Reverse engineering of complex dynamical networks in the presence of time-delayed interactions based on noisy time series

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Abstract. - Reverse engineering of complex dynamical networks is important for a variety of fields where uncovering the full topology of unknown networks and estimating parameters characterizing the network structure and dynamical processes are of interest. We consider complex oscillator networks with time-delayed interactions in a noisy environment, and develop an effective method to infer the full topology of the network and evaluate the amount of time delay based solely on noise-contaminated time series. In particular, we develop an analytic theory establishing that the dynamical correlation matrix, which can be constructed purely from time series, can be manipulated to yield both the network topology and the amount of time delay simultaneously. Extensive numerical support is provided to validate the method. While our method provides a viable solution to the network inverse problem, significant difficulties, limitations, and challenges still remain, and these are discussed thoroughly.

Time-delayed interactions are common in complex systems arising from various fields of science and engineering. Consider, for example, a coupled oscillator network in a physical environment where noise is present. Time delay can typically occur in the node-to-node interactions. Now suppose that no prior knowledge about the nodal dynamics and the network topology is available but only a set of noise-contaminated time series can be obtained through measurements. The question is whether it is possible to deduce the full topology of the network and to estimate the amount of average time delay using the time series only. This issue belongs to the recently emerged subfield of research in complex systems: reverse engineering of complex networks (or the inverse problem). While a number of methods address the network inverse problem have appeared, to our knowledge, the issue of time-delayed interactions has not been considered. Here we present an effective method to infer the full network topology and, at the same time, to estimate the amount of average time delay in the network. In particular, we develop a physical theory to obtain a formula relating the network topology and time delay to the dynamical correlation matrix, which can be constructed purely from time series. We then show how information about the time delay encrypted in the dynamical correlation matrix can be separated from that of network topology, allowing both to be inferred in a computationally extremely efficient manner. We present numerical examples from both model and real-world complex networks to demonstrate the working of our method. Difficulties, limitations, and challenges are also discussed. Reverse-engineering of complex dynamical systems has potential applications in many disciplines, and our work represents a small step forward in this extremely challenging area.

One of the outstanding issues in nonlinear and statistical physics, and also in network science and engineering, is to infer or predict the topology and other basic character-
istics of complex networks based only on measured time series. This “inverse” problem is relevant to a number of fields such as biomedical and techno-sciences where complex networked systems are ubiquitous. In defense, the problem of identifying various adversarial networks based on observations is also of paramount importance. Despite tremendous efforts in revealing the connection between network structures and dynamics [1, 3], how to infer the underlying topology from dynamical behaviors is still challenging as an inverse problem, especially in the absence of the knowledge of nodal dynamics.

Recent years have witnessed the emergence of a number of methods to address various aspects of the inverse problem, which include gene networks inference using singular value decomposition and robust regression [2], spike classification methods for measuring interactions among neurons from spike trains [7], symbolically reverse engineering of coupled ordinary differential equations [8], approaches based on response dynamics of a specific oscillator [9], $L_1$ norm in optimization theory [10], noise induced scaling laws [11], and the interplay between dynamical correlation and network structure in the presence of noise [12]. However, the issue of time delay has not been addressed yet. The purpose of this article is to present a general theory that leads to a completely data-driven and extremely efficient method to predict the network topology and the time delay at the same time.

Time delay is fundamental in natural systems, due to the finite propagation speed of physical signals. In addition to numerous examples in physics, situations where time delay is important include the latency times of neuronal excitations in neuroscience, finite reaction times of chemicals in chemistry, etc. In coupled oscillator networks, the effects of time delay on dynamics under various given network topologies have been studied extensively [13–17]. In our case, however, the network connections, the amount of the time delay, and other properties of the network are unknown a priori, and our goal is to predict these by using noisy time series only. To be concrete, we shall focus on complex oscillator networks. Our general point of view is that, information about the network topology and time delay has been encoded in noisy time series from various nodes in the network. The objective of solving the inverse problem is to decode such information from noisy time series.

Our idea is that, if the networked system suffers from a noisy environment so that the measured time series are noisy, it is possible to accomplish the task of decoding in a natural way. In particular, we construct a dynamical correlation matrix from all available time series, the elements of which are the average products of the deviations of all pair-wise time series from a mean value. We shall show analytically that information about the network structure and time delay can be decoded through this matrix. In fact, as we will show in developing our theory, information about the network topology can be separated from the time delay through a generalized inverse operation of the dynamical correlation matrix, enabling a complete prediction of the underlying networked system.

To provide numerical support for our theory, we exploit three representative dynamical systems on homogeneous and heterogeneous model complex networks and on a number of real-world networks as well. We find that the presence of a time delay results in a deviation in the distribution of the diagonal elements of the dynamical correlation matrix from a power law, which can be used as a preliminary criterion to determine whether there is a significant time delay in the underlying networked system. Computations reveal high accuracies in the prediction of both the network topology and the time delay for all combinations of dynamical systems and network models studied.

We present our theory and method by considering a network of $N$ coupled oscillators. Each oscillator, when decoupled, satisfies $\dot{\mathbf{x}}_i = \mathbf{F}_i[\mathbf{x}_i]$, where $\mathbf{x}_i$ denotes the $d$-dimensional state variable of node $i$. The dynamics of the whole time-delayed system in a noisy environment is described as:

$$
\dot{\mathbf{x}}_i(t) = \mathbf{F}_i[\mathbf{x}_i(t)] - c \sum_{j=1}^{N} L_{ij} \mathbf{H}[\mathbf{x}_j(t - \tau)] + \mathbf{\eta}_i(t),
$$

(1)

where $c$ is the coupling strength and $\mathbf{H}$ denotes the coupling function. $L_{ij}$ is Laplacian matrix, characterizing the topology of the underlying network that $L_{ij} = -1$ if $j$ connects to $i$ (otherwise 0) for $i \neq j$, and $L_{ii} = k_i$, where $k_i$ is the degree of node $i$. $\tau$ denotes the time delay, and $\mathbf{\eta}_i$ is a $d$-dimensional stochastic process representing noise on node $i$.\llap{16} (In the following, we use $\mathbf{\eta}$ on the head to denote the $d$-dimensional state variable). The standard procedure of linearization [1,13] can be carried out by letting $\mathbf{x}_i = \mathbf{\tilde{x}}_i + \mathbf{\zeta}_i$, where $\mathbf{\tilde{x}}_i$ is the counterpart of $\mathbf{x}_i$ in the absence of noise. The $d$-dimensional dynamical process governing the fluctuations on $i$th oscillator can then be obtained as the variational equation:

$$
\dot{\mathbf{\zeta}}_i(t) = D\mathbf{F}_i \cdot \mathbf{\zeta}_i(t) - c \sum_{j=1}^{N} L_{ij} D\mathbf{H} \cdot \mathbf{\zeta}_j(t - \tau) + \mathbf{\delta}_i(t),
$$

(2)

where $D\mathbf{F}_i$ and $D\mathbf{H}$ denote the $d \times d$ Jacobian matrices of the intrinsic dynamics $\mathbf{F}_i$ and the coupling function $\mathbf{H}$, respectively. Decomposing Eq. (2) in terms of the eigenmodes, we obtain

$$
\dot{\mathbf{\zeta}}_\alpha(t) = \sum_\beta D_{\alpha\beta} \mathbf{\zeta}_\beta(t) - c \lambda_\alpha D\mathbf{H} \cdot \mathbf{\zeta}_\alpha(t - \tau) + \mathbf{\delta}_\alpha(t).
$$

(3)

Here, instead of the index $i,j$ running on the real space of networks, the index $\alpha, \beta$ run on the eigen-space. $\mathbf{\zeta}_\alpha = \sum_i \psi_\alpha \mathbf{\tilde{x}}_i$, $\mathbf{\zeta}_\alpha = \sum_i \psi_\alpha \mathbf{\eta}_i$ and $D_{\alpha\beta} = \sum_i \psi_\alpha D\mathbf{F}_i \psi_\beta$, where $\psi_\alpha$ denotes the $\alpha$th normalized eigenvector of the Laplacian matrix, and $\lambda_\alpha$ is the corresponding eigenvalues that satisfy $0 = \lambda_0 < \lambda_1 \leq \cdots \leq \lambda_N$. Under the approximation $D\mathbf{F}_i \approx D\mathbf{F}$ so that $D_{\alpha\beta} = D\mathbf{F}_{\alpha\beta}$, the above equation can be reduced to

$$
\dot{\mathbf{\zeta}}_\alpha(t) = D\mathbf{F} \cdot \mathbf{\zeta}_\alpha(t) - c \lambda_\alpha D\mathbf{H} \cdot \mathbf{\zeta}_\alpha(t - \tau) + \mathbf{\delta}_\alpha(t).
$$

(4)
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From the covariance of Gaussian noise \( \langle \tilde{y}_t(t)\tilde{y}_t'(t') \rangle = \sigma^2 I_d \delta(t-t') \) with \( I_d \) the \( d \)-dimensional identity matrix and \( \sigma^2 \) the noise strength, we obtain \( \tilde{\zeta}_a(t)\tilde{\zeta}_a'(t') = \sigma^2 I_d \delta_{a,b}(t-t') \), which indicates the stochastic process we mapped into eig-space is still Gaussian noise. Assuming small time delay, we can apply the first-order approximation: \( \tilde{c}_a(t) = \tilde{c}_a(t) - \tau \tilde{c}_a(t) \), which yields

\[
(I_d - c\tau_\alpha D H) \tilde{c}_a(t) = -(c\lambda_\alpha D H - D F) \tilde{c}_a(t) + \tilde{\zeta}_a(t).
\]

Denote \( B = (I_d - c\tau_\lambda D H)^{-1} \), \( A = B(c\lambda_\alpha D H - D F) \), and follow the standard stochastic calculus \[18\], we get the solution:

\[
\tilde{c}_a(t) = e^{-At} \tilde{c}_a(0) + \int_0^t e^{-A(t-t')} B \tilde{\zeta}_a(t') dt'.
\]

Since we are interested in the regime where oscillator states are perturbed from the synchronized manifold by the noisy environment, we assume the system is in the absence of divergence of state variables, therefore in the long time limit, the initial condition term can be discarded and we have \[12\]:

\[
A \langle \tilde{c}_a \tilde{c}_a' \rangle + \langle \tilde{c}_a \tilde{c}_a' \rangle A = \sigma^2 B B^T.
\]

The general solution of \( \langle \tilde{c}_a \tilde{c}_a' \rangle \), the \( d \times d \) covariance matrix about \( d \)-dimensional states of the \( \alpha \)th oscillator in the eigen-space, can be written as \[19\]:

\[
\text{vec}(\langle \tilde{c}_a \tilde{c}_a' \rangle) = \sigma^2 \text{vec}(B B^T)/(I_d \otimes A + A \otimes I_d),
\]

where the operator \( \text{vec}(X) \) creates a column vector from a matrix \( X \) by stacking the columns of \( X \) below one another.

Although we obtain this solution, it is not practical in real applications. In follows, we approximate the state variables into one dimension such that \( D H = 1 \) and drop the notation “\(^\dagger\)”. In this way, the above solution is simplified to:

\[
\langle \tilde{c}_a \rangle = \frac{\sigma^2}{2c} \frac{1}{1 - c\tau_\alpha (\lambda_\alpha - DF/c)}.
\]

Return to real variables from the eigen-space by inserting \( \xi_i = \sum \psi_i \tilde{c}_a \) into the correlation function \( C_{ij} = \langle \xi_i \xi_j \rangle \) in the real space between any two nodes, we have \( C_{ij} = \sum_{\alpha=1}^{N-1} \psi_i \psi_j \langle \tilde{\zeta}_a \rangle \) such that

\[
C_{ij} = \frac{\sigma^2}{2c} \sum_{\alpha=1}^{N-1} \frac{\psi_i \psi_j}{(1 - c\tau_\alpha (\lambda_\alpha - DF/c))}.
\]

Under the approximation of negligible \( DF/c \) and reminding of the small time delay \( \tau \), Eq. \[7\] for the dynamical correlation can then be expanded as:

\[
C_{ij} \approx \frac{\sigma^2}{2c} \sum_{\alpha=1}^{N-1} \frac{1}{\lambda_\alpha} \psi_i \psi_j \psi_{ij} = \frac{\sigma^2}{2c} |L^1 + c\tau I_N|_{ij},
\]

wherein under the effect of noise \( \sigma^2 \), the dynamics in terms of correlation matrix \( C \) is connected explicitly with the time delay \( \tau \) and the structure information in terms of \( L^1 = \sum_{\alpha=1}^{N-1} \psi_i \psi_j / \lambda_\alpha \), the pseudo-inverse of Laplacian matrix. Note that the time delay has no effect on the cross-correlation elements except the auto-correlations due to the identity matrix. Following Eq. \[3\], the diagonal elements \( C_{ii} \) of the dynamical correlation matrix can be obtained by expanding \( L^1 \) in terms of the underlying network structure \[12\]:

\[
C_{ii} \approx \frac{\sigma^2}{2c} \left( K^{-1} + K^{-1} P K^{-1} + K^{-1} P K^{-1} P K^{-1} \right)_{ii} + \frac{\sigma^2}{2c} \sum_{\alpha=1}^{N-1} \psi_i \psi_j / \lambda_\alpha \psi_{ij} = \frac{2c}{\sigma^2} [L^1 + c\tau L^2]_{ii},
\]

where \( K = \text{diag}(k_1, \cdots, k_N) \) is the degree matrix, \( P \) is the adjacency matrix such that \( L = K - P \) and \( \langle k \rangle \) denotes the average degree. We see that the fluctuations \( C_{ii} \) at node \( i \) depend both on its local structure \( k_i \) and the time delay \( \tau \). When \( \tau = 0 \), this result is consistent with the recently discovered noise-induced scaling law \[11\], derived there by a power-spectral analysis.

The off-diagonal elements of \( L \) contain complete information about the network structure while its diagonal elements can be obtained from the off-diagonal ones. We thus focus on the off-diagonal elements. For \( i \neq j \), following Eq. \[7\], the generalized inverse matrix \( C^\dagger \) is

\[
C^\dagger_{ij} \approx \frac{2c}{\sigma^2} \sum_{\alpha=1}^{N-1} \frac{1}{\sigma_\alpha} \lambda_\alpha (1 - c\tau_\lambda_\alpha) \psi_i \psi_j = \frac{2c}{\sigma^2} [L + c\tau L^2]_{ij}.
\]

Considering \( L = K - P \), we can cast this equation in the following form:

\[
C^\dagger_{ij} = \frac{2c}{\sigma^2} [L + c\tau(K P + P K - K^2 - P^2)]_{ij}.
\]

For those off-diagonal elements \( i, j \), the diagonal matrix \( K^2 \) has no contributions and \( P^2 \) contributes \( l_{ij} \), where \( l_{ij} \) is the number of two-step paths connecting \( i \) with \( j \). By considering the negligible contribution of \( l_{ij} \) compared with degrees, we thus have:

\[
\frac{\sigma^2}{2c} C^\dagger_{ij} \approx \begin{cases} L_{ij} + c\tau(k_i + k_j), & \text{if } i \text{ connects with } j \\ 0, & \text{otherwise} \end{cases}
\]

Equation \[12\] is one of our main results for network inference, which indicates that the network structure can be inferred through the off-diagonal elements \( C^\dagger_{ij} \) of the dynamical correlation matrix based solely on the measured time series.

Once \( L \) is predicted, the time delay \( \tau \) can be estimated, e.g., from Eq. \[10\]. We obtain

\[
\tau \approx \left[ \frac{|L - \frac{\sigma^2}{2c} C^\dagger|_{ij}}{C^\dagger L^2|_{ij}} \right]_{i \neq j, L_{ij} \neq 0, (L^2)_{ij} \neq 0},
\]

where the subscript in the average \( \langle \cdot \rangle \) covers all possible pairs of \( i \) and \( j \) by excluding the diagonal elements in the matrices \( L \) and \( L^2 \), and all pairs with zero elements in the
Fig. 1: (Color online) Diagonal elements $C_{ii}$ of the dynamical correlation matrix as a function of node degree $k$ for three dynamical processes with different time delay $\tau$ on scale-free and random networks. Square, circle, triangle and reverse triangle denote $\tau = 0.01, 0.05, 0.07$ and 0.09, respectively. The curves are the theoretical prediction from Eq. (9). The sizes of model networks are 100 and the average degree is 10. The noise strength $\sigma^2$ is 0.1 and the coupling strength $c$ is 0.2.

matrix $L$ or $L^2$. Excluding zero elements can effectively reduce the estimation error for $\tau$.

We now demonstrate numerically our method by considering several model and real-world networks in the presence of noise and time delay. For each network, we implement three dynamical processes: (i) Consensus dynamics [20]:

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

(ii) Rössler dynamics [21]:

$$\begin{align*}
\dot{x}_i(t) &= -y_i - z_i + c \sum_{j=1}^{N} P_{ij} [x_j(t - \tau) - x_i(t - \tau)] \\
\dot{y}_i &= x_i + 0.2y_i + c \sum_{j=1}^{N} P_{ij} (y_j - y_i), \\
\dot{z}_i &= 0.2 + z_i(x_i - 9.0) + c \sum_{j=1}^{N} P_{ij} (z_j - z_i),
\end{align*}$$

and (iii) Kuramoto phase oscillators [22]:

$$\dot{\theta}_i = \omega_i + c \sum_{j=1}^{N} \sin[\theta_j(t - \tau) - \theta_i(t - \tau)] + \eta_i,$$

where $\theta_i$ and $\omega_i$ are the phase and the natural frequency of oscillator $i$.

Time series are then collected from all nodes. The element of the dynamical correlation matrix between two arbitrary nodes $i$ and $j$ is calculated as $C_{ij} = \langle |x_i(t) - \bar{x}(t)| \cdot |x_j(t) - \bar{x}(t)| \rangle_t$, where $\bar{x}(t) = (1/N) \sum_{i=1}^{N} x_i(t)$ and $\langle \cdot \rangle_t$ denotes the long time average. For the Rössler dynamics, $x_i(t)$ stands for the $x$ component of the $i$th oscillator and for the Kuramoto dynamics, $x_i(t)$ stands for the phase variable $\theta_i(t)$ of the $i$th oscillator.

Figure 1 provides an example of the dependence of fluctuations $C_{ii}$ on the time delay for three dynamical processes on both heterogeneous and homogeneous networks. The results are in good agreement with the theoretical prediction from Eq. (9). A non-ignorable deviation from the predicted fluctuations in noisy Rössler dynamics with time delay is observed, which is mainly due to the simplification of one-dimensional variable to get Eq. (9) while the state variable in Rössler dynamics has three dimension. Note that, in the absence of time delay, the dependence of $C_{ii}$ on the node degree $k_i$ can be described as a power law [11-12]: $C_{ii} \sim k_i^{-\alpha}$, regardless of the dynamics. For $\tau \neq 0$, the deviation of $C_{ii}$ from the power-law behavior can then be used to assess preliminarily whether there is a significant time delay in the underlying networked system: a more severe deviation suggests a larger value of the time delay.

After calculating the dynamical correlation matrix $C$, we can infer the details of the network connections through Eq. (12) via the generalized inverse of $C$. Figure 2(a) shows the distribution of the off-diagonal elements of
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\[ \frac{\sigma^2}{(2c)}C^\dagger \]. We observe a bimodal behavior with two peaks: one centered at a negative value which corresponds to existing links, and another centered at zero which indicates non-existent links. Without time delay, the hump in the distribution for the existent links should be centered at \(-1\). While with time delay, due to the contribution of the term \(c\tau(k_i + k_j) \approx 2c\tau(k)\), the center of the hump will shift toward zero. The larger the time delay, the more significant the shift will be. For example, as shown in Fig. 2(a), the amount of the shift in the negative peak is \(2c\tau(k) = 0.2\). Considering \(c = 0.2\) and \(k = 10\) in the example, we obtain \(\tau = 0.05\), which is exactly the pre-assumed value of the time delay in the system. To separate the two humps, a threshold is needed, where all existent links in the network are identified by the elements in \(C^\dagger\) which lie below the threshold. In particular, the subscript \(ij\) of a picked element below the threshold indicates a link between nodes \(i\) and \(j\). We set the threshold at the value which corresponds to the minimum value of the fitted curve between two humps. The performance of our prediction method can be characterized by the success rate \(S_e\) of the existent links, which is defined as the ratio of the number of successfully predicted existent links to the total number of existent ones. As shown in Figs. 2(b)-(d), our method yields high success rates for different values of the time delay \(\tau\), regardless of the nodal dynamics and of the network structures.

Fig. 3: (Color online) Predicted time delay \(\tau'\) from Eq. (13) versus the true (pre-assumed) values for the three dynamical processes on a number of model and real-world networks. The symbols denote the same networks as in Fig. 2. The lines are \(\tau' = \tau\). Other parameters are the same as in Fig. 1.

function which is conditionally approximated to the linear coupling function used in our theory.

We also examine the validity of our method for predicting coupled network system with inhomogeneous time delay. A random consensus network associated with random time delays within a certain range is considered. The success rate \(S_e\) as a function of the average time delay \(\tau\) among all pairs of nodes for different ranges of time delay is shown in Fig. 4(a). We see high success rate if the average time delay is not too large. Fig. 4(b) shows the predicted average time delay \(\tau'\) versus the original time delay \(\tau\) for different ranges of time delay. The predicted \(\tau'\) is in good agreement with \(\tau\). These results demonstrate that our approach is applicable to interacting units associated with inhomogeneous time delay.

While our theory and the prediction method are based on the system model Eq. (1), a similar theory and method can be developed for variants of the model. For instance, one can consider the following system:

\[ \ddot{x}_i(t) = F_i[\dot{x}_i(t)] - \varepsilon \sum_{j=1}^{N} P_{ij} \left( H[\dot{x}_i(t)] - H[\dot{x}_j(t - \tau)] \right) + \ddot{\eta}_i, \]  

(14)

with the Laplacian matrix in Eq. (11) replaced by \(P_{ij}\), the adjacency matrix of the underlying network. The difference is that, for the dynamics of a given node in Eq. (11), the time delay occurs only for the state information transmitted from its connected neighbors other than the dynamics of itself. Using similar analytical treatment, one may arrive at

\[ C^\dagger_{ij} \approx \frac{2\varepsilon}{c^2} (c\tau(k) - 1) P - c\tau P^2 \langle ij \rangle, \]

(15)

and

\[ \tau \approx \left\langle \frac{P + \frac{\tau^2}{c^2} C^\dagger}{c\langle k \rangle P - P^2 \langle ij \rangle} \right\rangle_{i\neq j,P_{ij}\neq 0,(P^2)_{ij}\neq 0}. \]

The network structures and time delay can again be predicted for various nodal dynamics and network structures,
as we verified through extensive numerical simulations (data are not shown here).

In summary, we have established a theory to address the inverse problem for complex networked systems in the presence of time delay and noise, based solely on measured time series from the network. Especially, we have obtained a formula relating the generalized inverse of the dynamical correlation matrix, which can be computed purely from data, to the structural Laplacian (or adjacency) matrix and the amount of time delay. Under reasonable approximations the network topology and the effect of time delay can be separated, leading to a computationally extremely efficient method for inferring the network topology and for estimating the time delay. The validity of the method has been tested numerically using a variety of combinations of nodal dynamics and network topology, including a number of real-world network structures. Our method is completely data driven, and we expect it to be applicable to the critical network inverse problems in a variety of fields, such as biomedical and social sciences where complex networked systems are ubiquitous.

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