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Assessing Dependences within Multivariate Time Series Partializing the Knowledge of Thirds

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Abstract—A method to estimate from multivariate measurements the dependences within a network of coupled dynamical systems is proposed. The method is non-parametric and resorts to a statistics of the eigen-spectrums of the time series partial correlation matrices. The method is successfully validated on numerically generated data, demonstrating its capability to distinguish between direct and indirect dependences.

1. Introduction

In modern experimental setups, with the growing availability of multiple parallel measurements, multivariate time series analysis has been raising as a key topic. In particular, inferring from measured data the functional interactions (dependences) between coupled dynamical systems has become a crucial step to unravel the principles governing the observable collective behaviors of concrete networks [1]. For instance, in population biology the interest is focused on interactions between different populations in a given territory [2], while in neuroscience a key question is how single neurons process a certain stimulus within functionally coherent neuronal assemblies [3].

Traditionally, this step consists in estimating the strength of dependences between measured signals (time series) with estimators such as linear cross-correlation, mutual information, measures of mutual predictability and phase dynamics [4, 5]. Unfortunately, these estimators are usually not viable in a multivariate context, either because of their computational complexity or because their inability to marginalize third knowledge. Indeed, when dealing with multivariate data, the computational costs might explode and direct and indirect dependences must be discerned [6].

An effective dependences estimator for multivariate stochastic processes is already available [6], while for deterministic processes contributions have started to appear only very recently (*e.g.* [7]).

Here, we present an approach to estimate the strength of dependences between multivariate time series that, theoretically, can be applied to both deterministic and stochastic processes. The method is non-parametric and represents an extension of a recently proposed multivariate dependences estimator [8].

The method is described in Sec. 2; in Sec. 3 its ability to correctly estimate dependences within networks of three dynamical systems is assessed on numerically generated data; finally, conclusions are given in Sec. 4.

2. Method

We first briefly recall the recently introduced dependence estimator, called S [8], then we explain how to correctly apply it on measurements from deterministic dynamical systems, and, finally, we will extend it to estimate dependences between two time series conditionally upon third ones.

2.1. S estimator

This estimator has been recently introduced to quantify the cooperativeness within a network of dynamical systems out of measured time series [8].

Given M time series, one from each dynamical system under study, we denote them by $\mathbf{Y} = \{\mathbf{y}_i\}$, $i = 1, \ldots, L$, where $\mathbf{y}_i \in \mathbb{R}^M$ is the $i-th$ sample observation vector and L is the number of available samples. Without loss of generality, we can consider $\mathbf{Y}$ as de-trended to zero mean and normalized to unitary variance.

Let us consider the $M \times M$ estimated correlation matrix of the time-series

$$\mathbf{C} = \frac{1}{L-1} \sum_{i=1}^{L} \mathbf{y}_i^T \mathbf{y}_i \,, \quad (1)$$

with elements $c_{ii} = 1$ and $c_{ij} = \rho_{ij}$, $i \neq j$, *i.e.* the correlation between the i-th and j-th time series. Called $\lambda'_i = \frac{\lambda_i}{M}$ the normalized eigenvalues of $\mathbf{C}$, the entropy-like quantity

$$H = -\sum_{i=1}^{M} \lambda'_i log\left(\lambda'_i\right) \quad (2)$$

is a measure inversely proportional to the amount of dependences between the M time series.

Indeed, it can be interpreted as a deviation from mutual orthogonality (lack of correlation) between the M signals.

In the case of M uncorrelated signals, $\mathbf{C} = \mathbf{I}$, the normalized eigenvalues are all equals $\lambda'_i = \frac{1}{M}$, and H is equal to $logM$. In the case of perfectly correlated signals, $\mathbf{C}$ has one unitary normalized eigenvalue and all the others zero, and H is equal to 0. To have a measure proportional to the amount of dependences, we can simply rearrange Eq. (2) as $S = 1 - \frac{H}{logM}$, which is 0 for uncorrelated signals, 1 for completely correlated ones, is monotonically increasing with respect to all correlation terms (*cf.* [8]), *i.e.* the off-diagonal elements of $\mathbf{C}$, and has been shown to scale with coupling strength when considering coupled deterministic non linear dynamical systems [8].

By reconstructing from the measured scalar time series, through embedding, the trajectory of the dynamical phenomena under observation, this estimator can explicitly account for the hypothesis of deterministic dynamical systems behind the measurements. However, in this case a normalizing step is necessary.

Given, for the sake of simplicity, two time series ($M = 2$), for which delay times ($\tau^{(1)}$ and $\tau^{(2)}$) and embedding dimensions ($m^{(1)}$ and $m^{(2)}$) have been estimated [5], we can consider the embedded multivariate trajectory $\mathbf{X} = \{\mathbf{x}_i\}$, where $\mathbf{x}_i \in \mathbb{R}^{\left(m^{(1)}+m^{(2)}\right)}$ and

$$\mathbf{x}_i = \left[\underbrace{y_i^{(1)}, \cdots, y_{i-\left(m^{(1)}-1\right)\tau^{(1)}}^{(1)}}_{\mathbf{x}_i^{(1)}}, \underbrace{y_i^{(2)}, \cdots, y_{i-\left(m^{(2)}-1\right)\tau^{(2)}}^{(2)}}_{\mathbf{x}_i^{(2)}}\right].$$

The corresponding estimated correlation matrix can be block partitioned to highlight the contribution of the two systems, *i.e.*

$$\mathbf{C} = \begin{bmatrix} \mathbf{C}^{(1,1)} & \mathbf{C}^{(1,2)} \\ \mathbf{C}^{(1,2)^T} & \mathbf{C}^{(2,2)} \end{bmatrix}, \tag{3}$$

where the $m^{(i)} \times m^{(i)}$ matrices $\mathbf{C}^{(i,i)}$, $i = 1, 2$, collect the *intra-system* correlation terms, *i.e.* the correlation between state-variables of the same system, while the $m^{(1)} \times m^{(2)}$ matrix $\mathbf{C}^{(1,2)}$ collects the *inter-system* correlation terms, which are the dependences in our interest.

To correctly estimate the *inter-dependence* between the two systems, independently of the *intra-dependences*, we proceed through a suitable linear transformation of the reconstructed state space $\mathbf{X}$ which reduces the $\mathbf{C}^{(i,i)}$ to identity matrices; in other words, we intra-orthogonalize the state variables of the two systems. As result of the transformation, the estimated correlation matrix for the transformed trajectory will have nonzero off-diagonal elements only within the *inter-dependence* block $\mathbf{C}^{(1,2)}$.

The transformation is given by

$$\mathbf{Z} = \left[\mathbf{Z}^{(1)}\ \mathbf{Z}^{(2)}\right] = \left[\mathbf{X}^{(1)}\ \mathbf{X}^{(2)}\right] \begin{bmatrix} \mathbf{T}^{(1)} & \mathbf{0} \\ \mathbf{0} & \mathbf{T}^{(2)} \end{bmatrix} = \mathbf{XT},$$

with $\mathbf{T}^{(1)} = \mathbf{C}^{(1,1)^{-\frac{1}{2}}}$ and $\mathbf{T}^{(2)} = \mathbf{C}^{(2,2)^{-\frac{1}{2}}}$, *i.e.* the principal square root matrices of $\mathbf{C}^{(1,1)^{-1}}$ and $\mathbf{C}^{(2,2)^{-1}}$ respectively, where the inverses are guaranteed to exist if an appropriate embedding is performed. Clearly, the estimated correlation matrix for the $\mathbf{Z}$ trajectory turns out to be

$$\mathbf{R} = \begin{bmatrix} \mathbf{I} & \mathbf{T}^{(1)^T}\mathbf{C}^{(1,2)}\mathbf{T}^{(2)} \\ \mathbf{T}^{(2)^T}\mathbf{C}^{(2,1)}\mathbf{T}^{(1)} & \mathbf{I} \end{bmatrix} = \begin{bmatrix} \mathbf{I} & \mathbf{R}^{(1,2)} \\ \mathbf{R}^{(1,2)^T} & \mathbf{I} \end{bmatrix}, \tag{4}$$

which can then be used, through Eq. (2), to correctly quantify the dependence between the two systems. If the two systems are uncorrelated, $\mathbf{R}^{(1,2)} = \mathbf{0}$, $\mathbf{R}$ will be diagonal, and $H = log\left(m^{(1)} + m^{(2)}\right)$, while if the two systems are "identical", it can be verified that $\mathbf{R}^{(1,2)}$ will have ones on the main diagonal and zeros elsewhere. Under this case the entropy of the normalized eigenvalues will depend on the embedding dimensions ($m^{(1)}$ and $m^{(2)}$). We do not have a closed form formula to compute it; though, it can be easily computed numerically and we denote with H_{min} its value. Knowing the extremes, we can finally rearrange Eq. (2) as

$$S = \frac{log\left(m^{(1)} + m^{(2)}\right) - H}{log\left(m^{(1)} + m^{(2)}\right) - H_{min}}, \tag{5}$$

getting a measure proportional to the amount of dependences and ranging from 0 to 1. Clearly, this procedure can be trivially extended to estimate the whole cooperativeness within M interacting dynamical systems.

2.2. Partial S estimator

In the previous section we have derived an estimate for the cooperativeness strength between coupled deterministic dynamical systems. However, this derivation is still not satisfactory because cooperativeness between systems may be merely incidental to the fact that all systems may be commonly correlated to another system. This difficulty can be overcome by considering the partial correlation matrix instead of the correlation one. Indeed, partial correlations are a well established statistical tool to examine correlations between signals conditionally upon thirds signals [9].

To illustrate the procedure, let us consider three deterministic systems, assuming that we want to estimate the dependence between the first two marginalizing the knowledge of the third one.

After a suitable embedding, the $M \times M$ (where $M = \sum_{j=1}^{3} m^{(j)}$) correlation matrix $\mathbf{C}$ of the embedded trajectory is estimated. $\mathbf{C}$ can be tri-partitioned similarly as Eq. (3) and, accounting for the partitioning, the $\left(m^{(1)} + m^{(2)}\right) \times \left(m^{(1)} + m^{(2)}\right)$ partial correlation matrix between the first two systems given the third one is written as [9]

$$\mathbf{P} = \begin{bmatrix} \mathbf{P}^{(1,1)} & \mathbf{P}^{(1,2)} \\ \mathbf{P}^{(1,2)^T} & \mathbf{P}^{(2,2)} \end{bmatrix} =$$
$$= \begin{bmatrix} \mathbf{C}^{(1,1)} & \mathbf{C}^{(1,2)} \\ \mathbf{C}^{(1,2)^T} & \mathbf{C}^{(2,2)} \end{bmatrix} - \begin{bmatrix} \mathbf{C}^{(1,3)} \\ \mathbf{C}^{(2,3)} \end{bmatrix} \mathbf{C}^{(3,3)^{-1}} \begin{bmatrix} \mathbf{C}^{(1,3)^T} & \mathbf{C}^{(3,2)} \end{bmatrix}.$$

From this point, we can proceed as in the previous section. Firstly, through a linear transformation of the state

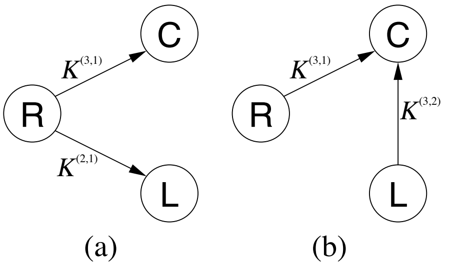

Figure 1: Networks of coupled Rössler (R), Lorenz (L) and Colpitt's (C) dynamical systems considered for the validation of the method. Cases of triangular dependences: (a) – common source; (b) – common child.

space[1], $\mathbf{P}$ is conveniently transformed in a form similar to Eq. (4); then, the dependence between the first two systems marginalized upon the third one is quantified through Eq. (5). From here on, we shall denote as pS the estimates of partial dependences. Once again, this procedure can be trivially extended to account of more than three systems.

3. Numerical Validation

The S and pS estimators have been validated on numerically generated data. We considered the two heterogenous networks of Fig. 1, which are composed of three structurally different dynamical systems; namely, a Rössler (R), Lorenz (L) and Colpitts (C) oscillator. These two coupling schemes are exemplary of the difficulties arising when estimating interactions among multivariate data. In scheme (a) a non existent (indirect) connection between L and C may be inferred because of the common source R, also called a confounder. In scheme (b), a non-existent interaction between R and L may be inferred because of their common destination C, or child.

The equations governing the dynamics of the two considered networks are given by

$$\begin{cases} \dot\theta_1^{(1)} = T\left[\theta_2^{(1)} + \theta_3^{(1)} + \eta_1^{(1)}\right], \\ \dot\theta_2^{(1)} = T\left[\theta_1^{(1)} + a\theta_2^{(1)} + \eta_2^{(1)}\right], \\ \dot\theta_3^{(1)} = T\left[b + \theta_3^{(1)}\left(\theta_1^{(1)} - c\right) + \eta_3^{(1)}\right], \\ \dot\theta_1^{(2)} = \sigma\left(\theta_2^{(2)} - \theta_1^{(2)}\right) + \mathcal{K}^{(2,1)}\left(\theta_1^{(1)} - \theta_1^{(2)}\right) + \eta_1^{(2)}, \\ \dot\theta_2^{(2)} = r\theta_1^{(2)} - \theta_2^{(2)} - \theta_1^{(2)}\theta_3^{(2)} + \eta_2^{(2)}, \\ \dot\theta_3^{(2)} = \theta_1^{(2)}\theta_2^{(2)} - \beta\theta_3^{(2)} + \eta_3^{(2)}, \\ \dot\theta_1^{(3)} = T\left[\frac{g}{Q(1-k)}\left(\alpha\left(1 - e^{-\theta_2^{(3)}}\right) + \theta_3^{(3)}\right) + \mathcal{K}^{(3,1)}\left(\theta_2^{(1)} - \theta_2^{(3)}\right) + \mathcal{K}^{(3,2)}\left(\theta_2^{(2)} - \theta_2^{(3)}\right) + \eta_1^{(3)}\right], \\ \dot\theta_2^{(3)} = T\left[\frac{g}{Qk}\left((1-\alpha)\left(1 - e^{-\theta_2^{(3)}}\right) + \theta_3^{(3)}\right) + \eta_2^{(3)}\right], \\ \dot\theta_3^{(3)} = -T\left[\frac{Qk(1-k)}{g}\left(\theta_1^{(3)} + \theta_2^{(3)}\right) + \frac{1}{Q}\theta_3^{(3)} + \eta_3^{(3)}\right], \end{cases} \quad (6)$$

where $\theta_j^{(1)}, \theta_j^{(2)}, \theta_j^{(3)}\; j = 1, 2, 3$ are the state variables of the Rössler, Lorenz and Colpitts oscillators, respectively; $a = 0.4$, $b = 0.4$, $c = 5.7$, $\sigma = 10$, $\beta = 8/3$, $r = 28$, $g = 10^{0.625}$, $Q = 10^{0.15}$, $\alpha = 0.996$, $k = 0.5$ are standard valued parameters; the time scale $T = 6$ adapts the relative speed differences between the three sub-systems; $\eta_j^{(i)}$, $i, j = 1, 2, 3$, are zero mean uncorrelated Gaussian random noises (set to at a strength of 1% of the energy of the right hand side along the uncoupled attractors); and the $\mathcal{K}^{(2,1)}$, $\mathcal{K}^{(3,1)}$, and $\mathcal{K}^{(3,2)}$ are the diffusive coupling strengths corresponding to the situations of Fig. 1, which in the simulations have been varied within the intervals $[0, 15]$ (the former) and $[0, 5]$ (the latter two).

[1]In reality the similarity transformation $\mathbf{P}' = \mathbf{T}^T\mathbf{P}\mathbf{T}$, with $\mathbf{T} = \begin{bmatrix} \mathbf{P}^{(1,1)-\frac{1}{2}} & \mathbf{0} \\ \mathbf{0} & \mathbf{P}^{(2,2)-\frac{1}{2}} \end{bmatrix}$ can be applied directly to the matrix $\mathbf{P}$.

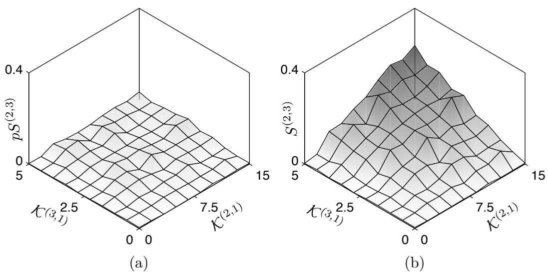

Figure 2: Estimated C – L dependence in the case of common source connection (*cf.* Fig. 1(a)): dependences of (a) – $pS^{(2,3)}$ and (b) – $S^{(2,3)}$ upon the coupling strengths $\mathcal{K}^{(2,1)}$ and $\mathcal{K}^{(3,1)}$.

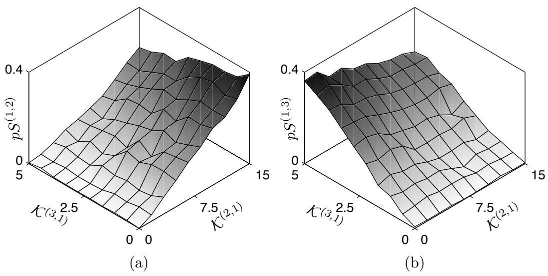

Figure 3: Estimated R – C and R – L dependences in the case of common source connection (*cf.* Fig. 1(a)): dependences of (a) – $pS^{(1,2)}$ and (b) – $pS^{(1,3)}$ upon the coupling strengths $\mathcal{K}^{(2,1)}$ and $\mathcal{K}^{(3,1)}$.

For every considered value of the couplings the network was simulated starting from random initial conditions. The transients were discarded, and time series of length $L = 5000$ were collected by sampling ($\delta T = 0.02$) the coupled variables $\theta_1^{(1)}$, $\theta_1^{(2)}$ and $\theta_1^{(3)}$ corrupted by zero-mean white Gaussian observational noise leading to 40 dB SNR. From these measurements, we reconstructed 4-dimensional state spaces by delay embedding the time series with $\tau^{(i)} = 0.18$, $i = 1, 2, 3$.

The results for the case of common source (Fig. 1 (a)) are shown in Figs. 2 and 3. Figure 2 reports the dependence of $pS^{(2,3)}$ ($= pS^{(3,2)}$) and $S^{(2,3)}$ upon the coupling strengths $\mathcal{K}^{(2,1)}$ and $\mathcal{K}^{(3,1)}$ evaluated at 100 evenly spaced points. Correctly, $pS^{(2,3)}$ stays close to zero and do not scale with neither of the coupling strengths, whilst the $S^{(2,3)}$ does scale, showing that the marginalization upon the mea-

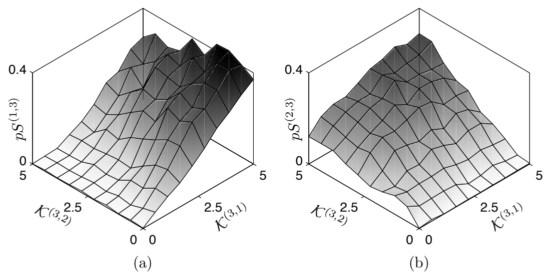

Figure 4: Estimated R – C and L – C dependences in the case of common child connection (*cf.* Fig. 1(b)): dependences of (a) – $pS^{(1,3)}$ and (b) – $pS^{(2,3)}$ upon the coupling strengths $\mathcal{K}^{(3,1)}$ and $\mathcal{K}^{(3,2)}$.

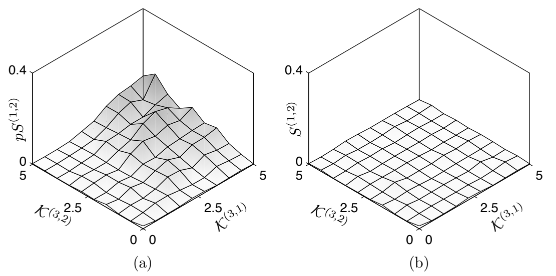

Figure 5: Estimated R – L dependence in the case of common child connection (*cf.* Fig. 1(b)): dependences of (a) – $pS^{(1,2)}$ and (b) – $S^{(1,2)}$ upon the coupling strengths $\mathcal{K}^{(3,1)}$ and $\mathcal{K}^{(3,2)}$.

surements from third system does improve the dependence estimation. Moreover, $pS^{(2,3)}$ is always inferior to $pS^{(1,2)}$ and $pS^{(1,3)}$, which, as shown in Fig. 3, scale correctly with the coupling strengths. Also, we remark that they decrease slowly with the increase of both coupling strengths. This phenomenon can be explained by the fact that the three systems influence each other and, consequently, become more and more similar, jeopardizing the reconstruction.

As a consequence of these results, one could think to consider only partial S for estimating dependences, disposing of S. However, this is not the case because of the so-called "marrying-parents" effect, commonly observable in the case, illustrated in Fig. 1(b), of a common child. For this case, as shown in Fig. 4, $pS^{(1,3)}$ and $pS^{(2,3)}$ scale correctly with the coupling strengths $\mathcal{K}^{(3,1)}$ and $\mathcal{K}^{(3,2)}$. However, as shown in Fig. 5(a), $pS^{(1,2)}$ does scale with the couplings, leading to the incorrect inference of a non-existent dependence between R and L. Though, the voidance of this coupling can be easily tested by means of the $S^{(1,2)}$ estimator which, as shown in Fig. 5(b), correctly stays close to zero.

From these two numerical experiments we can conclude that, by combining both S and pS estimators, we can correctly estimate the dependences within a network of coupled dynamical systems.

4. Conclusions

A new method to infer from measured time series the strength of interactions within a network of coupled dynamical systems has been proposed, and its ability to discriminating direct from indirect dependences has been demonstrated on numerical data.

The method proved eligible for the application on experimental data. However, toward a significant and appropriate experimental application, deeper and extensive simulation studies are needed. This is matter of ongoing research and will be presented in a later work.

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