics $c = 1$, $\sigma^2 = 2$ is used for a friendship network of karate club

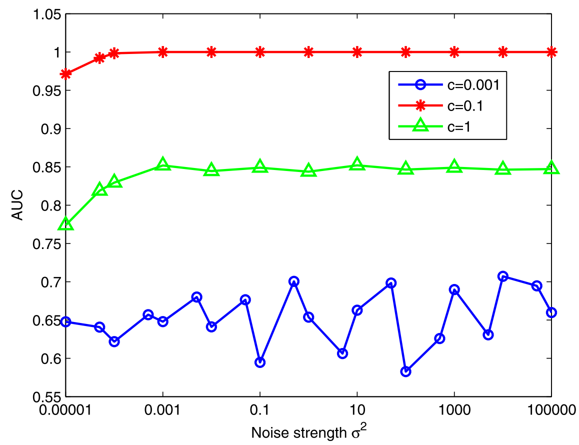

Fig. 9 The area under ROC curves as a function of the noise intensity. Here, consensus dynamics is used for a friendship network of karate club

that although the noise intensity improves, the value of AUC varies without no clear upward trend. It seems that AUC always goes up and down with the change in the noise intensity, observed in Fig. 9.

Then the coupling strength is set as $c = 0.1$ and consider the change of the noise intensity. It can be seen from Fig. 9 that only when the noise intensity is very small and close to zero, the value of AUC is less than 1. As the noise intensity increases, the value of AUC improves and remains in AUC = 1.

Finally, we set the coupling strength at $c = 1$. A similar phenomenon can be observed in Fig. 9 as when the noise intensity increases, the values of AUC rises and remains unchanged.

From Fig. 9 it is clear that topology identification is crucially determined by the coupling strength. When the coupling strength is large enough, the noise with extremely low intensity would have a negative effect on topology estimation. This is because when the noise intensity is close to zero, $\sigma^2/(2c)$ will approach zero, which results in $L = [\sigma^2/(2c)]C^+$ trending toward zero. This means that the accuracy and precision of topology identification falls but quite a little. That is to say, decreasing or increasing the noise intensity cannot clearly improve the effectiveness of topology identification. However, when the coupling is very weak, the value of AUC is always quite small, with wide fluctuations although the noise intensity increases, which implies that the noise intensity will make the effectiveness of topology identification vary irregularly in the case of weak coupling. In fact, Fig. 9 is another proof that the accuracy and efficiency of topology estimation is mainly determined by the coupling strength.

It is known that noise is of great importance to topology identification, since the presence of noise can guarantee that the dynamical correlation matrix C be generalized invertible. For weak coupling, changing the noise intensity will reduce to an irregular fluctuation. However, for strong coupling, the noise intensity has no much impact on the accuracy and efficiency of topology identification except the extremely low noise strength.

4 Conclusions

In brief, we have numerically provided concrete examples for showing a possible failure in topology identification from noisy time series. However, making good use of ROC curve analysis might easily lead to a higher SREL and SRNL, as the optimal threshold is selected to maximize the separation between existent links and non-existent links. Moreover, the area under a ROC curve has been used to analyze the impact of coupling strength and noise intensity on topology identification. It has been found that too strong or too weak coupling makes topology reconstruction of complex networks impossible. A network can be successfully identified if the coupling strength is large enough without resulting in synchronization. What is more, noise bridges dynamical correlation and network topology, but the noise intensity cannot remarkably improve the success rate of topology identification.

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