



OPEN ACCESS

Inferring network topology from complex dynamics

To cite this article: Srinivas Gorur Shandilya and Marc Timme 2011 *New J. Phys.* **13** 013004

View the [article online](#) for updates and enhancements.

You may also like

- [Changes of EEG phase synchronization and EOG signals along the use of steady state visually evoked potential-based brain computer interface](#)
Yufan Peng, Ze Wang, Chi Man Wong et al.
- [Inferring network topology via the propagation process](#)
An Zeng
- [Optimization of communication topology for persistent formation in case of communication faults](#)
Guo-Qiang Wang, , He Luo et al.

Inferring network topology from complex dynamics

Srinivas Gorur Shandilya^{1,2,5} and Marc Timme^{1,3,4}

¹ Network Dynamics Group, Max Planck Institute for Dynamics and Self-Organization, 37073 Göttingen, Germany

² Interdepartmental Neuroscience Program, Yale University, 333 Cedar Street, New Haven, CT 06510, USA

³ Bernstein Center for Computational Neuroscience, 37073 Göttingen, Germany

⁴ Faculty of Physics, University of Göttingen, 37077 Göttingen, Germany

E-mail: srinivas@nld.ds.mpg.de

New Journal of Physics **13** (2011) 013004 (12pp)

Received 9 July 2010

Published 5 January 2011

Online at <http://www.njp.org/>

doi:10.1088/1367-2630/13/1/013004

Abstract. Inferring the network topology from dynamical observations is a fundamental problem pervading research on complex systems. Here, we present a simple, direct method for inferring the structural connection topology of a network, given an observation of one collective dynamical trajectory. The general theoretical framework is applicable to arbitrary network dynamical systems described by ordinary differential equations. No interference (external driving) is required and the type of dynamics is hardly restricted in any way. In particular, the observed dynamics may be arbitrarily complex; stationary, invariant or transient; synchronous or asynchronous and chaotic or periodic. Presupposing a knowledge of the functional form of the dynamical units and of the coupling functions between them, we present an analytical solution to the inverse problem of finding the network topology from observing a time series of state variables only. Robust reconstruction is achieved in any sufficiently long generic observation of the system. We extend our method to simultaneously reconstructing both the entire network topology and all parameters appearing linear in the system's equations of motion. Reconstruction of network topology and system parameters is viable even in the presence of external noise that distorts the original dynamics substantially. The method provides a conceptually new step towards reconstructing a variety of real-world networks, including gene and protein interaction networks and neuronal circuits.

⁵ Author to whom any correspondence should be addressed.

Contents

1. Background	2
2. Theory of direct reconstruction from dynamical trajectories	3
3. Performance for different collective dynamics	4
3.1. Successful reconstruction from different dynamics	5
3.2. Quality of reconstruction	7
3.3. Required observation time	7
3.4. Robustness: substantial noise and unknown parameters	8
4. Recipe for network reconstruction	9
5. Conclusion	10
Acknowledgments	12
References	12

1. Background

Understanding the relationships between network topology and its collective dynamics is at the heart of current interdisciplinary research on networked systems [1]. Often it is possible to observe the dynamics of the individual units of the network, whereas the coupling strengths between them and the underlying network topology cannot be directly measured. Examples range from neuronal circuits in the brain and protein and gene interaction networks in the cell to the spreading of diseases on human travel networks and food webs [2–6]. Hence, various methods have been proposed to solve the inverse problem of inferring the network structure from observation and control of dynamics.

Perturbing a fixed point of a network dynamical system constitutes the simplest controlled intervention of a system. The method of Tegnér *et al* [7] perturbs the steady-state expression levels of selected genes. Their iterative algorithm can reveal the structure of an underlying gene regulatory network by analysing resultant dynamical changes in the pattern of gene expression levels. A similar iterative method based on multiple regression, coupled with transcriptional perturbations to the fixed points of a genetic network, has been used to successfully identify a nine-gene sub-network [8]. Faith *et al* [9] have extended and validated specific machine learning algorithms to infer interactions in large transcriptional regulator networks in *Escherichia coli*, leading to the prediction of several new links in the network. A method introduced by Timme [10] extends dynamical system reconstruction to networks of smoothly coupled limit-cycle oscillators with periodic collective dynamics. The underlying idea is that the asymptotic response dynamics of a network to different externally induced driving conditions are a function of its topology *and* of the (external) driving signals. Thus, measuring the response to suitable driving signals in different experiments restricts the set of network topologies that are consistent with the driving–response pairs, yielding the network’s topology for sufficiently many experiments.

Can one reconstruct a network displaying collective dynamics richer than simple fixed points or limit-cycles? Yu *et al* [11] introduced a synchronization method to identify networks of chaotic Lorenz oscillators up to $N = 17$ units. Assuming full knowledge of all model parameters, the network topology of a clone of the system is varied progressively via error minimization until it synchronizes with the original system. The topology of the clone is then

recognized as that of the original network. An extension of this synchronization method [12] involves additional ‘control signals’ to externally drive the system to steady states, allowing the inference of interaction topology for sparse, symmetric networks.

In this paper, we introduce a simple, direct and intervention-free method for reconstructing networks of arbitrary topology from the mere observation of generic collective dynamics. Here, a dynamical state is considered generic if it generates observations of state variables that imply linearly independent constraints (cf equation (2) below). Thus, reconstruction is possible for arbitrarily complex collective dynamics (for instance, high-dimensional and chaotic) but may not be possible for overly simple dynamical states. For instance, the interactions between coupled identical oscillators in an unperturbed, identically synchronized state cannot be reconstructed, because there are no effective interactions in the perfectly synchronized state. Given the functional form of the intrinsic and interaction dynamics, we show that all other factors of the network dynamical system, such as network topology and coupling strengths (and even typical parameters), can be reliably and efficiently reconstructed.

2. Theory of direct reconstruction from dynamical trajectories

Given an observation of the collective trajectory of a dynamical network, how can we infer its underlying topology? We consider a dynamical system consisting of N units, where the dynamics of each unit are specified by an arbitrary set of dynamical equations, and the interactions between the units take place via edges in the network. The units of the dynamical system are coupled on a directed graph of unknown connectivity with their dynamics satisfying

$$\frac{d}{dt} \mathbf{x}_i = \mathbf{f}_i(\mathbf{x}_i) + \sum_{j=1}^N J_{ij} \mathbf{g}_{ij}(\mathbf{x}_i, \mathbf{x}_j), \quad (1)$$

where $i, j \in \{1, 2, \dots, N\}$, and $\mathbf{x}_i = [x_i^{(1)}, x_i^{(2)}, \dots, x_i^{(D)}] \in \mathbb{R}^D$ describes the state of the i th unit and the functions $\mathbf{f}_i, \mathbf{g}_i: \mathbb{R}^D \rightarrow \mathbb{R}^D$ mediate intrinsic and interaction dynamics of the D -dimensional unit, and are known. Methods based on copy-synchronization [11, 12] rely on the construction of a new network, with dynamics governed by equation (1) and network parameters J'_{ij} that are tuned to that of the real network by an error minimization procedure. Here, we reduce the same reconstruction problem by evaluating the time series of state variables directly, recognizing that the only remaining unknowns in equation (1) are the time derivatives $\dot{x}_i^{(d)}$ as well as the coupling strengths, which are to be determined. A concise recipe for network reconstruction is provided in section 4.

The dynamics of the d th dimension of the i th unit is given by

$$\dot{x}_i^{(d)}(\tau_m) = f_i^{(d)}(\mathbf{x}_i(\tau_m)) + \sum_{j=1}^N J_{ij} g_{ij}^{(d)}(\mathbf{x}_i(\tau_m), \mathbf{x}_j(\tau_m)), \quad (2)$$

where $\tau_m \in \mathbb{R}$, $m \in \{1, \dots, M\}$, are the times we evaluate equation (1). We now write $\dot{z}$ for the rate of change $\frac{d}{dt}z$ of a scalar variable z . To obtain the data necessary for reconstruction, we sample the time series of state variables $x_i^{(d)}(t_m)$ at discrete times t_m and take $\tau_m := (t_{m-1} + t_m)/2$. We linearly interpolate according to

$$x_i^{(d)}(\tau_m) := \frac{x_i^{(d)}(t_{m-1}) + x_i^{(d)}(t_m)}{2} \quad (3)$$

and linearly estimate the time derivatives by

$$\dot{x}_i^{(d)}(\tau_m) := \frac{x_i^{(d)}(t_m) - x_i^{(d)}(t_{m-1})}{t_m - t_{m-1}}, \quad (4)$$

assuming that the sampling intervals $t_m - t_{m-1}$ are sufficiently small. From (2), we thus obtain M equations of the form

$$\dot{x}_{i,m}^{(d)} = f_{i,m}^{(d)} + \sum_{j=1}^N J_{ij} g_{ijm}^{(d)} \quad (5)$$

for each dimension d of the local dynamical systems $f_i^{(d)}$ separately. As the equations (5) are uncoupled for any two different dimensions d and d' , we treat these separately and drop the index (d) from now on.

Repeated evaluations of the equations of motion (2) of the system at different times τ_m thus comprise a simple and implicit restriction on the network topology J_{ij} as follows: writing $X_{i,m} = \dot{x}_{i,m} - f_{i,m}$, these equations constitute the matrix equation

$$X_i = J_i G_i, \quad (6)$$

where $X_i \in \mathbb{R}^{1 \times M}$, $J_i \in \mathbb{R}^{1 \times N}$ and $G_i \in \mathbb{R}^{N \times M}$. Here, the elements of the i th row of J are given by J_i and comprise the sequence $(J_{ij})_{j \in \{1, \dots, N\}}$ of all input coupling strengths to unit i .

Can we rewrite this equation explicitly for J_i ? Generically, $M > N$, and we wish to solve this overdetermined problem by minimizing the error function given by

$$E_i(\hat{J}_i) = \sum_{m=1}^M \left(x_{im} - \sum_{k=1}^N \hat{J}_{ik} g_{ikm} \right)^2 \quad (7)$$

for the best (in Euclidean (ℓ_2) norm) solution $\hat{J}_i$. Here $\hat{J}_{ik}$ represents the reconstructed value of the real coupling strength J_{ik} . Equating to zero the derivatives of the error function with respect to the matrix elements, $\frac{\partial}{\partial J_{ik}} E_i(\hat{J}_i) \stackrel{!}{=} 0$, yields an analytical solution to ℓ_2 error-minimization given by

$$\hat{J}_i = X G_i^T (G_i G_i^T)^{-1} \quad (8)$$

and thus the set of input coupling strengths (and input connectivity) of unit i . Evaluating such equations for all $i \in \{1, \dots, N\}$ yields the complete reconstructed network $\hat{J}$. This form of minimum ℓ_2 -norm solution is implemented in many mathematical software packages (e.g. as the `mrdivide` function in MATLAB [13]).

Other weighted linear forms of determining states and derivatives work equally well, substituting (3) and (4). For instance, one might take $\tau_m = t_m$, directly evaluate the states at the sampled times, $x_i^{(d)}(\tau_m) = x_i^{(d)}(t_m)$, and estimate the derivatives as $\dot{x}_i^{(d)}(\tau_m) = (x_i^{(d)}(t_m) - x_i^{(d)}(t_{m-1})) / (t_m - t_{m-1})$. This approach is used in estimating derivatives in reconstructions in figure 4.

3. Performance for different collective dynamics

How does this theoretical method perform in applications on data? To illustrate the performance of the method and its insensitivity to the type of dynamics, we apply it to four distinct collective

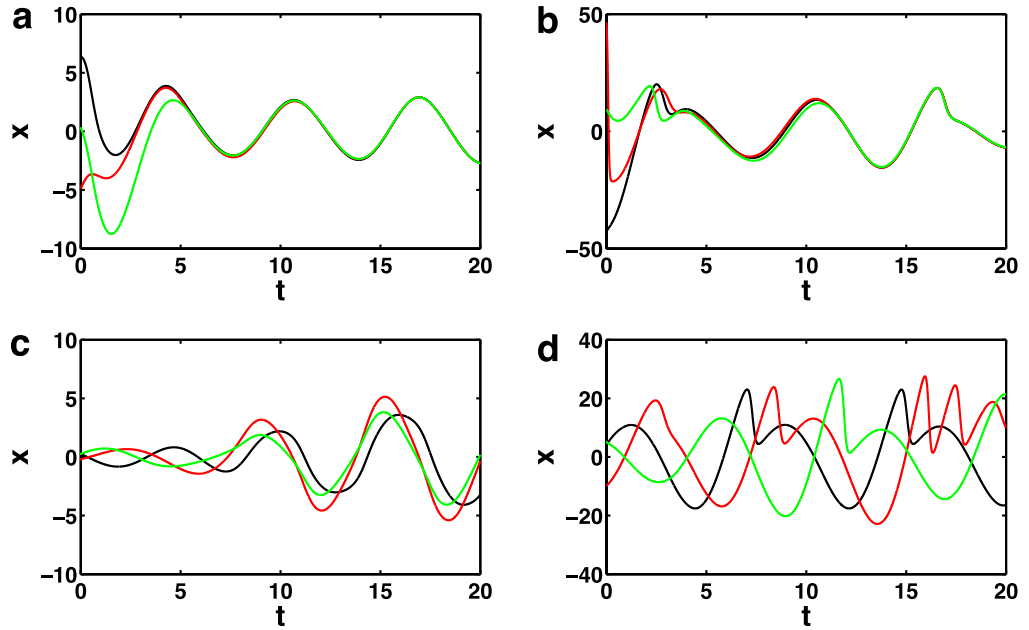


Figure 1. Reconstruction of networks is possible for various types of collective dynamics. A 32-unit random network of Rössler oscillators (9) with fixed connection probability $p = 0.5$ exhibiting (a) a synchronous periodic state ($a_i \equiv 0.2$, $b_i \equiv 1.7$ and $c_i \equiv 4.0$ for all units); (b) a synchronous chaotic state ($a_i \equiv 0.2$, $b_i \equiv 1.7$ and $c_i \equiv 13.0$ for all units); (c) an asynchronous periodic state (parameters randomly drawn independently from $a_i \in [0.10, 0.101]$, $b_i \in [0.10, 0.101]$ and $c_i \in \{4, 6, 12\}$); (d) an asynchronous chaotic state (parameters randomly drawn independently from $a_i \in [0.0, 0.38]$, $b_i \in [0.0, 2.0]$ and $c_i \in [13, 16]$). The x -values of three out of $N = 32$ oscillators are shown. Close to perfect reconstructions from all these distinct dynamics are shown in figure 2.

dynamical states ranging from simple periodic synchronous dynamics to very complex, highly chaotic asynchronous states. We choose networks of Rössler oscillators that can exhibit a rich repertoire of collective dynamics from multi-dimensional chaos to periodicity and from global synchrony to asynchrony (see figure 1), depending on local unit parameters and coupling functions. Unless otherwise stated, simulations were performed with Euler first-order integration at a fixed time step of $\delta t = 10^{-5}$, and observations were sampled at fixed time intervals separated by $t_{m+1} - t_m = \Delta t = 10^{-3}$.

3.1. Successful reconstruction from different dynamics

The dynamics of each Rössler oscillator [14] is given by the three ordinary differential equations

$$\begin{aligned}\dot{x}_i &= -y_i - z_i + \sum_{j=1}^N J_{ij} f(x_i, x_j), \\ \dot{y}_i &= x_i + a_i y_i, \\ \dot{z}_i &= b_i + z_i(x_i - c_i),\end{aligned}\tag{9}$$

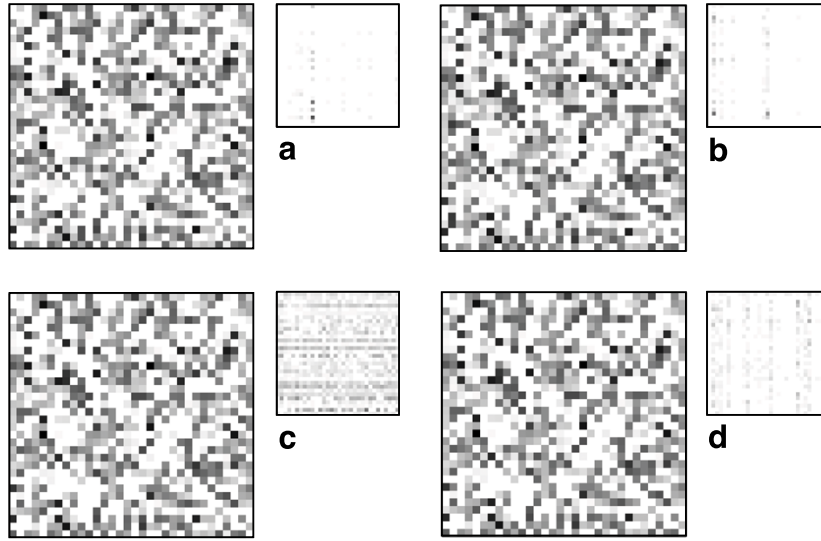


Figure 2. Successful reconstruction of the topology of networks from very different dynamics. Each panel (a)–(d) shows a reconstruction of the network’s topology from the dynamics shown in the respective panels (a)–(d) of figure 1. The smaller panels show absolute differences (c, d magnified by a factor of 10^3) from the actual network (picked randomly from an ensemble of networks with connection probability $p = 0.5$). The reconstructions (a)–(d) used trajectories from very different dynamical states, as shown in figures 1(a)–(d). Reconstructions in panels (c) and (d) have lower errors as they utilize whole dynamical trajectories, instead of transients towards synchronous states, as in panels (a) and (b).

where a_i , b_i and c_i are local parameters. The coupling function was set to $f(x_i, x_j) = x_j - x_i$ to induce synchronization and to $f(x_i, x_j) = \sin(x_j)$ to prevent it. The local unit parameters a_i , b_i and c_i of the Rössler oscillators are chosen to induce either chaotic or periodic dynamics. The parameters were treated as unknown and are not needed for the reconstruction of the network topology. This is the case in this example, since the equations where the parameters of network topology occur (in the x -dimension) do not contain any other (unknown) parameter. We now demonstrate a reconstruction of the network in all four dynamical paradigms illustrated in figure 1: periodic synchronous, chaotic synchronous, periodic asynchronous and chaotic asynchronous collective states.

Reconstruction *in praxis* works as follows: for networks exhibiting synchronized dynamics, the coupling function $f(x_i, x_j) = x_j - x_i$ is uniformly zero for all units in the synchronized state, revealing no information about the network topology. Nevertheless, the network can still be reconstructed from its *transient* dynamics towards the synchronous state. In general, by substituting $X_{i,m} = \dot{x}_i(\tau_m) + y_i(\tau_m) + z_i(\tau_m)$ and $G_{ij,m} = f(x_i(\tau_m), x_j(\tau_m))$ in (6), we find the least-squares reconstructed network according to (8). Since each unit has at most $N - 1$ incoming links of unknown weights, the diagonals in the reconstructed $\hat{J}$ are zero. A reliable reconstruction of the network from trajectories (as shown in figure 1) is illustrated in figure 2, for all four dynamical paradigms considered.

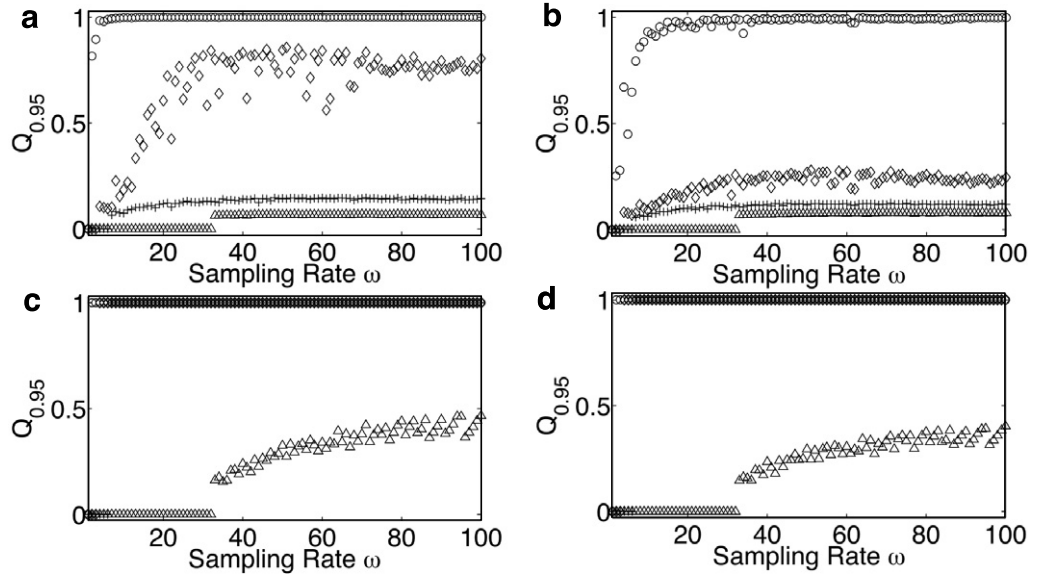


Figure 3. Quality of reconstruction ($Q_{0.95}$) as a function of sampling rate ω and observation time T . Good-quality reconstruction can be achieved even at low sampling rates. The underlying system dynamics used for reconstruction in panels (a)–(d) are shown in figures 1(a)–(d). The lengths of observations are $T = 1$ (Δ), $T = 5$ ($+$), $T = 10$ ($\diamond$) and $T = 20$ ($\circ$). Each point is the result of averaging over 50 networks.

3.2. Quality of reconstruction

How accurate is such a reconstruction? The quality of reconstruction

$$Q_\alpha := \frac{1}{N^2} \sum_{i,j} H((1 - \alpha) - \Delta J_{ij}) \in [0, 1] \quad (10)$$

is defined as the fraction of coupling strengths that are considered correct. Here $\alpha \leq 1$ is the required accuracy of the coupling strengths and H is the Heaviside step function, $H(x) = 1$ for $x \geq 0$ and $H(x) = 0$ otherwise. The normalized element-wise difference between the reconstructed and real networks is

$$\Delta J_{ij} := |\hat{J}_{ij} - J_{ij}| / (2J_{\max}), \quad (11)$$

where $J_{\max} = \max_{i',j'} \{|J_{i',j'}|, |\hat{J}_{i',j'}|\}$. Typically, the quality of reconstruction increases with both the sampling rate and the length of trajectory observed, becoming close to 1 even at lower sampling rates for longer times (see figure 3).

3.3. Required observation time

What is the minimum length of observation required to reconstruct a network? Assuming fixed sampling rate $\omega = (t_m - t_{m-1})^{-1}$, we define

$$T_{q,\alpha,\omega} := \min \{T \mid Q_\alpha(T) \geq q\} \quad (12)$$

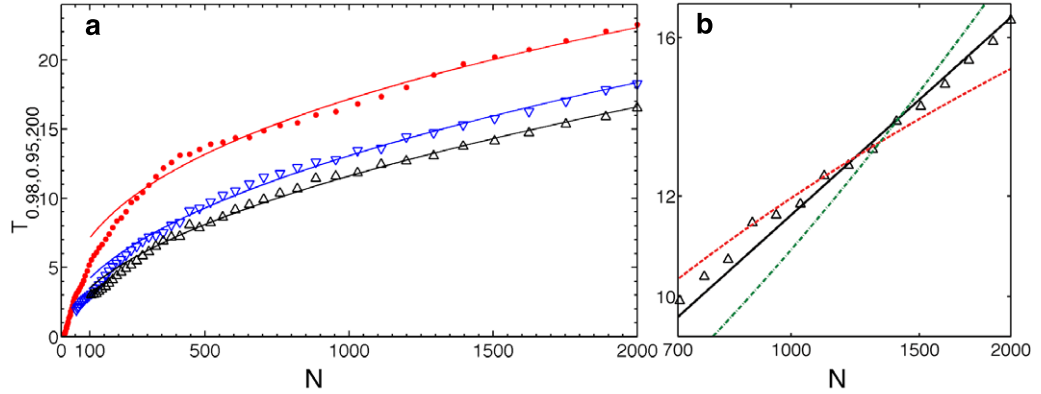


Figure 4. Sublinear scaling of reconstruction time with system size. (a) The minimum required time of observation for reconstruction ($q = 0.98$, $\alpha = 0.95$ and $\omega = 200$) grows sublinearly (presumably algebraically) with system size N for networks with various fixed indegrees $K = 10$ ($\bullet$), $K = 50$ (∇) and $K = 100$ ($\triangle$). The fit suggests that $T_{q,\alpha,\omega} \propto N^\gamma$, where the exponent of scaling $\gamma \approx 0.5$. (b) An algebraic scaling (black) fits the data ($K = 100$, $\triangle$) best. Data plotted on a bilogarithmic scale. Linear best-fits (green dashes) overestimate and logarithmic fits (red dots) underestimate reconstruction time. All fits to data from $N = 100$ to $N = 2000$. $\delta t = \Delta t = 0.005$.

to be the minimum length of time of observation required for accurate reconstruction at quality level q at accuracy α . A general observation is that with increasing sampling rate ω or increasing observation time T , the quality increases, due to more accurate information that is obtained about the system's states. In general, however, it is not only the total number $T \times \omega$ of restricting equations (per node and per dimension) that controls the quality. For instance, at a given observation time, high quality close to $Q_{0.95} = 1$ is reached even at lower sampling frequency if the collective dynamics are more irregular, cf figures 3(a) and (b) versus figures 3(c) and (d). We ascribe this to the lower degree of correlation among observations at different times that is required for accurate reconstruction numerics in (8), e.g. for irregular dynamics, sample points more distant in time provide more relevant information increase about the system as they are less correlated than closer-by points.

How does the minimum required observation time scale with system size? Figure 4 shows $T_{0.98,0.95,200}$, the minimum length of time of observation required to have at least $q = 98\%$ of the links accurate in strength to an accuracy of at least $\alpha = 0.95$, sampled at a rate of $\omega = 200$, as a function of N . The numerics suggest that, at fixed ω , $T_{q,\alpha,\omega}$ scales sublinearly with network size N for reasonably small $0 < 1 - \alpha \ll 1$ and $0 < 1 - q \ll 1$ (reasonably large α and q). This implies that the cost of observation does not grow prohibitively quickly, and that even large networks can be reconstructed by a single observation of the collective dynamics.

3.4. Robustness: substantial noise and unknown parameters

Is reconstruction still feasible in the presence of substantial noise? Is it possible to find unknown parameters of the local unit systems? In the preceding examples, none of the unknown parameters appeared in the dimension of coupling, making the problem of reconstructing

network topology distinct from that of inferring dynamical parameters. In the following example, we illustrate reconstructing networks with intrinsic unit dynamics that are governed by arbitrary functions with K unknown parameters and where the dynamics are influenced by substantial additive noise $\xi_i^{(d)}$. Assuming that all $\xi_i^{(d)}$ have a finite variance, we note that an observation of the dynamics of the system yields a system of equations linear in the $K + N$ unknowns, which we can solve as before. A simple example is a network of Lorenz oscillators [15], where the dynamics of each oscillator is given by

$$\begin{aligned}\dot{x}_i &= \sigma_i (y_i - x_i) + \sum_{j=1}^N J_{ij} (x_j - x_i) + \xi_i^{(x)}(t), \\ \dot{y}_i &= x_i (\rho_i - z_i) - y_i + \xi_i^{(y)}(t), \\ \dot{z}_i &= x_i y_i - \beta_i z_i + \xi_i^{(z)}(t),\end{aligned}\tag{13}$$

where the parameters σ_i , ρ_i and β_i are unknown, and chosen randomly from intervals where the Lorenz system is known to be chaotic: $\sigma_i \in [9, 11]$, $\rho_i \in [20, 35]$, $\beta_i \in [2, 3]$. The $\xi_i^{(d)}(t)$ represent external Gaussian white noise components, independent of all $d \in \{x, y, z\}$ and all $i \in \{1, \dots, N\}$, without bias, $\langle \xi_i^{(d)}(t) \rangle = 0$, and with correlation $\langle \xi_i^{(d)}(t) \xi_j^{(d')}(t') \rangle = 2\lambda \delta(t - t') \delta_{i,j} \delta_{d,d'}$; here λ is the noise strength. In our discrete time simulations of the continuous time dynamics, we take the first-order Euler method with time steps $\delta t = 0.001$ and $\lambda = 5$. The network topology *and* all parameters of the system can be reconstructed and the reconstruction method works despite substantial interference from noise. Figure 5 shows a successful reconstruction of the network and of all dynamical parameters for a network of heterogeneous Lorenz oscillators, where the noise amplitude is chosen such that it drastically alters the dynamics from its deterministic counterpart (black versus blue curve in figure 5(a)). This illustrates by example that the theory is insensitive to additive noise and capable of successful reconstruction, as desired for generic real-world systems.

4. Recipe for network reconstruction

Here, we briefly outline the method for reconstructing network connection topology from observed collective time series of state variables:

- (i) Observe the collective dynamical trajectory $\mathbf{x}_i(t)$ of all units of the network at times $t \in \{t_0, t_1, \dots, t_M\}$.
- (ii) Estimate states $x_i^{(d)}$ and derivatives $\dot{x}_i^{(d)}$ at times $\tau_m = \{\tau_1, \tau_2, \dots, \tau_M\}$ where $\tau_m := (t_{m-1} + t_m)/2$ by approximating to first-order (3)–(4).
- (iii) Use the observed state variables $x_i(\tau_m)$ and the estimated derivatives $\dot{x}_i(\tau_m)$ to compute $f_i^{(d)}(\mathbf{x}_i(\tau_m))$ and $g_{ij}^{(d)}(\mathbf{x}_i(\tau_m), \mathbf{x}_j(\tau_m))$ and set up the matrix equation (6).
- (iv) Using ℓ_2 optimization, solve for unknown coupling strengths (and, if applicable, for unknown parameters appearing linear in the system) according to (8).
- (v) If desired, threshold the resultant weighted adjacency matrix, as appropriate for the question under consideration.

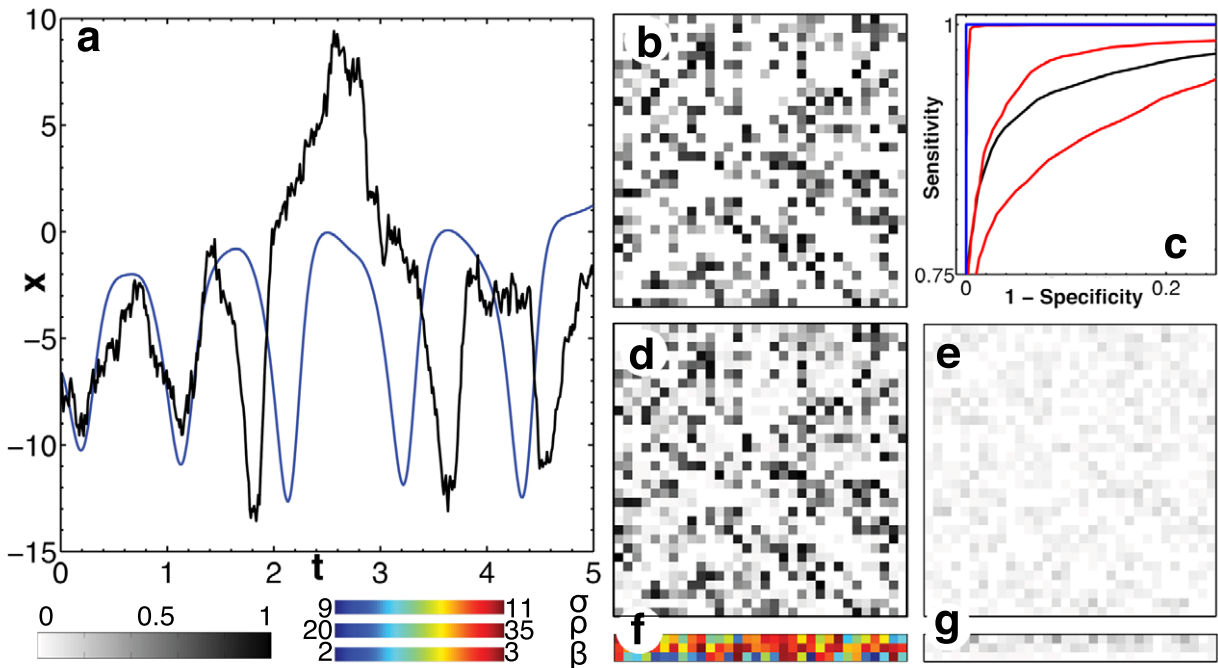


Figure 5. Reconstructing a network and unknown parameters for a system in the presence of substantial external noise $\lambda = 5$. (a) The dynamics of a unit in a network of 32 Lorenz oscillators in the noise-free (blue) and noise-driven (black) regimes. The network was a realization from an ensemble of networks with edge connection probability $p = 0.5$. Starting from the same initial condition, the noise-driven trajectory quickly deviates due to the chaotic nature of the system. Reconstruction of the network topology (d) and parameters (f) with corresponding absolute errors (e), (g). Panel (b) shows the actual network, and (c) shows the receiver operating characteristics (ROC) of reconstruction from noiseless (blue) and noisy (black, $\lambda = 5$) observations, as the detection threshold is varied. For the three red curves, the noise amplitude $\lambda \in \{0.1, 1, 10\}$. Simulation time step $\delta t = 0.001$, sampling interval $\Delta t = 0.01$.

5. Conclusion

In summary, we have introduced a simple robust method for inferring the connection topology from observations of deterministic and noisy network dynamical systems, where the functional form of the evolution equations is known.

Our method is unique in the following ways. A simple sufficiently long observation of the system dynamics suffices to reconstruct the network topology and coupling strengths. In many cases, experimental access to the system, say to introduce ‘control signals’, as in [10, 12] may not be possible, and the method proposed here does not require any form of system intervention. Furthermore, the type of collective dynamics is not restricted to, e.g., fixed points, periodic orbits, synchronous states or any other specific type of motion (cf [8, 10]). Using entire dynamical trajectories, including transients, for the reconstruction, we demonstrate robust reconstruction for a wide range of observed dynamical states, from asynchronous chaotic states to transient states towards global synchrony. Moreover, we treated the system as a

‘grey box’, where we know some general principles of the system (such as the coupling functions) but lack the details, such as network structure or intrinsic parameters. Given (e.g. experimental) dynamical observation data, our theory provides an explicit analytic solution to the inverse problem of finding the network structure. This solution is a direct restatement of the differential equations governing the dynamics of the system, and is thus conceptually simple. This simplicity may suggest high attainable quality for such inverse problems.

The method scales sublinearly with network size, seems robust against substantial addition of noise and thus provides a promising complement to existing reconstruction methods. Thus, our method offers a conceptual simplification over other methods that make the same assumptions we do, but rely on more complex techniques such as copy-synchronization (called auto-synchronization in [12]) or the use of topology estimating clone models or control signals [11]. Further, the method suggested here is capable of reconstructing the network structure from a simple observation of the system’s dynamics, without resorting to any external intervention to drive the system into or from some canonical state, as in [10].

Efforts to understand the general interplay of network structure and dynamics have yielded several promising approaches, mainly applicable to smaller systems. Notable among the forward methods, i.e. methods that predict dynamical features from the knowledge of network topology, are those that study the propagation of a harmonic perturbation through a network of coupled phase oscillators [16, 17] and methods for predicting disordered dynamics from the structures of strongly connected components in the network [18]. Cimponeriu *et al* [19] introduced two methods for estimating the interaction delay in weak coupling between two self-sustained oscillators from observed dynamical time series. Arenas *et al* [20] show that times of synchronization can reveal the hierarchical structure of a network, revealing a connection between synchronization dynamics and topological clustering. In an alternative approach, Memmesheimer and Timme [21, 22] present an analytical method for designing networks of spiking neurons that display a required spike pattern. Other inverse methods have relied on stochastic optimization [23] to fit a model of a network of spiking neurons to an observation of a real network to infer its topological parameters. Reconstructing gene regulatory networks has been shown to be useful in identifying targets of drugs from secondary responders [3]. For systems where good proxy models for the dynamics of single units and their interactions already exist, e.g. for interacting genes and proteins, for neural circuits and for generic systems of coupled oscillators (e.g. pacemaker networks), the new, simpler method developed here may be implemented in a straightforward way.

Several avenues for further research present themselves. As suggested by previous work [7, 10], minimizing the ℓ_1 norm, instead of the ℓ_2 norm as used here, may result in more efficient reconstruction of sparse networks [24]. In addition, our preliminary studies suggest that this highly overdetermined inverse problem can be reduced to an exactly determined problem by selectively choosing points on the time series to ensure that the resultant system of equations is maximally linearly independent. This reduction significantly reduces the cost of computation to reconstruct large networks. Furthermore, it is straightforward to extend this method to coupled map networks and to systems with delay. Finally, recent studies show that a method analogous to the one presented here for smoothly coupled systems is capable of reconstructing networks of pulse-coupled systems such as integrate-and-fire neurons [25].

Acknowledgments

We thank C Kirst and R-M Memmesheimer for valuable discussions. This work was partially supported by the Federal Ministry of Education and Research, Germany, via the Bernstein Center for Computational Neuroscience, Göttingen, under grant number 01GQ1005B and by a grant from the Max Planck Society to MT.

References

- [1] Strogatz S 2001 *Nature* **410** 268–76
- [2] Hu T and Leonardo A 2009 Reconstruction of sparse circuits using multi-neuronal excitation (RESCUME) *Advances in Neural Information Processing Systems* 22 NPIS Foundation (New York: Curran Associates)
- [3] di Bernardo D, Thompson M, Gardner T, Chobot S E, Eastwood E L, Wojtovich A P, Elliott S J, Schaus S E and Collins J J 2005 *Nat. Biotechnol.* **23** 377–83
- [4] Hufnagel L, Brockmann D and Geisel T 2004 *Proc. Natl Acad. Sci. USA* **101** 15124
- [5] Drossel B and McKane A J 2003 Modelling food webs *Handbook of Graphs and Networks* (Berlin: Wiley-VCH)
- [6] Palsson B O 2006 *Systems Biology: Properties of Reconstructed Networks* (Cambridge: Cambridge University Press)
- [7] Tegnér J, Yeung M, Hasty J and Collins J 2003 *Proc. Natl Acad. Sci. USA* **100** 5944–9
- [8] Gardner T, di Bernardo D, Lorenz D and Collins J 2003 *Science* **301** 102–5
- [9] Faith J J, Hayete B, Thaden J T, Mogno I, Wierzbowski J, Cottarel G, Collins S K J J and Gardner T S 2007 *PLoS Biol.* **5** 54–66
- [10] Timme M 2007 *Phys. Rev. Lett.* **98** 224101
- [11] Yu D, Righero M and Kocarev L 2006 *Phys. Rev. Lett.* **97** 188701
- [12] Yu D and Parlitz U 2008 *Phys. Rev. E* **77** 066221
- [13] 2006 MATLAB7 (Natick, MA: The Mathworks Inc.)
- [14] Rössler O 1976 *Phys. Lett. A* **57** 397–8
- [15] Lorenz E 1963 *J. Atmos. Sci.* **20** 130–41
- [16] Zanette D 2004 *Europhys. Lett.* **68** 356–60
- [17] Kori H and Mikhailov A 2004 *Phys. Rev. Lett.* **93** 254101
- [18] Timme M 2006 *Europhys. Lett.* **76** 367–73
- [19] Cimponeanu L, Rosenblum M and Pikovsky A 2004 *Phys. Rev. E* **70** 046213
- [20] Arenas A, Diaz-Guilera A and Perez-Vicente C 2006 *Phys. Rev. Lett.* **96** 114102
- [21] Memmesheimer R M and Timme M 2006 *Phys. Rev. Lett.* **97** 188101
- [22] Memmesheimer R M and Timme M 2006 *Physica D* **224** 182–201
- [23] Makarov V, Panetsos F and Feo O 2005 *J. Neurosci. Methods* **144** 265–79
- [24] Napoletani D and Sauer T 2008 *Phys. Rev. E* **77** 26103
- [25] van Bussel F, Kriener B and Timme M 2010 *Frontiers in Computational Neuroscience* under review