Recovering the Graph Underlying Networked Dynamical Systems under Partial Observability: A Deep Learning Approach

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Abstract

We study the problem of graph structure identification, i.e., of recovering the graph of dependencies among time series. We model these time series data as components of the state of linear stochastic networked dynamical systems. We assume partial observability, where the state evolution of only a subset of nodes comprising the network is observed. We propose a new feature-based paradigm: to each pair of nodes, we compute a feature vector from the observed time series. We prove that these features are linearly separable, i.e., there exists a hyperplane that separates the cluster of features associated with connected pairs of nodes from those of disconnected pairs. This renders the features amenable to train a variety of classifiers to perform causal inference. In particular, we use these features to train Convolutional Neural Networks (CNNs). The resulting causal inference mechanism outperforms state-of-the-art counterparts w.r.t. sample-complexity. The trained CNNs generalize well over structurally distinct networks (dense or sparse) and noise-level profiles. Remarkably, they also generalize well to real-world networks while trained over a synthetic network – namely, a particular realization of a random graph.

Introduction

Networked dynamical systems are characterized by a set of interconnected nodes or agents. The state of the nodes evolves over time according to their peer-to-peer interactions constrained by a support network of contacts (Barbier, Barthelemy, and Vespignani 2012; Liggett 2005; Robert 2003; Porter and Gleeson 2016). More concretely, the state of a node \(i\) is only immediately affected by the state of nodes that directly link to \(i\), i.e., nodes that bear a direct causal effect on node \(i\). This causal network is captured by a graph, which is often a latent structure underlying these systems.

Examples of networked dynamical systems include: i) Pandemics – the fraction of infections within each community of individuals is captured by a time series that is strongly influenced by contacts in neighboring communities. Knowledge of the contact network (which determines the main avenues of contagion) is critical for designing effective mitigation measures (Lahmanovich and James 1976; Ganesh, Massoulié, and Towsley 2005; Santos, Moura, and Xavier 2015; Braunstein et al. 2016; Ren et al. 2019). For example, a natural mitigation policy is network dismantling: aiming to quarantine a minimal set of nodes to promote a maximal disconnect of the underlying contagion network (Braunstein et al. 2016; Ren et al. 2019) – thus, hindering virus propagation across communities without disrupting the global function of the networked system; ii) Brain activity – based on temporal signals gathered from cranial probes, an important task is to infer the so-called Functional Connectivity Matrix, which represents the graph of interactions among the active regions of the brain (see, e.g., (Liégeois et al. 2020)). Recent evidence shows that the Functional Connectivity Matrix can be used to diagnose or predict the onset of motor activities or cognitive disorders (Dow et al. 2010; Ranasinghe et al. 2014; Oltar et al. 2021; Stam et al. 2007; Monajemi et al. 2016; van Mierlo et al. 2019; Lehnhert, Bröhl, and Rings 2020); iii) Finance – the dynamics of stock prices can be influenced by interactions between firms, and knowledge of this interaction network can inform government interventions, for instance (Fenn et al. 2009, 2012; Bazzi et al. 2016).

In most practical instances of the examples above, the node-level time series are readily accessible, but the underlying causal network – which is of fundamental importance in downstream tasks – is fully or partially unknown. To address this issue, a growing body of literature has developed methods for reconstructing the network from the observed node-level time series (Chen, Wang, and Shen 2022; Pereira, Ibrahim, and Montanari 2010; Materassi and Salapaka 2015; Matta, Santos, and Sayed 2020). In this work, we focus on linear stochastic networked dynamical systems, which is arguably one of the most natural settings for network identification from time series since a great class of nonlinear networked dynamical systems can be addressed via linearization about the equilibria under small-noise regimes (Ching and Tam 2017; Napoletani and Sauer 2008) or via appropriate embedding in higher dimensional spaces (Lim et al. 2015; Mauroy and Goncalves 2016).
The general goal of causal inference is to uncover the possible avenues of information flow: to recover from observation of the time series samples the underlying graph structure of dependencies defined by the Markov property. Typically, this is done by leveraging various forms of scalar measures between time series, e.g., transformations of the covariance matrix; regression (e.g., Granger estimator) (Geiger et al. 2015; Pereira, Ibrahimi, and Montanari 2010; Matta, Santos, and Sayed 2020); or other scalar graph metrics (Materassi and Salapaka 2015). The performance of the precise methods strongly depends on the data generative process and to whether the system is fully or partially observed.

Full-Observability

**Graphical models.** Classical algorithms (assuming i.i.d. samples) based on conditional independence tests, include the SGS (Spirtes, Glymour, and Scheines 2000), PC (Spirtes and Glymour 1991), GES (Chickering 2003), and FGS (Ramsey et al. 2016). The algorithms and sufficient conditions for consistency devised in these works rely on sparsity related structural constraints that hardly fit the connectivity pattern of general networks. The work (Anandkumar et al. 2012) offers an approach for the large scale setting under certain complying assumptions of sparsity. The independence tests are leveraged via conditional covariance tests. All structural constraints, revolving around sparsity, play a critical role to render the scaling of the independence tests amenable to computation, otherwise, the problem becomes quickly unfeasible (Bresler, Gamarnik, and Shah 2014; Bogdanov, Mossel, and Vadhan 2008).

**Networked dynamical systems.** For approaches in the signal processing literature, (Mateos et al. 2019) provides an overview highlighting regression plus regularization of the network sparsity methods for full-observability over distinct models – primarily promoting sparsity of the latent network, – including linear dynamical systems as vector autoregressive (VAR) models, as in (Mei and Moura 2017; Moneta et al. 2009; Kivits and Hof 2022). In this regard, (Pereira, Ibrahimi, and Montanari 2010) addresses the problem for linear stochastic differential equations (SDEs) via an optimization formulation that regularizes sparsity of the latent network. This problem is addressed by first converting the continuous-time SDE into a discrete-time linear dynamical system – a technique that yields the discrete-time model considered in this work. Other schemes exploit spectral-based methods (Granger 1969; Segarra, Scauba, and Jadbabaie 2017; Segarra et al. 2017). These leverage the spectral properties of the interaction matrix or support graph (Sandryhaila and Moura 2013) to characterize signatures that allow consistent estimation over certain sparse networks.

Partial-Observability

**Graphical models.** In general, the proposed approaches rely on conditional independence (CI) tests or measures thereof, e.g., conditional mutual information (CMI) or transfer entropy, and a causal link is declared whenever a test yields a positive CMI-based metric. Classical algorithms for causal inference under the presence of latent variables are the FCI (Spirtes, Meek, and Richardson 1995) and

\[
y(n+1) = Ay(n) + x(n+1)
\]
Problem Formulation

We consider the linear networked dynamical law

$$y(n + 1) = Ay(n) + x(n + 1),$$

where $y(n) = [y_1(n), y_2(n), \ldots, y_N(n)]^T \in \mathbb{R}^N$ represents the state-vector of the $N$-dimensional networked dynamical system at time $n$ that collects the states $y_i(n)$ of each node $i$ at time $n$; $x(n) \sim \mathcal{N}(0, \sigma^2 I_N)$ represents the excitation noise associated with the $N$ nodes of the system with covariance matrix $\sigma^2 I_N$, and independent across time $n$; $A \in \mathbb{R}^{N \times N}$ refers to the non-negative interaction matrix whose support represents the underlying graph linking the nodes. The dynamical system is assumed to be stable, i.e., $\rho(A) < 1$, where $\rho(A)$ stands for the spectral radius of $A$.

This work deals with the problem of recovering the support of the submatrix $A_S$, i.e., the graph structure of connections among the observed nodes in the subset $S$ from observation of the subvector $[y(n)]_S = [y_{m_1}(n), y_{m_2}(n), \ldots, y_{m_{|S|}}(n)]^T \in \mathbb{R}^{|S|}$ over time $n$, where $|S|$ is the cardinality of the subset $S$ (see Fig. 1).

**Structural Consistency**

Consider the following $k^{th}$ lag covariance matrix

$$R_k(n) \triangleq \mathbb{E}[y(n+k)y(n)^T]$$

associated with the process $(y(n))_{n \in \mathbb{N}}$. In addition, define the empirical counterpart of $R_k(n)$

$$\hat{R}_k(n) \triangleq \frac{1}{n} \sum_{\ell=0}^{n-1} y(\ell+k)y(\ell)^T.$$ (3)

We refer to a matrix-valued estimator as any map whose input is given by the (observed) time series and the output is given by a matrix, namely,

$$F(n) : \mathbb{R}^{|S| \times n} \rightarrow \mathbb{R}^{|S| \times |S|},$$

where $F(n)_{ij} = F(x_{ij}(n))$, for any given $n \in \mathbb{N}$. The idea is that the $ij^{th}$ entry of the output matrix $F(n)$ estimates the strength of the link from $i$ to $j$ from $n$ samples of the observed time series. For instance, the empirical covariance matrix $\hat{R}_k(n)$, under full-observability, or $[\hat{R}_k(n)]_{S}^{S}$, in the case of partial-observability, are examples of matrix-valued estimators.

**Definition 1** (structural consistency of a matrix). A matrix-valued estimator $F(n)$ is structurally consistent with high probability, whenever there exists a threshold $\tau$ so that

$$\mathbb{P}\left(F(n)_{ij} > \tau \right) \rightarrow 1 \implies i \leftrightarrow j,$$

i.e., $i$ links to $j$ if and only if the $ij^{th}$ entry of the estimator matrix $F(n)$ lies above the threshold $\tau$, provided that there is a large enough number of samples $n$. 

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As an example, the estimator $T^{(n)}$ whose $ij$th entry of the tensor output $\mathcal{T}^{(n)}$ is defined as

$$T^{(n)}_{ij} \triangleq \left( \left[ \hat{R}_{D}(n) \right]_{ij}, \left[ \hat{R}_{D+1}(n) \right]_{ij}, \ldots, \left[ \hat{R}_{L}(n) \right]_{ij} \right)$$

corresponds to an order-3 tensor-valued estimator. As we will show in the next section, if $D \leq 1$ and $L \geq 3$, then this estimator is linearly structurally consistent w.h.p.

**Features Separability & Explainability**

This section provides the explainability results underlying the ML approach for graph learning considered in this work.

**Assumption 1.** Let $\mathcal{E}^{(n)} := \{E_1^{(n)}, E_2^{(n)}, \ldots, E_M^{(n)}\}$ be a family of matrix-valued estimators such that for some $w := (w_1, w_2, \ldots, w_M) \in \mathbb{R}^M \setminus \{0\}$, the linear combination $E^{(n)}(w) = \sum_{i=1}^{M} w_i E^{(n)}_i$ is a structurally consistent w.h.p. matrix-valued estimator for the dynamics (1).

**Lemma 1.** For each pair $ij$, with $i \neq j$, define the associated feature vector as,

$$T_{ij}^{(n)} := \left( \left[ E_1^{(n)} \right]_{ij}, \left[ E_2^{(n)} \right]_{ij}, \ldots, \left[ E_M^{(n)} \right]_{ij} \right) \in \mathbb{R}^M.$$  

Then, under Assumption 1, the tensor-valued estimator $T^{(n)}$ is linearly structurally consistent w.h.p., or equivalently, the set of features $\{ T_{ij}^{(n)} \}_{i \neq j} \subset \mathbb{R}^M$ is consistently linearly separable w.h.p.

**Proof.** Since $E^{(n)}(w) = \sum_{i=1}^{M} w_i E^{(n)}_i$ is structurally consistent w.h.p. for some $w \in \mathbb{R}^M$, then there exists a threshold $\tau_w$ so that $[E^{(n)}(w)]_{ij} > \tau_w$ across connected pairs $ij$ and $[E^{(n)}(w)]_{ij} < \tau_w$ otherwise. Therefore, the affine map $\mathcal{L}_w(x) = x \cdot w - \tau_w$ consistently separates the set of features $\{ T_{ij}^{(n)} \}_{i \neq j}$ w.h.p. Indeed,

$$\mathcal{L}_w(T_{ij}^{(n)}) = T_{ij}^{(n)} \cdot w - \tau_w = [E^{(n)}(w)]_{ij} - \tau_w > 0 \quad (9)$$

for a connected pair $ij$ or

$$\mathcal{L}_w(T_{ij}^{(n)}) = [E^{(n)}(w)]_{ij} - \tau_w < 0, \quad (10)$$

otherwise. In other words, the hyperplane characterized by the linear map $\mathcal{L}_w : \mathbb{R}^M \rightarrow \mathbb{R}$ separates consistently the pairs $ij$ for all $i \neq j$, w.h.p.

**Theorem 1.** For each pair $ij$, with $i \neq j$, define the associated feature vector as,

$$T_{ij}^{(n)} := \left( \left[ \hat{R}_{D}(n) \right]_{ij}, \left[ \hat{R}_{D+1}(n) \right]_{ij}, \ldots, \left[ \hat{R}_{L}(n) \right]_{ij} \right),$$

with $D \leq 1$ and $L \geq 3$, and assume that the interaction matrix $A$ underlying the dynamics (1) is symmetric and the covariance matrix of the noise process $(x(n))_{n \in \mathbb{N}}$ is given by $\Sigma_x := \sigma^2 I_N$, for some $\sigma > 0$. Then, the set

$$\{ T_{ij}^{(n)} \}_{i \neq j} \subset \mathbb{R}^M$$

is consistently linearly separable w.h.p.
Number Structural Graph
Connectivity
samples
Directed
Network
Graph
Biochemical
Graph
Number
Graph
17
Accuracy
(a)
54
-236
-18
-91
200
279
279
367
391
Proof. Define the vector \( \mathbf{w} \in \{-1, 0, 1\}^M \)
so that \( E^{(n)}(\mathbf{w}) = \hat{R}_1(n) - \hat{R}_3(n) \), which is possible
since \( D \leq 1 \) and \( L \geq 3 \). According to Theorem 1 in (Chen,
Wang, and Shen 2022), \( E^{(n)}(\mathbf{w}) = \hat{R}_1(n) - \hat{R}_3(n) \) is
structurally consistent w.h.p. and the result now follows
from the previous Lemma 1.

Remark 2 (Locality of the structural estimation). Note
that, to compute the feature \( \tau_{ij}^{(n)} \) associated with each
pair \( ij \) defined in Theorem 1, we need only the time series
\( \{y_1(\ell), y_j(\ell)\}^{1}_{\ell=0} \) associated with the pair \( ij \) as
\[
\tau_{ij}^{(n)} := \frac{1}{n} \sum_{\ell=0}^{n-1} (y_i(\ell + D)y_j(\ell), \ldots, y_i(\ell + M)y_j(\ell)),
\]
which only involves information related to nodes \( i \) and \( j \).
As such, it is possible to reconstruct the connectivity pattern
in a pairwise manner. This is a special property that results
from the fact that each lag-moment, or covariance matrix,
in the feature vector can be locally estimated. Observe that
the majority of the matrix-valued estimators does not exhibit
this locality property. For example, to reconstruct the \( ij^{th} \)
entry of the Precision matrix \( \left( \hat{R}_0(n) \right)^{-1} \), one needs to know
the whole matrix \( \hat{R}_0(n) \) (or a large portion around the pair
\( ij \) thereof). This has the drawback of implying the observation
of a large set of nodes (or of the whole network) just to
estimate the corresponding entry \( ij \) of the Precision matrix.

Now, given a matrix-valued estimator \( F^{(n)} \), define its
identifiability gap as (Matta, Santos, and Sayed 2022)
\[
\Gamma \left( F^{(n)} \right) \triangleq \min_{ij : A_{ij} \neq 0} F^{(n)}_{ij} - \max_{ij : A_{ij}=0} F^{(n)}_{ij} \quad (11)
\]
i.e., the gap between the smallest entry of \( F^{(n)}_{ij} \) across con-
ected pairs and the largest entry of \( F^{(n)}_{ij} \) over disconnected
pairs. An estimator \( F^{(n)} \) is structurally consistent w.h.p.
if and only if \( \Gamma (F^{(n)}) > 0 \) w.h.p., or in other words, if
and only if connected pairs are separated from disconnected
pairs, in view of the entries of the matrix \( F^{(n)} \) for \( n \) large
enough. This statistical metric is a relevant parameter re-
garding the hardness of the classification. The larger the
identifiability gap, the easier the classification via thresh-
olding of the entries of the matrix \( F^{(n)} \) tends to be.

Similarly, define the identifiability gap \( \Gamma (T^{(n)}) \) associ-
ated with a tensor-valued estimator \( T^{(n)} \) as the maximum
distance among all parallel hyperplanes that consistently separate the features, as in Fig. 2. For example, the SVM al-
gorithm is designed to find these margins. More concretely,
\[
\Gamma \left( T^{(n)} \right) \triangleq \max_{(\mathbf{w}, \tau) \in \mathcal{H}} \frac{|\tau_1 - \tau_2|}{||\mathbf{w}||}, \quad (12)
\]
where \( \mathcal{H} \) indexes the set of linear maps that consistently sep-
are the features: \( (\mathbf{w}, \tau) \in \mathcal{H} \) if and only if the linear map
\( \mathcal{L}_{(\mathbf{w}, \tau)}(\mathbf{x}) := \mathbf{w} \cdot \mathbf{x} - \tau \) consistently separates the features.
Lemma 2. Let $T^{(n)}$ be a tensor-valued estimator whose underlying features at each pair $ij$ are defined as

$$T^{(n)}_{ij} := \left( \left[ E_1^{(n)} \right]_{ij}, \left[ E_2^{(n)} \right]_{ij}, \ldots, \left[ E_M^{(n)} \right]_{ij} \right) \in \mathbb{R}^M,$$

with identifiability gap $\Gamma^{(n)}_E = \Gamma(T^{(n)})$. Let $\tilde{A}^{(n)}$ be a matrix-valued estimator with identifiability gap $\Gamma^{(n)}_A = \Gamma\left( \tilde{A}^{(n)} \right)$. If both $\tilde{A}^{(n)}$ and $T^{(n)}$ are (linearly) structurally consistent w.h.p., then the tensor-valued estimator $\tilde{T}^{(n)}$ defined via the augmented features

$$\tilde{T}^{(n)}_{ij} := \left( \left[ \tilde{A}^{(n)} \right]_{ij}, \left[ E_1^{(n)} \right]_{ij}, \ldots, \left[ E_M^{(n)} \right]_{ij} \right) \in \mathbb{R}^M,$$

exhibits an identifiability gap obeying $\Gamma\left( \tilde{T}^{(n)} \right) \geq ||\Gamma^{(n)}||_2$ w.h.p., with $\Gamma^{(n)} = \begin{pmatrix} \Gamma^{(n)}_A & \Gamma^{(n)}_E \end{pmatrix}$. Lemma 2 asserts that, if further matrix-valued structurally consistent estimators are incorporated into the feature vector, the identifiability gap increases.

Proof. Let $Cv(S)$ denote the convex hull of a set $S \subset \mathbb{R}^M$, i.e., the smallest convex set containing $S$ (Hirata-Urruty and Lemaréchal 2001). Define $\tilde{C} = \left\{ \tilde{T}^{(n)}_{ij} \right\}_{ij : A_{ij} \neq 0}$ as the set of augmented features associated with connected pairs and $\tilde{D} = \left\{ \tilde{T}^{(n)}_{ij} \right\}_{ij : A_{ij} = 0}$ associated with disconnected pairs. Similarly, define $\tilde{C} = \left\{ T^{(n)}_{ij} \right\}_{ij : A_{ij} \neq 0}$ and $\tilde{D} = \left\{ T^{(n)}_{ij} \right\}_{ij : A_{ij} = 0}$. Let $R$ be the smallest entry of $\tilde{A}^{(n)}$ across connected pairs and $r$ be the greatest entry of $\tilde{A}^{(n)}$ across disconnected pairs and note that $r < R$ w.h.p. since $\tilde{A}^{(n)}$ is structurally consistent w.h.p. We have that

$$\Gamma\left( T^{(n)} \right) \geq \begin{pmatrix} d & 0 \\ A & 0 \end{pmatrix} \begin{pmatrix} d(Cv(\tilde{C}) \times [R, \infty)) & d(Cv(\tilde{D}) \times (\infty, r]) \\ d(Cv(C) \times [R, \infty)) & d(Cv(D) \times (\infty, r]) \end{pmatrix} \begin{pmatrix} d & 0 \\ A & 0 \end{pmatrix} \begin{pmatrix} \Gamma^{(n)}_E \\ \Gamma^{(n)}_A \end{pmatrix}^2 = \left( \begin{pmatrix} \Gamma^{(n)}_E \\ \Gamma^{(n)}_A \end{pmatrix} \right)^2 = ||\Gamma^{(n)}||_2^2$$

where for two subsets $\mathcal{X}, \mathcal{Y} \subset \mathbb{R}^M$, $d(\mathcal{X}, \mathcal{Y})$ is the distance

$$d(\mathcal{X}, \mathcal{Y}) = \inf_{x \in \mathcal{X}, y \in \mathcal{Y}} ||x - y||_2;$$

the first identity (a) conforms to an alternative dual characterization for the identifiability gap (refer to Theorem 13 in (Dax 2006)); (b) holds in view of the inclusions $\tilde{C} \subset C \times [R, \infty)$ and $\tilde{D} \subset C \times (\infty, r]$; (c) holds since $\tilde{C} \subset C \subset \mathbb{R}^M$ and $D \subset C \subset \mathbb{R}^M$ and the fact that the convex hull commutes with the Cartesian product over convex sets (Hirata-Urruty and Lemaréchal 2001); the identity (d) is straightforward from the definition of the distance $d(\cdot, \cdot)$. ❑

Methodology

In order to stratify the pairs of nodes into connected or disconnected from the observed time series, we address the linear separability property of the covariance-based features $\left\{ \Gamma^{(n)}_{ij} \right\}_{ij}$ established in Theorem 1, by studying the performance of trained classifiers, in particular, linear Support Vector Machines (SVMs) and Convolutional Neural Networks (CNNs). The training set is given by

$$\mathcal{T}^{(n)} = \left\{ \left( \tilde{T}^{(n)}_{ij}, 1_{\{A_{ij} \neq 0\}} \right) \right\}_{i \neq j}$$

where we have introduced the normalized feature vectors

$$\tilde{T}^{(n)}_{ij} = \frac{\tilde{T}^{(n)}_{ij}}{\max_{i \neq j} ||\tilde{T}^{(n)}_{ij}||_\infty},$$

with the unnormalized features given by,

$$\tilde{T}^{(n)}_{ij} = \begin{pmatrix} \tilde{R}^{(n)}_{-100}(ij) \\ \tilde{R}^{(n)}_{-99}(ij) \\ \ldots \\ \tilde{R}^{(n)}_{100}(ij) \end{pmatrix}.$$}

In other words, for training, we provide a normalized feature $\tilde{T}^{(n)}_{ij}$ associated with the pair $ij$ as input to a classifier and the output should be the ground truth $1_{\{A_{ij} \neq 0\}}$. The normalization in the training set is motivated by the following observation. With infinitely many samples,

$$\tilde{T}^{(n)^\pi} = \sigma^2 \begin{pmatrix} [\tilde{R}_D]_{ij} & [\tilde{R}_{D+1}]_{ij} & \ldots & [\tilde{R}_{M}]_{ij} \end{pmatrix}$$

where $\tilde{R}_k$ is the $k$-lag covariance matrix (equation (2)) of the normalized process $(y(t)/\sigma)_{t \in \mathbb{N}}$, i.e., the process whose noise is normalized to unit variance. With the proposed normalization in equation (17), the multiplicative factor $\sigma^2$ is cancelled out, which decreases the role played by the noise-level in the performance of the trained CNNs. Furthermore, this normalization renders the generalization performance of the trained CNNs robust across structurally distinct graphs.

To generate the matrix $A$ to obtain the full sequence data $(y(t))_{t \geq 0}$, given a graph $G$, the following procedure was considered. Let $G$ be a given graph without self-loops, i.e., $G_{ii} = 0$ for all $i$. Define the interaction matrix $A$ as

$$A_{ij} = \begin{cases} 1 & \text{if } i \neq j \\ 0 & \text{if } i = j \end{cases}$$

where $A$ is the number of nodes. Throughout, we assume that we can only observe the time series data from $|S| = 20$ nodes, that is, we assume $S = \{1, 2, \ldots, 20\}$. 9043
Simulation Results

In the numerical results considered, we define accuracy as the number of directed pairs correctly classified over the total number of directed pairs in the underlying graph. We consider 1000 Monte Carlo runs across all plots.

Fig. 3 (a) – (f) depict the sample-complexity performance of the estimators across structurally distinct networks, considering: i) Granger under partial observability $\left[\tilde{R}_1(n)\right]_S \left[\tilde{R}_0(n)\right]_S^{-1}$ that is provably structurally consistent (Santos, Matta, and Sayed 2020; Matta, Santos, and Sayed 2020) for distinct regimes of network connectivity; ii) The one-lag estimator $\tilde{R}_1(n)$, which is also consistent for several network connectivity regimes (Matta, Santos, and Sayed 2022); iii) the $\tilde{R}_1(n) - \tilde{R}_3(n)$ that is structurally consistent (Chen, Wang, and Shen 2022); iv) the linear SVM; and v) the trained CNNs. For classification, we apply Gaussian mixture over the sorted entries of the matrix-valued estimators in order to stratify the connected and disconnected pairs. Our results show the overall superiority in performance for the CNN-based classifier. Figs. 3 (a) – (b) refer to real-world networks obtained from the database (Rossi and Ahmed 2015), with (a) for a Brain structural connectivity matrix of a monkey and (b) for an enzyme biochemical network; (c) – (d) refer to symmetric regimes where the underlying support graph of the networked dynamical system is undirected; and (e) – (f) refer to directed graph regimes. $N$ and $p$ stand for the number of nodes and probability of edge/arrow drawing in the random graph models. It should be remarked that while the CNN is trained over a synthetic network, namely, a particular realization of an Erdős–Rényi (for undirected networks) random graph model with $p = 0.5$ and $N = 100$, it generalizes well over real-world networks as demonstrated in Figs. 3 (a) – (b).

Fig. 4a illustrates the robustness of both the trained CNNs and the linear SVMs against distinct noise-level regimes. The CNNs and SVMs are trained with a noise variance of $\sigma^2 = 0.5$, but generalize well over an extended range of noise variance. Fig. 4a shows that the performance of these classifiers is not sensitive to the variance of the input noise in the dynamics (1). Fig. 4b shows the gain in performance when the Granger estimator is included in the feature vector. In particular, when we include in the feature vector

$$T_{ij}^{(n)} \triangleq \left[\tilde{A}_S\right]_{ij}, \left[\tilde{R}_{-100}(n)\right]_{ij}, \ldots, \left[\tilde{R}_{100}(n)\right]_{ij}$$

the additional component $\tilde{A}_S \triangleq \left[\tilde{R}_1(n)\right]_S \left[\tilde{R}_0(n)\right]_S^{-1}$ that is the Granger under partial observability, with only $|S| = 20$ nodes observed. This is consistent with Lemma 2, motivating the search for feature vectors built on other matrix-valued structurally consistent estimators. It motivates the following causal inference paradigm: i) characterize matrix-valued structurally consistent estimators; ii) define feature vectors that collect these consistent estimators; iii) use these new features to train classifiers like a CNN.

Concluding Remarks

This paper considered the problem of determining the graph that captures the fundamental dependencies among time series of data. These time series are indexed as nodes in linear stochastic networked dynamical systems. Only the time series of some nodes are observed (partial observability). We proposed a novel feature-based paradigm and proved that the features were consistently linearly separable. With this separability property, our features can be used as an input to a variety of machine learning pipelines in order to design new state-of-the-art algorithms for causal inference of linear networked dynamical systems. In particular, CNNs trained over this set of features exhibited remarkable sample-complexity performance, significantly reducing the number of samples required to reach a certain level of accuracy, as compared with other state-of-the-art estimators, which require a much larger number of samples. Simulation results show the superiority of the CNN-based approach. It was further shown that the inclusion of structurally consistent matrix-valued estimators in the feature vectors increases the performance of structure identification. This motivates further study of new structurally consistent matrix-valued estimators as building blocks for feature vectors or tensor-valued estimators.
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