

## RESEARCH ARTICLE

# A Novel Method for Estimating Accuracy of Network Structure Recovery Model

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**ABSTRACT** Many practical systems can be considered as networks of nodes interacting. Explicit network topology is a straightforward method to understand the actual system, so it is of practical significance to obtain the complete network topology from the empirically measured time series. With the premise that the dynamics equations and coupling matrix are known, a method to reconstruct the network topology from the measured time series is proposed, and based on regression theory the estimated matrix form of the adjacency matrix is given. Also, the method is suitable for predicting arbitrary weights of network connections, and its practicality is verified by numerical simulations. Importantly for the 0–1 matrix, a new method for judging the prediction performance of the model using the false negative rate is proposed. It can estimate the accuracy of model prediction with only partial sampling data when the information of network topology is unknown. In addition, a method that can control false positives is proposed, and the feasibility of the method is verified by numerical simulation. Finally, two factors that affect model performance, the amount of sample data and the intensity of noise, are discussed.

**INDEX TERMS** Reconstruction, false negative rate, regress theory.

## I. INTRODUCTION

A complex network is a network structure composed of a huge number of nodes and intricate relationships between nodes. Complex systems are ubiquitous in nature, such as weather systems [1], electric power systems [2], and gene regulation systems [3], which can be abstracted into complex networks for study. By representing the individuals in a system as nodes of a network and the interactions between individuals as connections between nodes, the nature of the network can be used to understand and control the function of the actual system [4], [5]. Complex networks are now widely used in various scientific fields, such as biology, engineering and sociology [6], [7], [8], [9], [10]. However, the topology of complex networks is often unknown, yet the structure affects the functionality of the system, so an important issue for complex networks is the structure problem.

In recent years, more and more attention has been paid to the study of network topology. In order to show the topology

structure of the network directly, it can be simplified into a graph for study. The Laplacian matrix [11] of the graph can be estimated under some observed data, which is usually expressed by the adjacency matrix, and the Laplacian matrix can reflect the properties of the graph [12], [13], so the Laplacian matrix can be used for topological reconstruction. For example, Ying et al. proposed to learn sparse graphs from the Laplacian constrained Gaussian graph model [14]. Sandeep et al. proposed a variety of algorithms that can simultaneously learn the graph structure and their weights [15]. The study of network topology is helpful to solve many problems in the real world [16], [17], [18].

The reconstruction of topology and dynamics from time series data has been the focus of research in the problem of studying network topology [19]. Various methods have been proposed and validated in recent years. For example, network reconstruction is based on missing complements and spurious screening of connection relationships, so link prediction can be used as a method for network reconstruction. Using this method, future links and existent yet unknown links in the network can be obtained [20], [21]. LÜ discussed structural

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similarity-based and maximum likelihood estimation-based link prediction methods to predict unknown connections in networks, which can be applied to social networks and protein interaction networks, etc [22]. In addition, the correlation method can be used to determine whether there are links between nodes based on the correlation of the node time series, which can be applied to establish a gene-coexpression network [23]. It can also be applied to the economic and financial spheres. R.N.Mantegna studied the hierarchical organization that exists within the stock market through correlation coefficient matrices [24]. For the problem of delay effects affecting each other in real systems, L.Kullmann, Zhang et al. transformed it into a delay correlation problem of time series and gave the corresponding links between nodes to reconstruct the network structure according to this method [25], [26].

A classical idea of reconstructing networks from time series is to transform a nonlinear system of dynamical equations into a linear system by certain methods to solve the network reconstruction problem. In recent years, methods based on this idea have been proposed and continuously promoted. Compressed sensing is gradually applied to network reconstruction and becomes the focus of research [27], which is applicable to sparse networks. For problems with large amounts of experimental data and low practicality, sparse solutions can be obtained using compressed sensing theory to identify the node connectivity relationships contained in the sparse solutions [28], [29]. For the problem that the dynamic basis function of network nodes is unknown, Li et al. proposed a new method based on Taylor expansion and compressive sensing to reconstruct the network topology [30]. Under the intra-network interaction functions to be known, Levnajic Z proposed a method for reconstructing dynamic networks from time series, and derived a simple equation that directly yields the adjacency matrix [31]. In the presence of significant noise and low data availability in sparse networks, Napoletani and Sauer used linearization of the dynamics around the center of a neighborhood of data points, and constrained optimization technology based on L1 norm to reconstruct the topology of sparse connected networks [32]. André Fujita et al. proposed the Sparse Vector Autoregressive model to estimate gene regulatory networks, which can infer true positive links even under conditions in which the number of samples is smaller than the number of genes, and proposed the use of statistical tests to control the false discovery rate for the first time in gene regulatory networks [33]. Shandilya S G proposed the analytical solution to the inverse problem of finding the network topology from observing a time series of state variables only, provided that the kinetic and coupling functions are known. [34].

The focus of these methods is to transform the system into linear equations. The network reconstruction problem is transformed into a mathematical problem of equation solving coefficients. Based on this idea, we propose a simple and straightforward method to build a network structure recovery model based on time series using regression

theory. It is possible to reconstruct various types of network topologies. The practicality of the method is verified by numerical simulation experiments. In addition, the method is extended to predict the nonzero weights of connections between network nodes. Two factors, sample data and noise intensity, which affect the recovery performance of the model are analyzed.

The traditional evaluation methods for 0-1 matrix require information on the topology of the prophetic network [32], [33], [35], while in practical systems it is generally not possible to obtain an explicit adjacency matrix, which limits its application. To overcome this difficulty, we propose a model evaluation method that does not rely on the original adjacency matrix: the false negative rate. The method relies only on sample data, which makes it possible to estimate the accuracy of model predictions with incomplete a priori information and is more realistic. In addition, for the overall hypothesis testing problem of regression coefficients, we propose to control the false discovery rate (False Discovery Rate) by statistical tests, and we adopt the *BH* method [36] to control the number of false positives within a predetermined range.

This paper is divided into three parts. The first part introduces the network structure reconstruction model, gives the form of the estimation matrix of the adjacency matrix, and additionally introduces the necessary statistical knowledge; The second and third parts evaluate the reconstruction performance of the model using numerical simulation methods and illustrate the feasibility and practicality of selecting the false-negative rate as the evaluation index. The cases in which the model reconstructs the network topology and the case in which the model predicts the connection weights between the network nodes are simulated, respectively. Two factors affecting the performance of the model are discussed.

## II. METHOD

Regression analysis is a statistical method used to determine the quantitative relationship of interdependence between two or more variables. The actual network system studied in this paper contains multiple independent variables and shows a linear relationship between the dependent and independent variables. Therefore, multiple linear regression model can be used to reconstruct the node connection relationship of the actual network.

### A. NETWORK STRUCTURE RECONSTRUCTION MODEL

Consider a complex system consisting of  $N$  interacting units, which is represented as a network of  $N$  nodes, with the dynamics of the  $i$ -th node being described by

$$\dot{x}_i = f_i(t, x_i) + \sum_{j=1}^N c_{ij} A x_j + \varepsilon_i, \quad i = 1 \dots N \quad (1)$$

where  $x_i = (x_{i1}, x_{i2} \dots x_{id})^T$  is  $d$ -dimensional state variables;  $f_i$  describing the local dynamics of node  $i$ ;  $C = (c_{ij})_{N \times N}$  represents the adjacency matrix, describing the connection status between node  $i$  and node  $j$ .  $c_{ij} = 1$  ( $i \neq j$ )

means that there is a connection between node  $i$  and node  $j$ ,  $c_{ij} = 0$  ( $i \neq j$ ) means that there is no connection between node  $i$  and node  $j$ , and its diagonal elements are defined as  $c_{ii} = -\sum_{j=1, j \neq i}^N c_{ij}$ .  $A$  represents the internal coupling matrix;  $\epsilon_i$  represents the error, which is assumed to be mutually independent and obey  $N(0, \sigma^2)$  distribution.

In the network represented by (1), assuming that  $f_i$  and  $A$  are known. The network structure reconstruction model is established to reconstruct the network topology by using the  $x_i$  obtained from the observable records, that is, to predict  $C$ . Thus the problem of recovering the network topology can be interpreted as estimating  $C$  from the measurable data  $X$  and  $Y$  in the form  $Y = XC + \epsilon$ , where  $C$  is an  $N \times N$  matrix. Considering it as a multiple linear regression problem, the reconstruction can be achieved by letting the error sum of squares be minimized, that is

$$\min(Y - \hat{Y})^2$$

where  $Y$  and  $\hat{Y}$  represent the observed and predicted values, respectively. In order to recover the topology of the network (1), it can be transformed into the above form for analytical discussion.

Since the system dynamics equation is known, equation (1) can be rewritten as

$$\dot{x}_i - f_i(t, x_i) = \sum_{j=1}^N c_{ij}Ax_j + \epsilon_i, \quad i = 1 \dots N \quad (2)$$

Since  $x_i$  is a  $d$ -dimensional variable, one has  $\dot{x}_i = (\dot{x}_{i1}, \dot{x}_{i2} \dots \dot{x}_{id})^T$ . Then for the  $i$ -th node the  $k$  ( $k = 1 \dots d$ ) components have

$$\dot{x}_{ik} - f_{ik}(t, x_i) = \chi_{ik}C_i + \epsilon_{ik} \quad (3)$$

where

$$\begin{aligned} \chi_{ik} &= (\mathbf{1}, \mathbf{A}_{k1}\mathbf{x}_{11} + \mathbf{A}_{k2}\mathbf{x}_{12} + \dots + \mathbf{A}_{kd}\mathbf{x}_{1d}, \\ &\quad \mathbf{A}_{k1}\mathbf{x}_{21} + \mathbf{A}_{k2}\mathbf{x}_{22} + \dots + \mathbf{A}_{kd}\mathbf{x}_{2d}, \dots, \\ &\quad \mathbf{A}_{k1}\mathbf{x}_{N1} + \mathbf{A}_{k2}\mathbf{x}_{N2} + \dots + \mathbf{A}_{kd}\mathbf{x}_{Nd}) \\ C_i &= (c_{i0}, c_{i1}, c_{i2}, \dots, c_{iN})^T \end{aligned}$$

The  $m$ -group time series obtained from the experimental observation records as sample data, the following equation for the  $k$ -th dimension of the  $i$ -th node in the form of  $Y = CX + \epsilon$ :

$$\begin{aligned} Y_{ik} &= \begin{pmatrix} \dot{x}_{ik}(t_1) - f_{ik}(t_1, x_i) \\ \dot{x}_{ik}(t_2) - f_{ik}(t_2, x_i) \\ \vdots \\ \dot{x}_{ik}(t_m) - f_{ik}(t_m, x_i) \end{pmatrix} \\ &= \begin{pmatrix} \chi_{ik}(t_1) \\ \chi_{ik}(t_2) \\ \vdots \\ \chi_{ik}(t_m) \end{pmatrix} C_i + \epsilon_{ik} = X_{ik}C_i + \epsilon_{ik} \end{aligned}$$

The problem of restoring the network topology structure is transformed into the problem of solving multiple linear regression parameter  $C$ . Here the approach of individual regression analysis is taken for each node, and each column

$C_i$  ( $i = 1, \dots, N$ ) of the adjacency matrix  $C$  is estimated by the sum of squares of the minimum error, and the predicted adjacency matrix  $\hat{C}_i$  is obtained. The loss function utilizes the form of the mean square error, which is also the objective function, that is

$$L(C_i) = \frac{1}{2}(X_{ik}C_i - Y_{ik})^T (X_{ik}C_i - Y_{ik}) \quad (4)$$

To determine the parameter  $C$  of the model and make the predicted value as close to the real value as possible, it is equivalent to finding the minimum value of  $L(C_i)$ . The objective function (4) contains the parameter  $C$  required to be solved, so the parameter  $C$  in model (3) can be solved in the process of solving the minimum value of (4). Here, the least square method is selected for solving. The point where the first partial derivative of  $C_i$  is  $0$  is the minimum point of (4).

$$\begin{aligned} \nabla_{C_i}L(C_i) &= \frac{1}{2}\nabla_{C_i}(X_{ik}C_i - Y_{ik})^T (X_{ik}C_i - Y_{ik}) \\ &= \frac{1}{2}\nabla_{C_i} \left( C_i^T X_{ik}^T - Y_{ik}^T \right) (X_{ik}C_i - Y_{ik}) \\ &= \frac{1}{2}\nabla_{C_i} \left( C_i^T X_{ik}^T X_{ik}C_i - C_i^T X_{ik}^T Y_{ik} \right. \\ &\quad \left. - Y_{ik}^T X_{ik}C_i + Y_{ik}^T Y_{ik} \right) \\ &= \frac{1}{2}\nabla_{C_i} \text{tr} \left( C_i^T X_{ik}^T X_{ik}C_i - C_i^T X_{ik}^T Y_{ik} \right. \\ &\quad \left. - Y_{ik}^T X_{ik}C_i + Y_{ik}^T Y_{ik} \right) \\ &= \frac{1}{2} \left[ \nabla_{C_i} \text{tr} \left( C_i^T X_{ik}^T X_{ik}C_i \right) \right. \\ &\quad \left. - \nabla_{C_i} \text{tr} \left( C_i^T X_{ik}^T Y_{ik} \right) - \nabla_{C_i} \text{tr} \left( Y_{ik}^T X_{ik}C_i \right) \right] \\ &= \frac{1}{2} \left( X_{ik}^T X_{ik}C_i + X_{ik}^T X_{ik}C_i \right. \\ &\quad \left. - X_{ik}^T Y_{ik} - X_{ik}^T Y_{ik} \right) \\ &= X_{ik}^T (X_{ik}C_i - Y_{ik}) \\ &= 0. \end{aligned}$$

where  $\text{tr}(A) = \sum_{i=1}^n a_{ii}$  denotes the trace of the matrix  $A$ . It follows that  $\hat{C}_i = (X_{ik}^T X_{ik})^{-1} X_{ik}^T Y_{ik}$  is the least-squares estimate of  $C_i$ , and the method is applicable to the case when the inverse matrix of  $X_{ik}^T X_{ik}$  exists ( $m > N$ ). When the inverse matrix does not exist, it adopts the form of pseudo-inverse.  $\hat{C}_i$  is an unbiased estimate of  $C_i$ , and unbiasedness ensures that the least squares estimate has a better result, where notation  $\hat{C}_i = (\hat{c}_{i0}, \hat{c}_{i1}, \dots, \hat{c}_{iN})^T$ .

### B. FALSE-NEGATIVE EVALUATION MODEL

After the regression result of adjacency matrix  $C$  is obtained by estimating the parameters of model (3), the regression coefficient needs to be tested to determine whether there is a connection between nodes. Hypothesis testing is adopted in this paper. Since the adjacency matrix of the study network is a  $0 - 1$  matrix, there are only two hypotheses  $c_{ij} = 0$  and  $c_{ij} = 1$ , where  $c_{ij} = 0$  means there is no connection

between node  $i$  and node  $j$  and  $c_{ij} = 1$  means there is connection between node  $i$  and node  $j$ , and one and only one of these two hypotheses will occur. In order to find which nodes are connected to each other, that is, to judge which position elements in the matrix are 1, we can consider from its opposite. Firstly, we assume  $c_{ij} = 0$ . If there are good reasons why it is not true, then we can accept  $c_{ij} = 1$ . Therefore, the following assumptions are established:

$$H_0^{ij} : c_{ij} = 0, \quad H_1^{ij} : c_{ij} = 1$$

The hypothesis testing method chosen in this paper is the  $t$ -test. Knowing  $\hat{c}_{ij} \sim N(c_{ij}, \sigma^2 w_{jj})$ , construct the test statistic when the hypothesis  $H_0^{ij}$  is true

$$t_{ij} = \frac{\hat{c}_{ij}}{\sqrt{w_{jj} \hat{\sigma}^2}} \sim t(m-N-1)$$

where  $t(m-N-1)$  denotes the  $t$ -distribution with  $(m-N-1)$  degrees of freedom,  $w_{jj}$  is the  $(j+1)$ -th diagonal element of  $(X_{ik}^T X_{ik})^{-1}$ ,  $\hat{\sigma}^2 = \frac{Se}{m-N-1}$  is the unbiased estimate of  $\sigma^2$ ,  $Se = (X_{ik} \hat{C}_i - Y_{ik})^T (X_{ik} \hat{C}_i - Y_{ik})$  is the residual sum of square.  $t_{ij}$  is the statistic used to test whether  $c_{ij}$  is equal to 0. Taking the significance level as  $\alpha$  ( $0 < \alpha < 1$ ), we select  $\alpha = 0.05$ . The null hypothesis  $H_0^{ij}$  is rejected and the alternative hypothesis  $H_1^{ij}$  is accepted when  $|t_{ij}| \geq t_{1-\frac{\alpha}{2}}(m-N-1)$ . In this case,  $c_{ij} = 1$  in the adjacency matrix  $\hat{C}$  is considered; Conversely when the null hypothesis is not rejected, it is considered that  $c_{ij} = 0$ . The predicted matrix is denoted  $\hat{C}$ , whose diagonal elements are defined as  $\hat{c}_{ii} = -\sum_{j=1, j \neq i}^N \hat{c}_{ij}$  and called  $\hat{C}$  as the estimation matrix.

Define evaluation metrics:

$E = \frac{d}{D}$  is the model unrecognized rate, where  $d$  denotes the number of connections between network nodes that are not recognized by the model, and  $D$  denotes the number of true connections between network nodes;

$FPR = \frac{l}{L}$  is the model false positive rate, where  $l$  denotes the number of network nodes that are not connected to each other but are recognized by the model as connected, and  $L$  denotes the number of network nodes that are not connected to each other;

$FDR = \frac{k}{K}$  is the model false discovery rate, where  $K$  denotes the number of nodes between which the model identifies the network as having connections.

The rejection region of the hypothesis test is  $W = \left\{ |t| \geq t_{1-\frac{\alpha}{2}}(m-N-1) \right\}$ . When  $c_{ij}$  falls into the rejection domain then the null hypothesis should be rejected and  $c_{ij} \neq 0, c_{ij} = 1$ . When  $H_0^{ij}$  is true,  $\hat{c}_{ij} \sim N(0, \sigma^2 w_{jj})$ . There are two types of errors that can be made when making judgments. If there is an error in which the null hypothesis  $H_0^{ij}$  is not valid, but the  $c_{ij}$  does not in the rejection region  $W$ , the error is said to be a false negative error. The false negative

rate is

$$\begin{aligned} \beta &= p(\hat{c}_{ij} \notin W | c_{ij}=1) \\ &= p\left(|t| < t_{1-\frac{\alpha}{2}}(m-N-1) | c_{ij}=1\right) \\ &= p\left(-t_{1-\frac{\alpha}{2}}(m-N-1) < \frac{\hat{c}_{ij}}{\sqrt{w_{jj} \hat{\sigma}^2}} \right. \\ &\quad \left. < t_{1-\frac{\alpha}{2}}(m-N-1) | c_{ij}=1\right) \\ &= p\left(-t_{1-\frac{\alpha}{2}}(m-N-1) - \frac{1}{\sqrt{w_{jj} \hat{\sigma}^2}} < \frac{\hat{c}_{ij}-1}{\sqrt{w_{jj} \hat{\sigma}^2}} \right. \\ &\quad \left. < t_{1-\frac{\alpha}{2}}(m-N-1) - \frac{1}{\sqrt{w_{jj} \hat{\sigma}^2}} | c_{ij}=1\right) \\ &= \Phi\left(t_{1-\frac{\alpha}{2}}(m-N-1) - \frac{1}{\sqrt{w_{jj} \hat{\sigma}^2}}\right) \\ &\quad - \Phi\left(-t_{1-\frac{\alpha}{2}}(m-N-1) - \frac{1}{\sqrt{w_{jj} \hat{\sigma}^2}}\right) \end{aligned} \quad (5)$$

where  $\Phi(u) = \frac{1}{\sqrt{2\pi}} \int_{-\infty}^u e^{-\frac{x^2}{2}} dx$  ( $u \geq 0$ ) denotes the normal distribution function.

Evaluating the predictive performance of the network structure reconstruction model using the unrecognized rate  $E$ ,  $ROC$  and  $AUC$  requires knowledge of the topology of the network, while the adjacency matrix  $C$  cannot be obtained in practice. This difficulty can be solved by our proposed false-negative rate  $\beta$ , which estimates the accuracy of the model when  $C$  is unknown, based on only partial sample data. This allows us to calculate the accuracy of model reconstruction with incomplete a priori information about the system.

### C. CONTROL FOR FALSE POSITIVE

If there is an error in which the null hypothesis holds but  $c_{ij}$  falls into the rejection region  $W$ , the error is said to be a false positive error (Type I error). In the Neyman-Pearson hypothesis test, the false positive rate can be required to be within an acceptable range. The test level  $\alpha=0.05$  is set to limit the probability of committing a Type I error, through which error control of statistical inferences from single-weighted hypothesis tests is achieved. The false positive rate is controllable within a single hypothesis test, but for multiple hypotheses as a whole, the false positive results increase with the number of tests and become invalid beyond a predetermined range. Therefore, multiple hypothesis tests should be conducted for the regression coefficient  $C$  as a whole. The Benjamini-Hochberg method is selected to control FDR, which can control FDR below the statistically significant level  $\alpha$ . Adjust the  $p$ -value to control the false discovery rate. The process is as follows:

For the hypothesis test  $\{H_0^{ij}\}_{i,j=1 \dots N, i \neq j}$ ,  $H_0^{ij}$  denotes the null hypothesis for the  $ij$ -th test. The  $p$ -values of all tests are sorted to generate sequential numbers

$\{p_k\}, k=1, \dots, s$ . Let  $q_{\max}=p_{\max}$ . Define

$$q_k = \min \left\{ p_k \frac{s}{k}, p_{k-1} \right\}, \quad k=1, \dots, s-1$$

where  $s$  represents the number of tests. When  $q_k < \alpha$ , the first  $k$  hypotheses are rejected and the nodes in the network are considered to be connected to each other.

### III. NETWORK STRUCTURE RECONSTRUCTION RESULTS AND ANALYSIS

#### A. NUMERICAL SIMULATION

Consider a network consisting of *Lorenz* systems as nodes, which consists of 10 bidirectionally coupled *Lorenz* oscillators [37], whose topology is shown in Figure 1.

Its adjacency matrix is as shown at the bottom of the page. The nodal dynamics is described as a *Lorenz* system:

$$f_i(x_i) = \begin{cases} a(x_{i2} - x_{i1}) \\ cx_{i1} - x_{i1}x_{i3} - x_{i2} \\ x_{i1}x_{i2} - bx_{i3} \end{cases}$$

where  $a, b, c$  are real parameters,  $a=10, b=8/3, c=28$ . Take the internal coupling matrix as

$$A = \begin{pmatrix} 0 & 0 & 0 \\ 0 & 0 & 0 \\ 0 & 0 & 1 \end{pmatrix}$$

The fourth-order Runge-Kutta algorithm is used to generate  $M$  sets of time series in (2), in which any  $m$  sets are taken as sample data. Experimental observations were fixed at a uniform time interval  $\Delta t=0.01$  sampling, selected Gaussian white noise with  $\sigma^2=0.5$ , and use model (3) to reconstruct the connection relationship between network nodes. Since the experiments are subject to randomness, the following experiments are taken to average the results of multiple experiments.

By linear approximation the time derivative as

$$\dot{x}_{ik}(t_q) := \frac{x_{ik}(t_{q+1}) - x_{ik}(t_{q-1})}{t_{q+1} - t_{q-1}}, \quad q=1, \dots, m$$

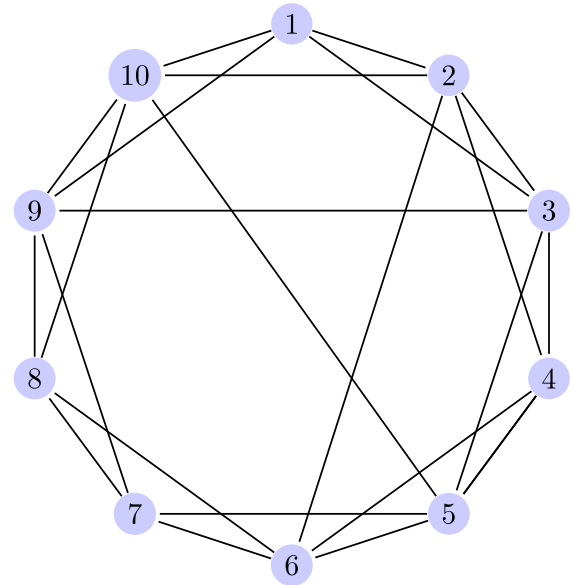


FIGURE 1. Network topology.

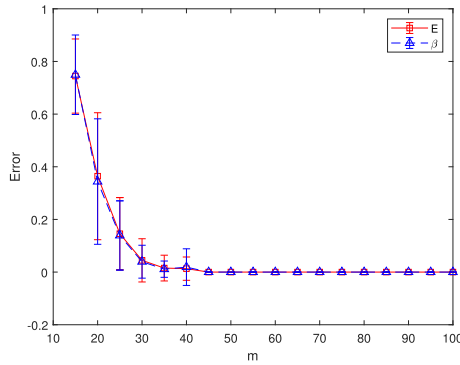
#### B. FALSE NEGATIVE RATE

The null hypothesis  $H_0^{ij} : c_{ij}=0$  to the alternative hypothesis  $H_1^{ij} : c_{ij}=1$ , taking the significance level  $\alpha=0.05$ .  $\hat{C}$  is the adjacency matrix reduced using model (3), and the unrecognized rate  $E$  of the model can be obtained from the network topology and the number of node connections predicted by the model.

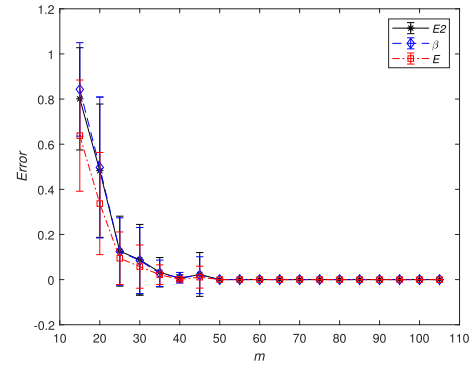
The rejection region of the hypothesis test is  $W = \left\{ |t| \geq t_{1-\frac{\alpha}{2}}(m-N-1) \right\}$ . The experiment was set to  $m=25$ , and the experimental results showed a rejection rate of 0.4698 by hypothesis testing, among which 2 rejection errors, accounting for only 0.0515, which indicates that it is feasible to restore the network topology by using this model in this case. The false negative rate can be calculated by equation (4).

From Figure 2, it can be found that for different sample data amounts  $m$ , the two curves correspond to basically the same error rate, and the false-negative rate  $\beta$  can be a good judge of the structural recovery performance of the model. It can be observed that when calculating the unrecognized rate  $E$ , the

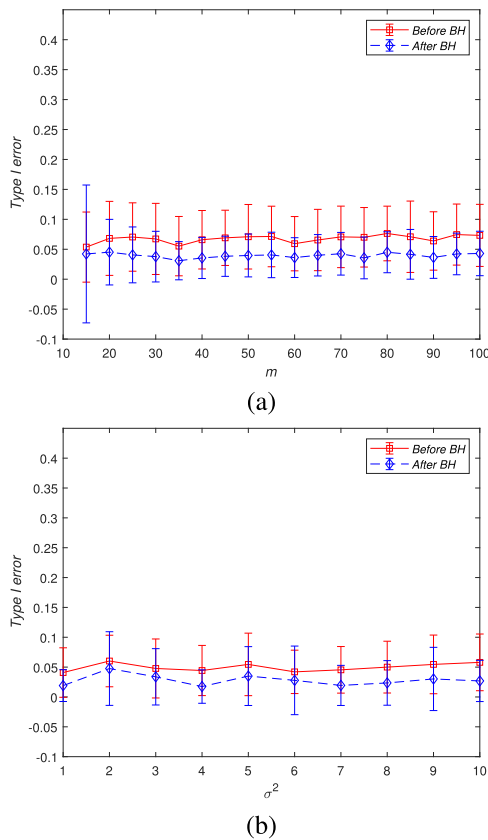
$$C = \begin{pmatrix} -4 & 1 & 1 & 0 & 0 & 0 & 0 & 0 & 1 & 1 \\ 1 & -5 & 1 & 1 & 0 & 1 & 0 & 0 & 0 & 1 \\ 1 & 1 & -5 & 1 & 1 & 0 & 0 & 0 & 1 & 0 \\ 0 & 1 & 1 & -4 & 1 & 1 & 0 & 0 & 0 & 0 \\ 0 & 0 & 1 & 1 & -5 & 1 & 1 & 0 & 0 & 1 \\ 0 & 1 & 0 & 1 & 1 & -5 & 1 & 1 & 0 & 0 \\ 0 & 0 & 0 & 0 & 1 & 1 & -4 & 1 & 1 & 0 \\ 0 & 0 & 0 & 0 & 0 & 1 & 1 & -4 & 1 & 1 \\ 1 & 0 & 1 & 0 & 0 & 0 & 1 & 1 & -5 & 1 \\ 1 & 1 & 0 & 0 & 1 & 0 & 0 & 1 & 1 & -5 \end{pmatrix}$$



**FIGURE 2.** For the network structure reconstruction model (3), the unrecognized rate  $E$  and the false negative rate  $\beta$  with their standard deviations for different sample data amounts  $m$ .



**FIGURE 4.** For the network structure reconstruction model (3), the unrecognized rate  $E$  and the false negative rate  $\beta$  with their standard deviations under different sample data volume  $m$  after using FDR correction, the red and black lines represent the unrecognized rate  $E$  before and after correction, respectively.



**FIGURE 3.** For the network structure reconstruction model (3), the probability and standard deviation of false positive rate under different sample data amount  $m$  and different noise intensity  $\sigma^2$ .

topology of the network must be known, which is difficult to obtain in reality. However, our method can accurately calculate the recovery performance of the model only when the sample data is known. Therefore, it is perfectly feasible and more concise to assess the accuracy of the reconstructed network structure by the false negative rate, which is more practical.

After applying FDR correction to the overall multiple hypotheses, it can be seen from Figure 3 that the false positive rate after correction will decrease compared with that before,

which achieves the purpose of controlling the false positive results. The false positive rate will always be within the range of  $(0, 0.05)$ , but it will increase the number of false negatives to some extent.

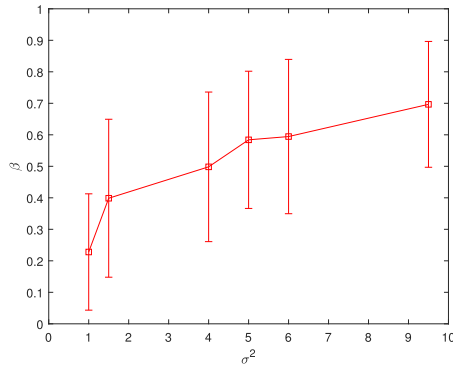
False positive error and false negative error cannot be increased or decreased simultaneously with a fixed amount of sample data. Therefore, FDR correction will inevitably increase false negative errors after reducing false positive errors. As shown in Figure 4, only by increasing the amount of sample data can both types of errors be reduced simultaneously, and the recovery performance of the model reaches a steady state at about 50 sample data. After FDR correction, it is still feasible to use the false negative rate to evaluate the accuracy of model prediction.

### C. EFFECT OF $m$ AND $\sigma^2$ ON MODEL ACCURACY

In the actual system, the sample data will be disturbed by the acquisition method or the internal noise of the system, which will have some influence on the results. Two factors affecting the results of model reconstruction are considered. First, the accuracy of the model recovery connection is affected by the amount of sample data, and the prediction performance of the model with different amount of sample data is analyzed. Second, the system is affected by internal noise and thus cannot obtain high-quality sample data, and the impact of noise on the prediction performance of the model is analyzed.

#### 1) EFFECT OF SAMPLE DATA SIZE $m$ ON THE RESULTS

In general, the model prediction results are influenced by the amount of sample data  $m$ . As  $m$  increases, the larger the amount of system state information obtained, the better the prediction performance of the model. From Figure 2, it can be found that the curve shows an obvious decreasing trend with the increase of  $m$ . The  $\beta$  and  $E$  unrecognized rate of the model are gradually decreasing, which indicates that the model has a significant effect on the recognition between nodes gradually. When  $m=25$ ,  $\beta=0.1392$ , the  $\beta$  is small, and the model can effectively identify the network topology. When the amount of sample data reaches about 50, the false



**FIGURE 5.** For the network structure reconstruction model (3), the false negative rate  $\beta$  at different noise intensities  $\sigma^2$ .

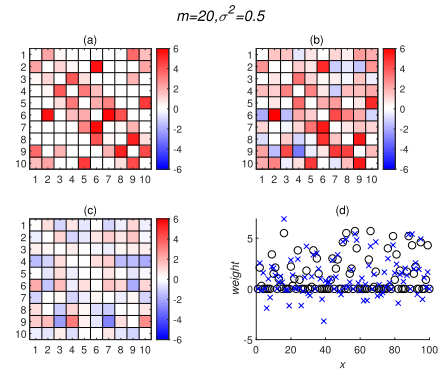
negative rate is close to 0, which indicates that the model can efficiently identify the connection relationship between nodes. Moreover, further increase in the sample data volume does not have a great impact on the model prediction results, maintaining a relatively stable state.

2) EFFECT OF NOISE INTENSITY  $\sigma^2$  ON THE RESULTS

When  $\sigma^2=0$ , model (3) has  $\beta=0.1033$  with 70 sample data, which indicates that the model can restore the topology better. Consider the effect of different noise intensity  $\sigma^2$  on the model recovery results. Figure 5 shows the experiments conducted under 25 sample data. From the figure, it can be found that the false negative rate  $\beta$  predicted by the model gradually increases with the increase of  $\sigma^2$ , that is, the more inaccurate the model identifies the connection relationship between the nodes. This is because with the increase of  $\sigma^2$ , the sample data becomes more and more polluted, and the network information cannot be efficiently reflected, resulting in a decrease in the number of node connections found by the model.

**IV. WEIGHTED NETWORK STRUCTURE RECOVERY MODEL AND ANALYSIS**

The network structure in Figure 1 is chosen as the study object, and weights are assigned to the connections between its nodes. After determining the connection relationship between nodes, it is also necessary to predict the weight value of their connections. Assuming that the rest of the



**FIGURE 6.** Matrix color block diagram. (a) represents the adjacency matrix  $C_{ij}$ , (b) represents the estimated matrix  $\hat{C}_{ij}$  predicted using the network reconstruction model (3), (c) represents the error between them, and (d) represents the comparison of the weight of each connection between nodes,  $x$  is the number of zero weight and non-zero weight,  $C_{ij}(\circ)$ ,  $\hat{C}_{ij}(x)$ .  $r_{ex}=0.8207$ ,  $r_{no}=0.8888$ .

network conditions remain unchanged, the adjacency matrix is as shown at the bottom of the page.

**A. MODEL EVALUATION**

Using model (3) to predict the weight of connections between network nodes. In order to quantify the predictive performance of this method on the weight of connections between nodes, the evaluation index prediction error,  $r_{ex}, r_{no}$  is defined as:

$$r_{ex} = \frac{\sum_i 1^{M_{ex}} (\hat{C}_{ex} - C_{ex})}{M_{ex}}$$

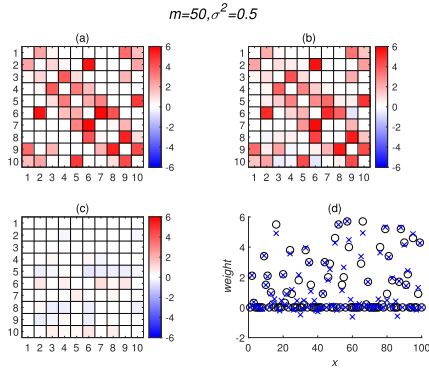
where  $\hat{C}_{ex}$  denotes the predicted value of the matrix with connections,  $C_{ex}$  denotes the actual value of the matrix with connections, and  $M_{ex}$  denotes the number of connections between nodes;

$$r_{no} = \frac{\sum_i 1^{M_{no}} (\hat{C}_{no} - C_{no})}{M_{no}}$$

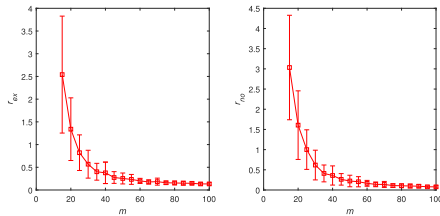
where  $\hat{C}_{no}$  denotes the predicted value of the matrix without connections,  $C_{no}$  denotes the actual value of the matrix without connections, and  $M_{no}$  denotes the number of no connections between nodes.

According to the aforementioned method, different time series can be obtained. The adjacency matrix of the network can be reconstructed by using these data according to model (3), and the estimated matrix  $\hat{C}$  can be obtained. The experiment is conducted under 20 sample data and  $\sigma^2=0.5$ , and the results are shown in Figure 6 with  $r_{ex}=0.8207$  and

$$C = \begin{pmatrix} -7.3 & 2.1 & 0.3 & 0 & 0 & 0 & 0 & 0 & 3.4 & 1.5 \\ 2.1 & -11 & 1 & 0.2 & 0 & 5.5 & 0 & 0 & 0 & 2.2 \\ 0.3 & 1 & -7.8 & 3.8 & 0.9 & 0 & 0 & 0 & 1.8 & 0 \\ 0 & 0.2 & 3.8 & -8.5 & 3 & 1.5 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0.9 & 3 & -13.4 & 2 & 2.9 & 0 & 0 & 4.6 \\ 0 & 5.5 & 0 & 1.5 & 2 & -18.7 & 5.7 & 4 & 0 & 0 \\ 0 & 0 & 0 & 0 & 2.9 & 5.7 & -10.5 & 0.2 & 1.7 & 0 \\ 0 & 0 & 0 & 0 & 0 & 4 & 0.2 & -10.3 & 5.2 & 0.9 \\ 3.4 & 0 & 1.8 & 0 & 0 & 0 & 1.7 & 5.2 & -16.4 & 4.3 \\ 1.5 & 2.2 & 0 & 0 & 4.6 & 0 & 0 & 0.9 & 4.3 & -13.5 \end{pmatrix}$$



**FIGURE 7.** Matrix color block diagram. (a) represents the adjacency matrix  $C_{ij}$ , (b) represents the estimated matrix  $\hat{C}_{ij}$  predicted using the network reconstruction model (3), (c) represents the error between them, and (d) represents the comparison of the weight of each connection between nodes,  $x$  is the number of zero weight and non-zero weight,  $C_{ij}$  (o),  $\hat{C}_{ij}$  (x).  $r_{ex}=0.1645$ ,  $r_{no}=0.1901$ .



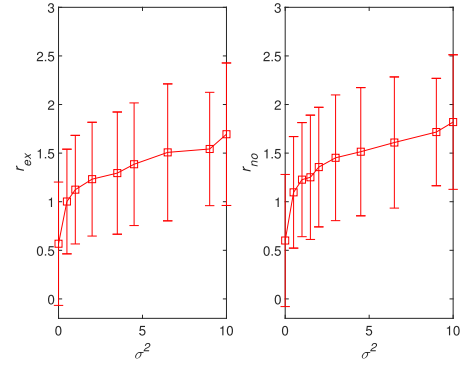
**FIGURE 8.** For the network structure reconstruction model (3), the prediction errors  $r_{ex}$ ,  $r_{no}$ , and their standard deviations for different sample data amounts  $m$ .

$r_{no}=0.8888$ . It can be found that the reconstruction of the model is feasible for the zero weight and non-zero weight of inter-node connections, but the prediction accuracy is not good. This is because the predicted results are affected by the experimental data containing the system state information. Next, the sample size of the experiment is increased. 50 sample data and  $\sigma^2=0.5$  are selected and the adjacency matrix is reconstructed using them. The results are shown in Figure 7 with  $r_{ex}=0.1645$  and  $r_{no}=0.1901$ . It can be found that the accuracy of predicting the weights of connections between network nodes using model (3) increases with the amount of data.

### B. EFFECT OF $m$ AND $\sigma^2$ ON MODEL ACCURACY

As can be seen from Figure 6, the accuracy of the model in predicting node connection weights differs greatly under the same sample data amount. This represents that the system state information contained in the time series affects the prediction quality. To assess the impact of the sample data amount  $m$  on the prediction performance of the model, the following experiments are taken to average the results of 100 experiments.

As shown in Figure 8, the prediction accuracy of model (3) for the connection weight increases with the increase of sample data amount  $m$ . When  $m=25$ ,  $r_{ex}=0.895$ ,  $r_{no}=1.024$ , the model can predict the weights between nodes well, and when the sample data amount reaches about 60, it can predict



**FIGURE 9.** For the network structure reconstruction model (3), the prediction errors  $r_{ex}$ ,  $r_{no}$ , and their standard deviations at different noise intensities  $\sigma^2$ .

the zero and non-zero weights between nodes efficiently. And the increase of the sample data volume does not have a large impact on the model results, maintaining a relatively stable state.

Figure 9 shows the effect of noise intensity  $\sigma^2$  on the model prediction discussed under 25 sample data. It can be found from the figure that as  $\sigma^2$  increases, the prediction error of the model  $r_{ex}$ ,  $r_{no}$  gradually increases, that is, the more inaccurate the model identifies the size of the connection weights between nodes. This is because as  $\sigma^2$  increases, the sample data is more contaminated, and the connection weight between nodes cannot be accurately predicted.

## V. CONCLUSION

It is of great practical significance to clarify the network topology structure. We propose a network reconstruction model based on regression theory. The relationship between network structure and linear regression model is illustrated, and a separate regression analysis is performed for each node. The model requires that the dynamics equations and coupling matrix are known, while the network topology and system noise can be unknown. With experimentally measured time series, the model provides a relatively simple form of estimation matrix  $\hat{C}$  for predicting the adjacency matrix  $C$ . It relies only on randomly selected time series and does not require additional human intervention, demonstrating that it is theoretically feasible and concise to reconstruct the network topology based on time series. The feasibility of the proposed method is verified by simulation experiments in a bidirectional coupling network composed of *Lorenz* system nodes.

After the regression coefficients are obtained by least squares estimation, the regression coefficients need to be tested to determine whether there are connected edges between nodes. The hypothesis test method used in this paper is the t-test, at which time the network topology recovery problem is transformed into a classification problem to be solved. The prediction matrix  $\hat{C}$  of the adjacency matrix  $C$  can be obtained, and a statistical test is needed to determine its accuracy. A novel method is proposed to evaluate the



prediction results of the model by the false negative rate  $\beta$ , which has certain advantages compared with the unrecognized rate  $E$ . This is demonstrated by numerical simulations. Calculating  $E$  requires prior knowledge of the network topology, while  $\beta$  can judge the prediction results of the model without knowing the network topology, which relies only on experimentally obtained random time series. At the same time, it illustrates that the model can know the overall network structure well by sample cases only. This advantage makes its application scope wider. Traditional hypothesis test can only control the false positive rate of a single hypothesis, but for the regression analysis as a whole, the false positive results will increase with the number of tests, beyond our preconceptions. Therefore, multiple hypothesis testing is required and the Benjamini-Hochberg method is selected to control the overall false positive rate.

In addition, two factors affecting the topological structure of the model recovery are discussed, the amount of sample data  $m$  and the noise intensity  $\sigma^2$ . First, the system information contained in the sample data reflects the state of the nodes. Therefore, with the increase of  $m$ ,  $\beta$  gradually decreases, that is, the connections between the nodes are well identified. When  $m=25$ ,  $\beta=0.1392$ , the beta is small, and the model can effectively identify the network topology. When  $m$  is about 50, the model reaches a better prediction result, at which time the effect of further increase in  $m$  on the model prediction is no longer significant. Second, noise interferes with the sample data. Therefore, the larger the noise  $\sigma^2$  intensity is, the more serious the sample data pollution is, and the less accurate the network information can be reflected, leading to a reduction in the number of node connections found by the model.

Finally, based on the above identification of connection relationships between nodes, the method is extended to predict arbitrary connection weight between nodes, transforming the problem into a regression problem for solution. The feasibility of using the model to predict zero weight and non-zero weight of inter-node connections is demonstrated by numerical simulations. Two factors that affect the accuracy of weight prediction are discussed. First, the amount of sample data, when  $m=25$ ,  $r_{ex}=0.895$ ,  $r_{no}=1.024$ , the model can predict the weights between nodes well, and when the sample data amount reaches about 60, it can predict the zero and non-zero weights between nodes efficiently, at this time, the influence of  $m$  increase on the model prediction is no longer significant. Second, the noise will interfere with the systematic information of the sample data, so it will affect the prediction of the weight size between nodes.

In summary, our method can reconstruct the network topology under arbitrary experimental data, and the method is applied to predict arbitrary weights of the connections. Importantly for 0–1 matrix, the proposed false-negative rate can be used to estimate the accuracy of the model prediction based on only part of the sampled data in the case of incomplete prior information.

## NOMENCLATURE

$AUC$	Area Under the Curve
$E$	unrecognized rate
$ROC$	Receiver Operating Characteristic
$FDR$	False Discovery Rate
$FPR$	False Positive Rate
$m$	sample data
$\beta$	false negative rate
$\sigma^2$	noise intensity
$C$	adjacency matrix
$A$	internal coupling matrix

## DATA AVAILABILITY

The data used to support the results of this study are available from the paper.

## CONFLICT OF INTEREST

The authors declare no conflict of interest with the publication of this article.

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