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Accelerated reference frames (ARFs) reveal networks from time series data

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Abstract

Inferring direct interactions in complex networked systems from time series data constitutes a challenging open problem of current research. Major obstacles include the often limited number of time points accessible, unknown or inaccurate dynamical systems models in many practical applications, the impossibility to infer topological information from invariant collective dynamics such as synchronized states, and the required computational effort. Here, we propose and analyze a mathematical scheme that transforms observed transient dynamics towards invariant states in to accelerated reference frames to reveal network interactions. The transformation yields simple linear constraints relating a number of short observed time series (of only a few data points) of the dynamics to estimates the absence, presence and strength of direct physical interactions in a computationally efficient way. As we illustrate numerically, the scheme applies across transient dynamics towards periodic and chaotic, phase-locked and other synchronized states. Reconstruction robustly reveals the entire connectivity of network dynamical systems with increased reconstruction quality for large and for sparse networks.

The collective dynamics of a networked system is shaped by its underlying interaction topology [1–8]. Yet, whereas recording the dynamics of individual units of networks is becoming more accessible in experimental settings, directly measuring the physical interaction topology of networks is often infeasible. Researchers routinely resort to indirect methods to infer the physical interactions from the networks' collective dynamics [9]. State-of-the-art approaches infer physical interactions via ODE modeling using large repertoire of functions [10–14]. Such approaches require the entire dynamics to admit a sparse representation in the chosen repertoire, which is difficult to satisfy if no prior information is provided. More recent approaches bypass the need for sparsity and reconstruct the full interaction topology by either imposing functional decompositions in grouped variables [15], or by driving the network dynamics with known constant signals [16]. While the former strategy carries along a high computational complexity that may become intractable in large networks, the latter demands an accurate (and often infeasible) control of network dynamics.

Moreover, the dynamics of systems in invariant sets (such as synchronized states), for mathematical reasons, is generically not capable of revealing complete topological interaction patterns [17–19]. This constraint comes about because in invariant states, the dynamics of each unit exhibits a strict functional dependence on the dynamics of the other units in the system such that the information contained in observed time series is insufficient for inferring interactions, no matter how many time series and how many data points per series are observed. As a consequence, practical approaches [14, 20–24] exploit transient dynamics towards synchronized or locked states such that the dynamics are not exactly invariant and do contain sufficient information for inferring network interactions, at least in principle. For simple classes of phase oscillators with constant, state-independent frequencies exhibiting exactly phase-locked or fully synchronous dynamics, transforming time series to a frame of reference that is co-moving with the dynamics is often possible by subtracting a term $-\Omega t$, containing the collective frequency Ω of the phase dynamics of each oscillator. However, such simple transformations are useless if intrinsic oscillator frequencies and collective frequencies are state-dependent, if

individual oscillators have more than one variable and in particular if collective dynamics is non-periodic and for instance chaotic.

In this article, we propose a tractable and model-free approach for inferring the interaction topology of networks relying only on transient dynamics towards stable attractors such as synchronized or phase-locked states. Specifically, we introduce the concept of accelerated reference frames (ARFs) in network dynamical systems and show how a nonlinear transformation of time series by subtracting reference variables that are accelerated and state-dependent themselves can reveal direct physical (as opposed to correlative statistical) interactions. Reconstruction is feasible for dynamics towards phase-locked or otherwise synchronized states with periodic or aperiodic and chaotic collective dynamics. Transformations in to co-moving ARFs enables linearizations about fixed points in the transformed dynamics, and thus mapping of the original inference problem to one for transient relaxations towards linearly stable fixed points. The ARF transformation thereby opens up solving a previously hardly accessible range of inference problems in a computationally effective, model-independent way.

1. Network inference on accelerated reference frames

To understand how ARFs aid in revealing the connectivity of networked systems, consider N coupled dynamical units of the form

$$\dot{x}_i = f_i(\Lambda^i \mathbf{x}), \quad (1)$$

where $x_i(t) \in \mathbb{R}$ represents the state of unit $i \in \{1, 2, \dots, N\}$ at time t , $\dot{x}_i = dx_i/dt$ denotes time derivative, $f_i: \mathbb{R}^N \rightarrow \mathbb{R}$ is an unknown continuously differentiable function determining the dynamics of i and $\mathbf{x} := [x_1, x_2, \dots, x_N]^T \in \mathbb{R}^N$ is a vector containing the state of all units in the network. The *explicit dependency matrices* $\Lambda^i \in \{0, 1\}^{N \times N}$ for $i \in \{1, \dots, N\}$, introduced in [15], are diagonal and their entries indicate which other units in the network directly affect the dynamics of unit i [15]. Specifically, if a unit j does not directly affect the dynamics of i , we have $\partial f_i / \partial x_j \equiv 0$ for all times t , and define $\Lambda_j^i = 0$ and if it does, we have $\partial f_i / \partial x_j \neq 0$ and define $\Lambda_j^i = 1$. Thus the diagonal entries Λ_j^i are non-zero if and only if the element A_{ij} of an adjacency matrix A , defining the dependency structure in a graph-theoretic setting, is non-zero.

Our aim is to transform the dynamics (1) to new variables $\mathbf{y}(t)$ such that these exhibit convergence to a fixed point if the original variables $\mathbf{x}(t)$ exhibit convergence to some form of synchronized state (see below for details). We propose to represent the dynamical units in (1) by subtracting an ARF as

$$y_i = x_i - g_i(\mathbf{x}), \quad (2)$$

where $g_i: \mathbb{R}^N \rightarrow \mathbb{R}$ indicates the location of i th component of the reference frame. Especially, the function $\mathbf{g}(\mathbf{x}) := [g_1(\mathbf{x}), g_2(\mathbf{x}), \dots, g_N(\mathbf{x})]^T \in \mathbb{R}^N$ represents an accelerated frame because it moves in dependence with the network state \mathbf{x} . We note that the reference frame is ‘accelerated’ with acceleration identically zero if $d^2 g_i / dt^2(\mathbf{x}) \equiv 0$ for all times t .

The time evolution of units in the accelerated frame is then given by

$$\dot{y}_i = \dot{x}_i - \nabla g_i(\mathbf{x}) \dot{\mathbf{x}}, \quad (3)$$

where ∇ is the gradient operator, and it follows that

$$\dot{y}_i = f_i(\Lambda^i \mathbf{x}) - h_i(\mathbf{x}), \quad (4)$$

with

$$h_i(\mathbf{x}) := \sum_{k=1}^N \frac{\partial g_i(\mathbf{x})}{\partial x_k} f_k(\Lambda^k \mathbf{x}). \quad (5)$$

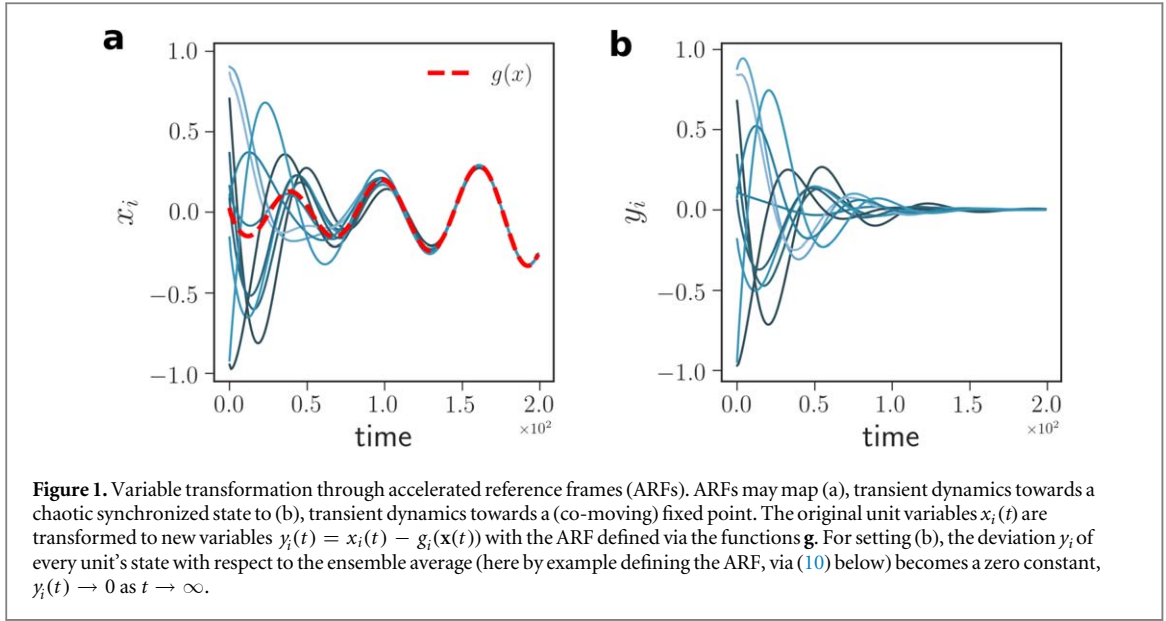
Assuming that \mathbf{y} is sufficiently small, we may approximate (4) around $\mathbf{g}(\mathbf{x})$ to first order in the y_i as

$$\dot{y}_i \doteq f_i(\Lambda^i \mathbf{g}(\mathbf{x})) - h_i(\mathbf{g}(\mathbf{x})) + \sum_{j=1}^N C_{ij}(\mathbf{g}(\mathbf{x})) y_j, \quad (6)$$

where

$$C_{ij}(\mathbf{g}(\mathbf{x})) := \frac{\partial f_i(\mathbf{g}(\mathbf{x}))}{\partial x_j} \Lambda_j^i - \frac{\partial h_i(\mathbf{g}(\mathbf{x}))}{\partial x_j}. \quad (7)$$

The first two terms on the right hand side of (6) define the intrinsic local dynamics of the transformed variables y_i , whereas C_{ij} , appearing in the third term and defined via (7), quantifies the effective coupling strength from unit j to i in the accelerated frame.



Our goal is to identify which of the Λ_j^i are zero and thus where there is no direct physical interaction from j onto i and which Λ_j^i are one, indicating a direct interaction. We remark that the quality of the inference options discussed below depend on the resulting transformation of interactions (7), as it depends on the degree the relative influence of the first term versus that of the second term in (7). This quality thus depends on the dynamics of the accelerated frame also set by properties of the system dynamics f_i , the ARF transformation functions g_i and on the actual size and sparsity of the network, as we will discuss shortly. Independent of those details, the connectivity properties of the original system (1) should be identifiable if the second term in (7) is sufficiently small. We need to carefully choose a reference frame to enforce a (ideally very strong) correlation between $C_{ij}(\cdot)$ and Λ_j^i , reflecting the coupling between the accelerated and original dynamical variables.

The long term behavior of a range of systems exhibiting attractors with oscillatory, periodic or chaotic dynamics, may be transformed to relaxations towards fixed points if appropriate reference frames are chosen. For instance, phase oscillators evolving towards phase-locked states ($x_i(t) - x_j(t) = \Delta_{ij}$) or identically synchronizing oscillators ($x_i(t) - x_j(t) = 0$) may be considered as relaxing towards a fixed point if we subtract the average state variable across all oscillators from each individual oscillator's state, see figure 1 below. In such ARFs, differences with respect to the average phase change as the system evolves towards the phase-locked state and remain constant once the system reaches such final state, see figure 1 for illustration.

In mathematical terms these properties mean that for such attractors there are functions $\mathbf{g}(\cdot): \mathbb{R}^N \rightarrow \mathbb{R}^N$ that satisfy $x_i(t) - g_i(\mathbf{x}(t)) \rightarrow y_i^*$ for all i as $t \rightarrow \infty$. Thus, we propose that an analogous system $\dot{y}_i(t) = \tilde{f}_i(\mathbf{y}(t))$ evolving towards a fixed point in the accelerated frame may be approximated around that point $\mathbf{y}^* := [y_1^*, y_2^*, \dots, y_N^*]^T \in \mathbb{R}^N$ as

$$\dot{y}_i(t) \doteq \sum_{j=1}^N A_{ij} [y_j(t) - y_j^*], \quad (8)$$

where $\tilde{f}_i: \mathbb{R}^N \rightarrow \mathbb{R}$ is an unknown function determining the evolution of y_i and $A_{ij} := \partial \tilde{f}_i(\mathbf{y}^*) / \partial y_j$ may be used as a proxy for a interaction strength from unit j to i .

So, given a collection of M transient states $\{\mathbf{y}(t_m), \dot{\mathbf{y}}(t_m)\}$ towards \mathbf{y}^* , we pose the reconstruction problem as the error minimization

$$\hat{\mathbf{J}}_i = \arg \min_{\{\mathbf{J}_{ij}\}} \left\| \sum_{m=1}^M \left(\dot{y}_i(t_m) - \sum_{j=1}^N A_{ij} [y_j(t_m) - y_j^*] \right) \right\|_2^2, \quad (9)$$

where $\hat{\mathbf{J}}_i := [\hat{J}_{i1}, \hat{J}_{i2}, \dots, \hat{J}_{iN}] \in \mathbb{R}^N$ represent the inferred incoming links to unit i . In particular, minimization (9) may be efficiently solved using the Moore–Penrose pseudoinverse [25] if $M > N$, and it can be solved for different units in parallel [9].

2. Average network states as examples of Accelerated Reference Frames (ARFs)

As an illustrative example, consider the average over the units' states to define an appropriate ARF for a class of systems exhibiting transient dynamics towards phase-locked or otherwise synchronous dynamics. We start focusing on phase-locking where $x_j(t) - x_i(t) \rightarrow \Delta_{ij}$ for all i, j as $t \rightarrow \infty$ and illustrate more complex collective dynamics below. Examples of phase-locking systems are networks of phase oscillators and other network dynamical systems exhibiting collective synchronization (where $\Delta_{ij} = 0$ for all i, j in case of identical synchronization).

We compute the average network state as

$$\mathbf{g}(\mathbf{x}(t)) = \frac{1}{N} \mathbf{1}^T \mathbf{x}(t), \quad (10)$$

where $\mathbf{1} \in \{1\}^N$ is a vector full of ones, and T denotes transpose. This definition with components

$$g_i(\mathbf{x}) = \frac{1}{N} \sum_{j=1}^N x_j \quad (11)$$

provides a reference frame that is accelerated, because

$$\frac{dg_i}{dt} = \sum_{j=1}^N \frac{\partial g_i}{\partial x_j} \dot{x}_j = \frac{1}{N} \sum_{j=1}^N f_j(\mathbf{x}) \quad (12)$$

which in general is non-constant in time. The units' state and rate of change defined through (2) and (3) yield

$$y_i(t) = x_i(t) - \frac{1}{N} \sum_{j=1}^N x_j(t), \quad (13)$$

$$\dot{y}_i(t) = \dot{x}_i(t) - \frac{1}{N} \sum_{j=1}^N \dot{x}_j(t). \quad (14)$$

In particular, in locked-like states, all units move together with the same collective velocity, thereby $y_i(t) \equiv y_i^*$ for all t (see figure 1(b)). So, any perturbation that evolves towards such state may be seen as a relaxation towards a fixed point in the y_i variables, where $\lim_{t \rightarrow \infty} (y_i(t) - y_i^*) = 0$ for all i .

How can the optimization (9) reveal network links considering transformed variables in this ARF? We gain insights about the effects of the frame on the proxies \hat{f}_i of (9) by evaluating (7) on (10) to result in

$$C_{ij}(\mathbf{g}(\mathbf{x}(t))) := \frac{\partial f_i(\mathbf{g}(\mathbf{x}(t)))}{\partial x_j} \Lambda_j^i - \frac{1}{N} \sum_{k=1}^N \frac{\partial f_k(\mathbf{g}(\mathbf{x}(t)))}{\partial x_j} \Lambda_j^k. \quad (15)$$

To obtain an intuition about the conditions when inference of a present versus absent original connection (Λ_j^i) may be feasible, assume for the sake of argument that the derivatives are of the same order of magnitude a , $\frac{\partial f_\ell(\mathbf{g}(\mathbf{x}(t)))}{\partial x_{\ell'}} \approx a$ for all ℓ, ℓ' , if they are non-zero. Then for a given link (i, j) we have

$$C_{ij} \approx a \Lambda_j^i - \frac{n_j^+}{N} a \quad (16)$$

where $n_j^+ = \sum_{k=1}^N \Lambda_j^k$ is the number of outgoing connections from unit j , i.e. its node degree in a graph-theoretic perspective. Now the task is to distinguish the case where the link is actually *present* in the network, $\Lambda_j^i = 1$ and thus $|C_{ij}| \approx \left| a - \frac{n_j^+}{N} a \right|$, from the case where it is absent, $\Lambda_j^i = 0$ and thus $|C_{ij}| \approx \left| \frac{n_j^+}{N} a \right|$. Thus, the form of (15) intuitively suggests that the distinction between present and absent links is simpler if the network is sparser (and thus the n_j are smaller) and, intriguingly, if the network is larger. The above analysis together with the intuitive arguments suggest that the average network state indeed is an appropriate ARF, at least for systems exhibiting synchronizing and locked-like dynamics. The numerical analyses presented below confirm this picture.

3. Reconstructing networks of phase-locking and synchronizing oscillators

To test our theory practically, we reconstructed the connectivity of coupled oscillators from their transient time evolution towards some locked or synchronizing states. To start simple, we first reconstructed directed networks of Kuramoto oscillators, figure 3, [26, 27] with dynamics

$$\dot{x}_i = \omega_i + \frac{1}{n_i^-} \sum_{j=1}^N J_{ij} \sin(x_j - x_i), \quad (17)$$

where $J \in \mathbb{R}^{N \times N}$ is given by $J = L \odot A$, the operator \odot stands for entry-wise-matrix product, A is the adjacency matrix, and both the ω_i and L_{ij} are randomly drawn from uniform distributions on the intervals $\omega_i \in (0, 1]$ and $L_{ij} \in [0.5, 1]$, and the initial conditions $x_i(0)$ of the system are taken from the uniform distribution $x_i(0) \in [-0.5, 0.5]$. Moreover, n_i^- as above indicates the number of incoming connections to unit i , figure 3.

To also assess the generality of our theory beyond phase-locking dynamics of one-dimensional (phase) oscillators, we inferred the connectivity of networks of synchronizing Roessler oscillators [28] in periodic and chaotic regimes, of synchronizing chaotic Lorenz oscillators [29] and of periodic Goodwin oscillators [30] serving as simple paradigmatic models of gene regulatory circuits. Each Roessler oscillatory unit evolves according to a network of three-dimensional dynamical units defined as

$$\dot{x}_i^{(1)} = -x_i^{(2)} - x_i^{(3)} + \frac{1}{n_i^-} \sum_{j=1}^N J_{ij}(x_j^{(1)} - x_i^{(1)}), \quad (18a)$$

$$\dot{x}_i^{(2)} = x_i^{(1)} + ax_i^{(2)}, \quad (18b)$$

$$\dot{x}_i^{(3)} = b + x_i^{(3)}(x_i^{(1)} - c), \quad (18c)$$

where the entries of J are set as before. The periodic and chaotic dynamics were generated with parameters $(a, b, c) = (0.2, 1.7, 4.0)$ and $(0.1, 0.1, 18.0)$, respectively, and the initial conditions were drawn from the uniform distribution $x_i^{(1)}(0), x_i^{(2)}(0), x_i^{(3)}(0) \in [-5, 5]$.

The dynamics of each Lorenz oscillator is determined by

$$\dot{x}_i^{(1)} = \sigma(x_i^{(2)} - x_i^{(1)}) + \frac{1}{n_i^-} \sum_{j=1}^N J_{ij}(x_j^{(1)} - x_i^{(1)}), \quad (19a)$$

$$\dot{x}_i^{(2)} = x_i^{(1)}(\rho - x_i^{(3)}) - x_i^{(2)}, \quad (19b)$$

$$\dot{x}_i^{(3)} = x_i^{(1)}x_i^{(2)} - \beta x_i^{(3)}, \quad (19c)$$

with $(\sigma, \rho, \beta) = (10.0, 28.0, 2.5)$ and initial conditions selected from the uniform distribution $x_i^{(1)}(0), x_i^{(2)}(0), x_i^{(3)}(0) \in [-5, 0]$.

The dynamics of each Goodwin oscillator is given by

$$\dot{x}_i^{(1)} = [1 + (x_i^{(3)})^p]^{-1} - ax_i^{(1)}, \quad (20a)$$

$$\dot{x}_i^{(2)} = x_i^{(1)} - bx_i^{(2)} + \frac{1}{n_i^-} \sum_{j=1}^N J_{ij}(x_j^{(2)} - x_i^{(2)}), \quad (20b)$$

$$\dot{x}_i^{(3)} = x_i^{(2)} - cx_i^{(3)}, \quad (20c)$$

where $p = 17$ and $(a, b, c) = (0.4, 0.4, 0.4)$ with initial conditions drawn from the uniform distribution $x_i^{(1)}(0), x_i^{(2)}(0), x_i^{(3)}(0) \in (0, 3]$.

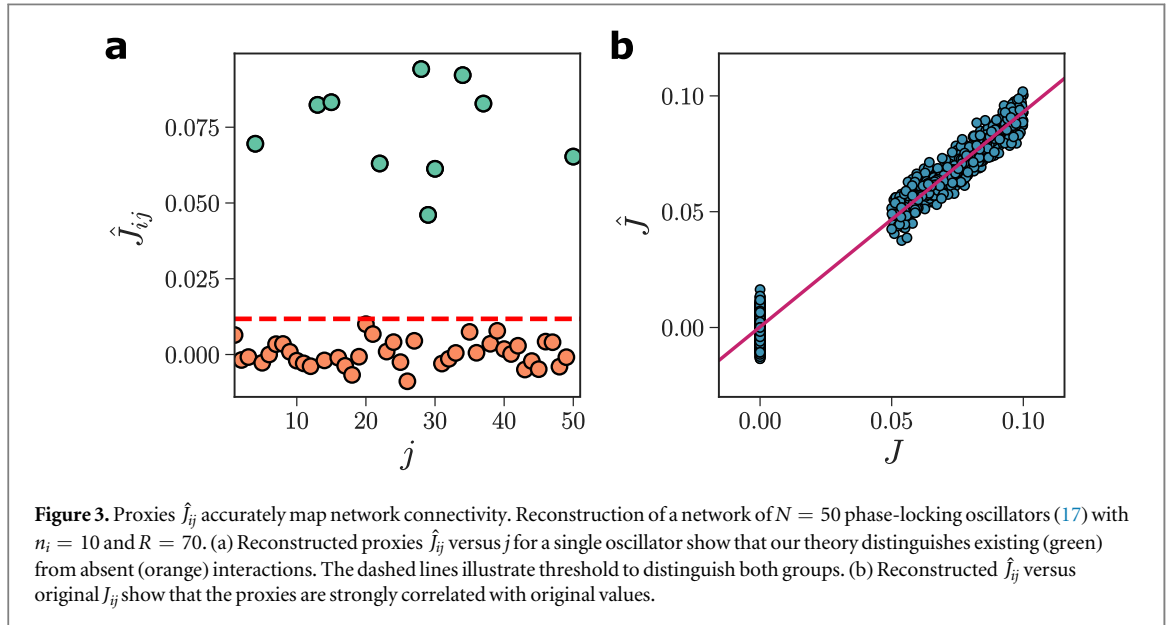
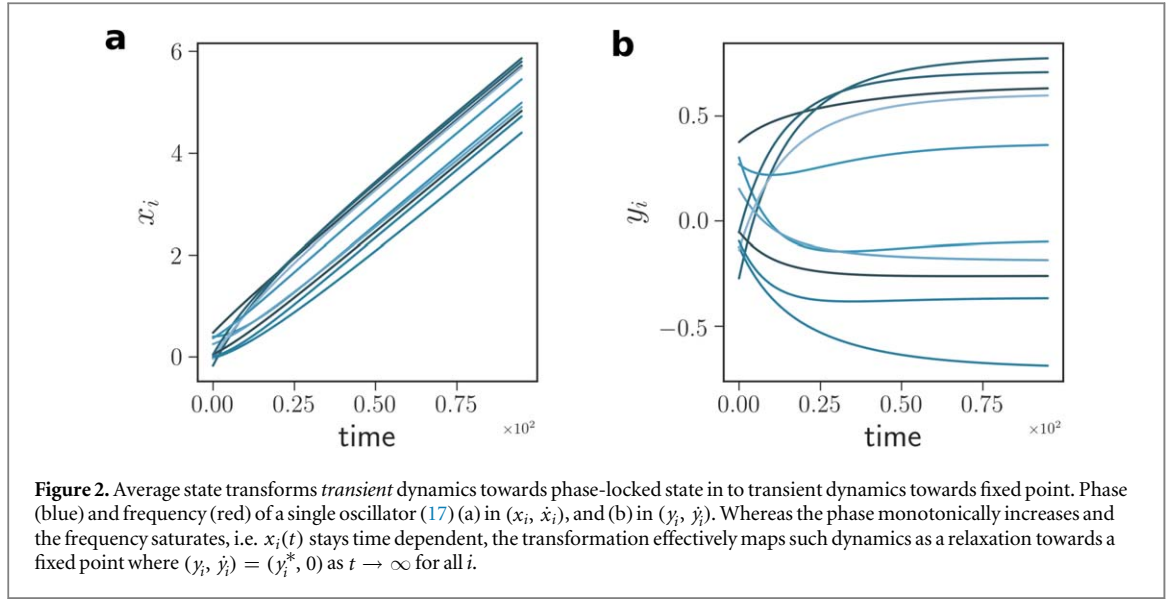
To emulate perturbations away from the locked-like state, we started the systems from random initial conditions and recorded R different transient trajectories towards synchrony. All simulations were performed in a time interval $t \in [0, 10]$ with $\Delta t = 0.1$. Only the first $M = 5$ time points per relaxation were used for reconstruction. Thus, the total number of time points used for reconstruction is

$$T = MR. \quad (21)$$

Simulations of phase-locking oscillators (17) confirm that (10) transforms their dynamics in to relaxations towards fixed points, figure 2. Inferring links from such relaxations via (9) demonstrates that our theory fully distinguishes between existing and absent interactions, figure 3(a). Moreover, our results indicate that the proxies obtained for the coupling strengths are strongly correlated with the actual coupling strengths employed in simulations, figure 3(b).

To study the effects of network sparsity on our framework, we systematically reconstructed networks of different levels of sparsity $s := 1 - n_i^-/N$ solving (9) via the Moore–Penrose pseudoinverse [25] and LASSO [31]. The latter is a standard regularization technique for fitting sparse models to data. In our context, the network connectivity represents the sparse model to fit. Furthermore, to compare both methods, we evaluated the quality of reconstructions in terms of the Area Under the Receiver-Operating Curve (AUC score) which is equal to 1 for perfect reconstruction and equal to 1/2 for reconstructions equivalent to random guessing [32].

Our numerics show that the quality of reconstruction increases with networks of greater sparsity for both Moore–Penrose pseudoinverse and LASSO, figures 4(a)–(b). However, the former shows best performance for increasing number of trajectories (especially for dense networks), figures 4(a)–(c). Moreover, the

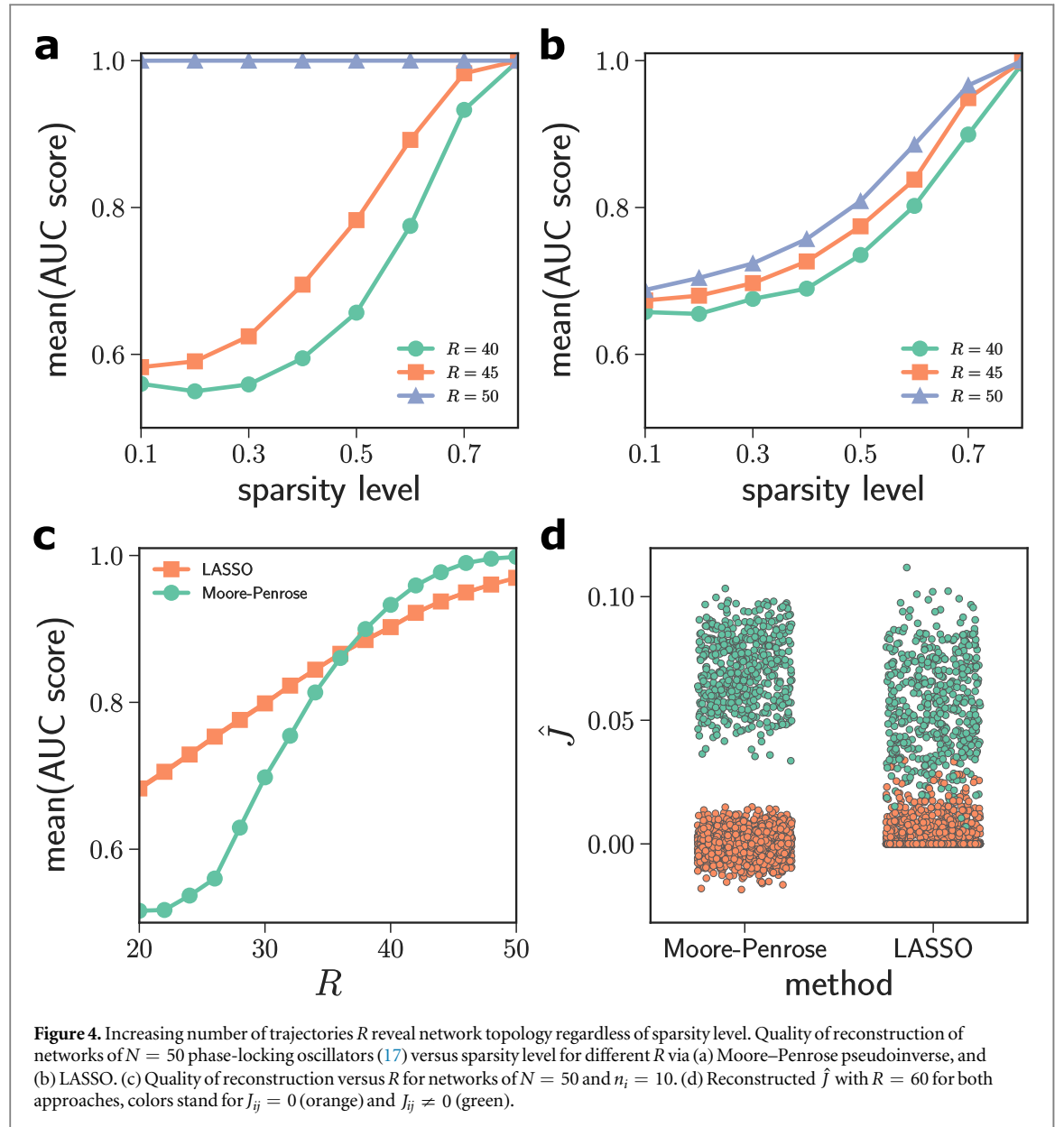


Moore–Penrose pseudoinverse shows superior performance at separating existing from absent connections, despite not being an approach specifically designed for variable selection as LASSO [31].

Can our theory reveal the connectivity of networks showing more complicated dynamics? Networks of synchronizing dynamical systems may evolve in time with a common yet variable rate of change once the network has relaxed back to the synchronized (locked-like) state.

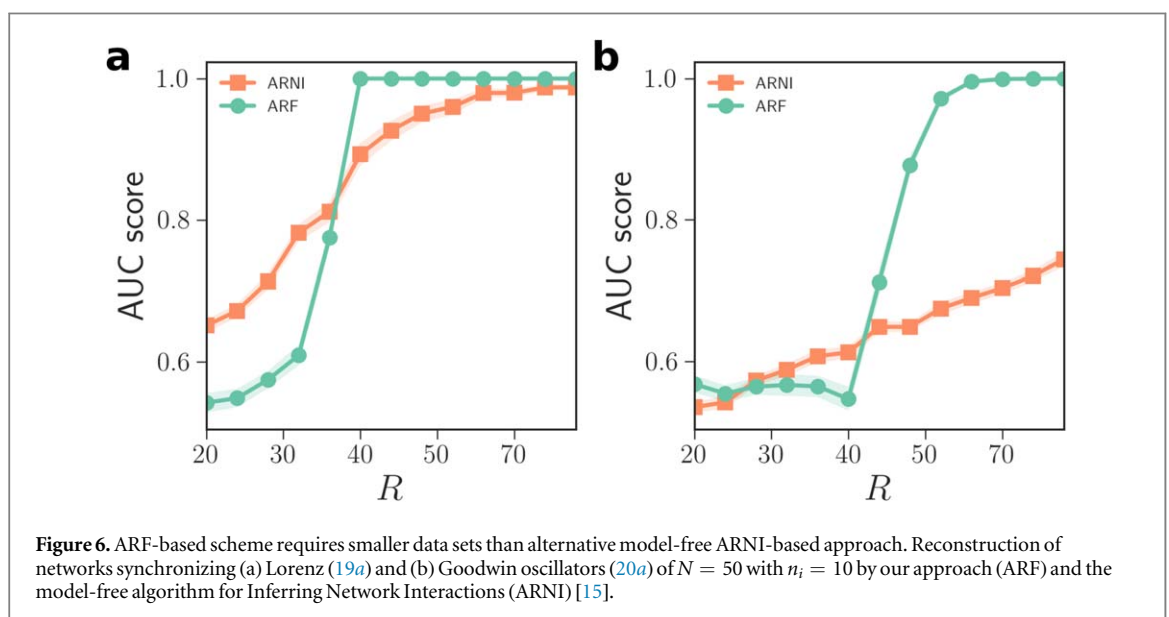
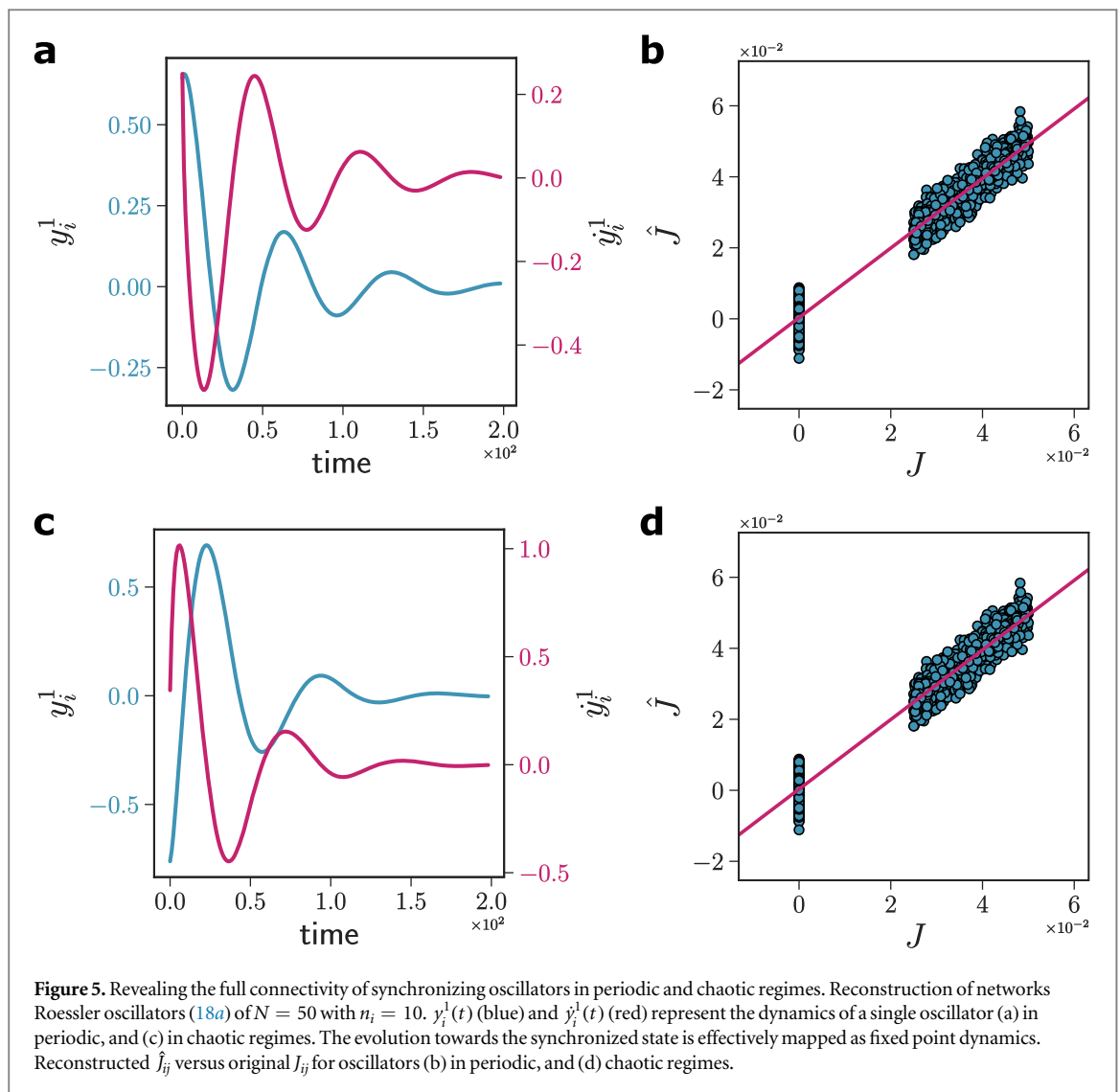
Simulations of networks of synchronizing Rössler oscillators (18a) whose rate of change on the synchronized state changes in time show again that (9) and (10) are effective at mapping the network evolution as fixed point dynamics and reveal the full network topology regardless of whether the oscillators operate in periodic or chaotic regimes¹, figure 5. These results are further supported by simulations of networks of Lorenz (19a) and Goodwin (20a) oscillators. Specifically, we compared the reconstruction quality on such systems using ARF and using the model-free algorithm for Inferring Network Interactions (ARNI) [15], figure 6. The results show that the ARF-based theory proposed here requires smaller data sets than ARNI to reveal the full topology of both systems. These results highlight the advantage of ARFs for inferring the structural connectivity of synchronizing network dynamical systems.

¹ To transform the synchronizing dynamics in to fixed point dynamics, we computed averages for $x^{(1)}$, $x^{(2)}$ and $x^{(3)}$ separately. In general, the reconstruction process may be performed in all components. We here selected the component showing a clear distinction between groups of existing and absent connections.



Summary and Conclusions. We presented a model-independent theory for inferring the interaction topology of synchronizing networks from solely recording their transient collective dynamics. Specifically, we introduced and exploited the concept of ARFs in the general context of network dynamical systems to reveal their full interaction topology under sufficiently weak, otherwise uncontrolled external perturbations. In particular, we demonstrated that accelerated frames may transform the dynamics of networked systems in to transient relaxation dynamics towards fixed points, which can readily be used for network inference. We illustrated this idea on networks exhibiting phase-locking and synchronization and showed that our theory is robust to non-trivial dynamical features such as periodic orbits with position-dependent velocities and collective chaos. For the specific ARF defined through network-wide state averages, the scheme exhibits optimal performance in the limit of large sparse networks, i.e. $n_i^-/N \rightarrow 0$.

Whereas exactly synchronous or phase-locked dynamics in principle can generally not reveal the complete network topology, inferring from transient dynamics towards synchrony or locking was so far restricted to driving-response settings with known signals [16] or to general model-free approaches using a large repertoire of functions [11, 12, 14, 15]. While the former strategy allows to create linear mappings from recorded dynamics to network topology, the latter allows to infer links from transient dynamics following an unknown driving or perturbation.



The theory presented in this article combines the advantages of both strategies simultaneously (i) allowing to create linear mappings from dynamics to topology, and (ii) allowing to work with transients generated by unknown drivings. It also refines the settings (ii) in the sense that fewer data points on trajectories are needed and simultaneously less computational efforts. These advantages may make the ARF scheme a promising concept for network inference in its own right.

Given that the theory only requires networks to operate around a steady state in some appropriate reference frame, this technique may well be transferable to other systems if functions $g(\cdot)$ are appropriately designed. For generalized settings such as delayed or generalized synchronization as well as other forms of spatio-temporally ordered dynamics, such transformation functions need to be identified in the future and perhaps be constructed on demand depending on the type of attractor the networked system describes, for instance by means of expansions in basis functions or other techniques of model selection. The proposed theory may thus pave a novel way for network inference applicable to a range of time series data obtained in systems where controlled driving is infeasible, only short transients are available, or individual measurements are costly.

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