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Block Partial Directed Coherence: a New Tool for the Structural Analysis of Brain Networks

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Abstract. We present an extension of partial directed co-herence (PDC), a popular frequency domain cau-sality measure valid for scalar time series taken from a multivariate (MV) data set, aimed to formal-ize its application on MV vector time series. A new causality measure, denoted as block PDC (bPDC), is defined through block-partitioning of the coeffi-cient matrices of the parametric model describing the observed MV dataset. Using theoretical MV processes, we show that the bPDC is able to cap-ture directional interactions between time series blocks in a straightforward way compared to the PDC. Then, we demonstrate its applicability to multichannel EEG time series, showing that utiliza-tion of the bPDC simplifies the structural analysis of networks composed by multiple brain regions each characterized by several recording channels.

Keywords: Brain Connectivity; Frequency Domain Causality; Multivariate Autoregressive Models; Physiological Time Series

1. Introduction

The partial directed coherence (PDC) [Baccala and Sameshima, 2001] is a frequency domain tool for the detection of linear causal relations between pairs of time series belonging to a multivariate (MV) data set. The PDC is probably the most widely used tool for inferring the effective connectivity of brain regions from neurophysiological MV time series such as the electroencephalogram (EEG). The popularity of this tool is mainly due to its frequency domain nature, which allows disclosing connectivity mechanisms related to specific neural rhythms (alpha, beta, etc.), and to its ability of eliciting direct causal effects between two series in the MV representation, which allows performing accurate structural analysis of brain networks [Faes et al., 2012].

The PDC is computed from the coefficients of a MV autoregressive (MVAR) model which is fitted on the available MV time series. With this representation, the PDC is defined only between a pair of scalar processes, each modeling a single channel of the observed data. Hence, in order to assess causality between two regions of interest each characterized by more than one recorded channel, the PDC has to be computed individually between all pairs of channels from the two regions and then the multiple estimated PDCs have to be arbitrarily reduced to a single causality measure. Moreover, separate computation of the PDC for each pair of series does not take the internal dynamics within each region of interest into account.

The above limitations can be overcame only when all time series from a given region are modeled as a realization of a vector stochastic process. In this study we introduce a novel frequency domain causality measure, denoted as block PDC (bPDC), which extends the classic PDC analysis to the study of multiple blocks of time series. The new measure is defined through proper block partitioning of the MVAR coefficient matrices, illustrated in comparison with the PDC for a theoretical example of multiple interacting vector processes, and tested in the practical analysis of multichannel EEG recorded during a visuomotor integration task.

2. Methods

Let us consider a network of Q interacting zero-mean scalar stationary stochastic processes, $y_1(n),...,y_Q(n)$, grouped in a way such that an equivalent network of M vector processes $Y_1(n),...,Y_M(n)$, of dimensions $M_1,...,M_M$, is also formed. Assuming that the overall vector process

$Y(n)=[y_1(n)\cdots y_Q(n)]=[Y_1(n)^T\cdots Y_M(n)^T]^T$ of dimension $Q=M_1+...+M_M$ admits an autoregressive (AR) representation, it can be described by means of the multivariate AR (MVAR) model of order p [Lutkepohl, 2005]:

$$Y(n)=\sum_{k=1}^{p}\mathbf{A}(k)Y(n-k)+U(n) \tag{1}$$

where $\mathbf{A}(k)$ is the $Q\times Q$ matrix of the model coefficients and $U(n)$ is a vector composed of Q zero-mean scalar innovation processes with positive definite covariance matrix $\mathbf{\Sigma}=\{\sigma^2_{ij}\}=\mathrm{E}[U(n)U(n)^T]$.

With reference to the scalar process representation of the network, a common frequency-domain measure of causality based on the MVAR model in Eq. 1 is the so-called partial directed coherence (PDC) [Baccala and Sameshima, 2001]. The PDC is computed from the elements of the $Q\times Q$ spectral matrix $\bar{\mathbf{A}}(f)=\{\bar{A}_{ij}(f)\}$ that is obtained transforming the coefficient matrix $\mathbf{A}(k)$ in the frequency domain:

$$\overline{\mathbf{A}}(f)=\mathbf{I}-\sum_{k=1}^{p}\mathbf{A}(k)e^{-\mathbf{j}2\pi f k} \tag{2}$$

where f is the normalized frequency and $\mathbf{j}=\sqrt{-1}$. Specifically, the squared modulus of the PDC from y_j to y_i ($i,j=1,...,Q$), expressed in its generalized formulation, is defined as [Baccala et al., 2007]:

$$\pi_{ij}^2(f)=\frac{\phi_{ii}\left|\overline{A}_{ij}(f)\right|^2}{\bar{\mathbf{a}}_j^*(f)\mathbf{\Phi}\bar{\mathbf{a}}_j(f)}=\frac{\phi_{ii}\left|\overline{A}_{ij}(f)\right|^2}{\sum_{q=1}^{Q}\phi_{qq}\left|\overline{A}_{qj}(f)\right|^2} \tag{3}$$

where $\bar{\mathbf{a}}_j(f)=[\bar{A}_{1j}(f)\cdots\bar{A}_{Qj}(f)]^T$ is the j-th column of $\bar{\mathbf{A}}(f)$ and $\mathbf{\Phi}=\mathrm{diag}\{\phi_{ii}\}$ is a $Q\times Q$ diagonal matrix having the inverse of the i-th innovation variance, $\phi_{ii}=1/\sigma^2_{ii}$, as i-th diagonal element (the superscript * stands for Hermitian transpose). The squared PDC is commonly adopted to infer the structure of the network of the Q scalar processes, as it can be shown that $\pi^2_{ij}(f)>0$ if and only if there is significant direct causality from y_j to y_i at the frequency f [Faes et al., 2012].

An extension of Eq. 3 useful to measure frequency domain causality for the vector process representation of the network may be provided through proper block-partitioning of the time and frequency domain $Q\times Q$ matrices. Specifically, noting that $\bar{\mathbf{A}}(f)$ and $\mathbf{\Phi}$ can be expressed as composed of M^2 blocks, with the (i,j) block having dimensions $M_i\times M_j$, we define the block partial directed coherence (bPDC) from the vector process Y_j to the vector process Y_i ($i,j=1,...,M$) as:

$$\pi_{ij}^{(b)}(f)=1-\frac{\left|\sum_{\substack{m=1\\m\neq i}}^{M}\overline{\mathbf{A}}_{mj}^*(f)\mathbf{\Phi}_{mm}\overline{\mathbf{A}}_{mj}(f)\right|}{\left|\sum_{m=1}^{M}\overline{\mathbf{A}}_{mj}^*(f)\mathbf{\Phi}_{mm}\overline{\mathbf{A}}_{mj}(f)\right|} \tag{4}$$

where $\bar{\mathbf{A}}_{mj}(f)$ is the (m,j) block of $\bar{\mathbf{A}}(f)$ and $\mathbf{\Phi}_{mm}$ is the (m,m) block of $\mathbf{\Phi}$.

The definition of Eq. 4 is motivated by the fact that the resulting bPDC generalizes to the study of vector processes the traditional PDC, while preserving the peculiar features desired for a frequency domain causality measure. Indeed, it can be shown [Faes and Nollo, 2013] that the bPDC is a normalized measure of causality between vector processes, which captures direct causal effects only and reduces to the classic PDC for scalar processes, as formalized by the following properties: $\pi_{ij}^{(b)}(f)$ is well defined at each f if the overall vector process $Y(n)$ can be represented as a finite order stationary MVAR process; $0\leq\pi_{ij}^{(b)}(f)\leq1$; $\pi_{ij}^{(b)}(f)=0$ when $\bar{\mathbf{A}}_{ij}(f)=0$; $\pi_{ij}^{(b)}(f)=1$ when $\bar{\mathbf{A}}_{mj}(f)=0$ for each $m\neq j$; $\pi_{ij}^{(b)}(f)=\pi^2_{ij}(f)$ if Y_i and Y_j are scalar processes ($M_i=M_j=1$).

3. Illustrative Example

The proposed bPDC measure is illustrated, in comparison with the classic PDC, with reference to the network identified by the following equations:

$$\begin{cases} y_1(n) = 1.456y_1(n-1) - 0.81y_1(n-2) + u_1(n) \\ y_2(n) = k_1y_1(n-1) + u_2(n) \\ y_3(n) = a_1y_2(n-1) - 0.81y_3(n-2) + u_3(n) \\ y_4(n) = a_2y_2(n-2) + k_2y_3(n-1) + k_3y_5(n-1) + u_4(n) \\ y_5(n) = c_1y_6(n-1) - c_1y_6(n-2) + u_5(n) \\ y_6(n) = b_1y_3(n-1) + b_2y_4(n-2) + u_6(n) \end{cases} \quad (5)$$

where $u_1(n),...,u_6(n)$ are white and uncorrelated innovation processes, and the observed scalar processes $y_1(n),...,y_6(n)$ are connected with each other as depicted in Fig. 1 (in this study, a_1=0.3, a_2=0.2, b_1=0.5, b_2=-0.4, c_1=0.6, k_1=0.3, k_2=0.2, k_3=-0.2). In this example we assume that the network of Q=6 scalar processes defined in (5) underlies an equivalent network of M=3 vector processes of dimensions M_1=2, M_2=3, M_3=1, such that $Y_1(n)=[y_1(n)\ y_2(n)]^T$, $Y_2(n)=[y_3(n)\ y_4(n)\ y_5(n)]^T$, and $Y_3(n)=y_6(n)$.

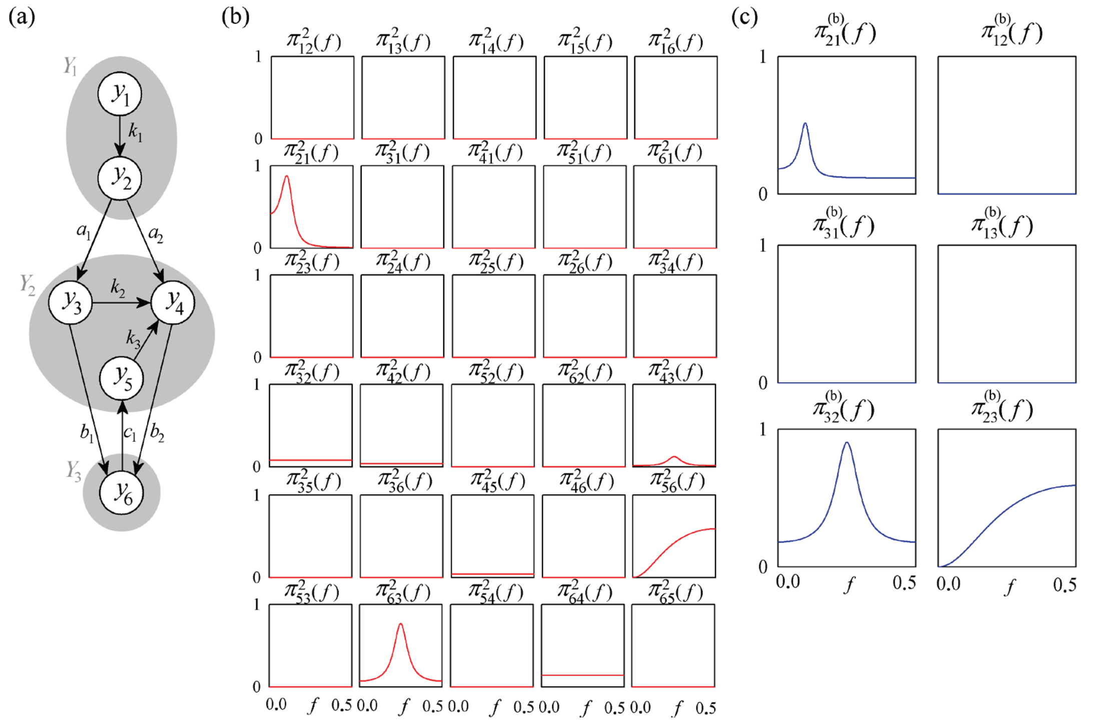

Figure 1. *(a) Graphical representation of the multivariate processes described by (5); (b) theoretical profiles of frequency domain causality estimated for the network of the scalar processes $y_1,...y_6$ through the PDC $\pi^2_{ij}(f)$ (i,j=1,...,6); (c) theoretical profiles of frequency domain causality estimated for the network of the vector processes Y_1, Y_2, Y_3 through the bPDC $\pi^{(b)}_{ij}(f)$ (i,j=1,2,3).*

As shown in Fig. 1a, the direct connections set for the network of the scalar processes are $y_1 \rightarrow y_2$, $y_2 \rightarrow y_3$, $y_2 \rightarrow y_4$, $y_3 \rightarrow y_4$, $y_3 \rightarrow y_6$, $y_4 \rightarrow y_6$, $y_6 \rightarrow y_5$, and $y_5 \rightarrow y_4$. These direct connections are correctly represented in the frequency domain by the nonzero profiles of the squared PDCs π^2_{21}, π^2_{32}, π^2_{42}, π^2_{43}, π^2_{63}, π^2_{64}, π^2_{56}, and π^2_{45} (Fig. 1b), thus confirming the usefulness of the PDC in determining the network structure for scalar processes. On the contrary, structure determination for the network of the vector processes is not straightforward if the PDC is used, because direct causality among Y_1, Y_2, and Y_3 should be assessed condensing in an arbitrary way the information provided by the large number of squared PDCs of Fig. 1b. This limitation can be overcame using the new defined bPDC function, which is devised to assess interactions between vector processes. Being computed for the Y_i's in place of the y_i's, the bPDC provides indeed a compact representation of frequency domain causality for the network of the vector processes (see Fig. 1c). In this representation, nonzero bPDC profiles are detected only over the directions for which direct causality effects are set (i.e. $Y_1 \rightarrow Y_2$, $Y_2 \rightarrow Y_3$, and $Y_3 \rightarrow Y_2$), while $\pi^{(b)}$ is uniformly zero over all other directions.

Moreover, the comparison between scalar and block measures may suggest, in some circumstances, a higher sensitivity of the block measure in conditions of weak coupling. As an example, causality detection from Y_1 to Y_2 seems difficult if performed on the basis of the very low values of π^2_{32} and π^2_{42}, while it seems a much more easy task when looking at the clear nonzero profile of the bPDC $\pi_{21}^{(b)}$. We ascribe the difference to the fact that the two PDCs π^2_{32} and π^2_{42} do not account for the internal dynamics of the source vector process Y_1, which in this case are very strong as documented by the sharp peak of the PDC π^2_{21}. On the contrary, the bPDC accounts for the dynamics occurring either *between* and *within* the constituent scalar processes of the investigated pair of vector processes; in this case, the profile of $\pi_{21}^{(b)}$ is magnified by the important information transfer occurring within Y_1.

4. First Application to Neurobiological Time Series

In this Section we report a practical application of the proposed bPDC to the study of neurophysiological interactions between multiple blocks of EEG time series. We considered EEG recordings acquired from a healthy subject during the execution of a visuomotor task combining precise grip motor commands with sensory visual feedback [Erla et al., 2012]. Briefly, the subject was asked to track the variations in size of a square target displayed on a monitor by acting on a pinch grip through his right hand thumb and forefinger. Visual feedback about his performance was provided to the subject by displaying on the monitor another square reflecting the exerted force (the task required to continuously match the two rectangles). EEG signals were acquired (earlobes common reference; sampling rate: 576 Hz) according to the standard 10-20 electrode placement enlarged with intermediate positions in cortical areas of interest for the specific task performed (Fig. 2a).

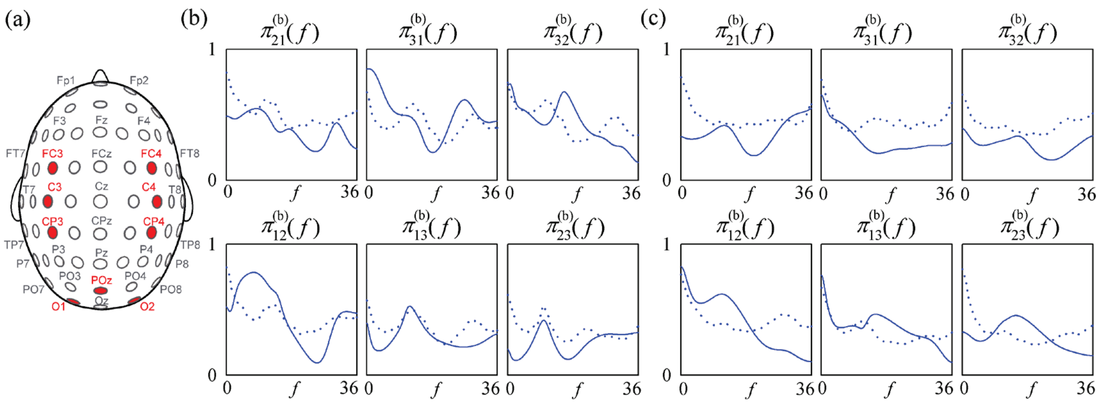

Figure 2. *(a) Schematic of EEG electrode placement for the practical application, with electrodes selected for the analysis depicted in red; (b) profiles of the bPDC (solid lines) and corresponding threshold for significance (dotted lines) estimated between each pair of time series blocks (Y_1: FC3, C3, CP3; Y_2: FC4, C4, CP4; Y_3: O1, POz, O2) before the execution of the visuo-motor task; (c) same as (b) with analysis performed during execution of the task.*

Here we present the results of bPDC analysis performed for M=3 regions of interest selected as representative of the scalp areas involved in visuomotor integration processes, i.e., left central (block 1, electrodes FC3, C3, CP3) and right central (block 2, electrodes FC4, C4, CP4) motor cortex areas, and posterior-parietal visual area (block 3, electrodes O1, POz, O2). Signals were bandpass filtered (3-45 Hz) and then downsampled to 72 Hz to reduce redundancy. Two stationary, artifact-free windows of ten seconds, selected before and during execution of the combined visuomotor task, were considered for the analysis. The coefficients and input covariance of the MVAR model fitting the Q=9 time series were estimated by classic vector least squares identification, and the model order was set according to the Akaike criterion [Faes et al., 2012]. The bPDC between each pair of block time series was then computed from the coefficient estimates, and compared with its corresponding threshold for significance determined by means of a specific procedure based on surrogate data generation (see [Faes et al., 2010] for details about surrogate data analysis). The frequency domain analysis was focused on the alpha (8-13 Hz) and beta (13-30 Hz) frequency bands, to investigate connectivity mechanisms related to long- and medium-range brain interactions [von Stein and Sarnthein, 2000].

Results of bPDC analysis before and during task execution are reported in Fig. 2b and Fig. 2c, respectively. The comparison between each bPDC and its corresponding threshold for significance indicates that, in both the analyzed time windows, a significant unidirectional interaction from the right to the left motor cortex is detected inside the alpha frequency band (Fig. 2b and 2c, $\pi_{12}^{(b)}$ is higher than the threshold). More interestingly, the direction of the interaction between visual (Y_3) and motor (Y_1, Y_2) areas, which results as unidirectional and significant mostly in the beta band, is reversed with the execution of the visuomotor task: before task execution the significant bPDC measures are $\pi_{31}^{(b)}$ and

$\pi_{32}^{(b)}$ (Fig. 2b); after task execution the significant bPDC measures are $\pi_{13}^{(b)}$ and $\pi_{23}^{(b)}$ (Fig. 2b). These results agree with findings suggesting that a functional link is activated between motor and visual brain cortices during tasks evoking processes of visuo-motor integration. Specifically, the emergence of a clear unidirectional interaction from the posterior area to both left and right central areas during task execution supports the hypothesis that visual feedback plays an active role in driving the beta oscillations recorded at the level of the motor cortex [Goodale, 1998].

5. Discussion

The new bPDC measure introduced in this study for the analysis of frequency domain causality between MV vector processes constitutes a suitable generalization of the very popular PDC measure originally defined to deal with MV scalar processes. Indeed, the bPDC has been shown to possess desirable properties of a frequency domain causality measure, such as being normalized between 0 and 1, reflecting direct causal effects between time series blocks, and reducing to the existing PDC measure in the case of univariate blocks [Faes and Nollo, 2013]. Main advantages with respect to the PDC are the compact representation of between-blocks interactions that is achieved without the need of arbitrary post-processing of multiple PDC profiles, and the ability to capture within-block interactions that would favor the correct detection of causality between weakly coupled blocks of time series. As also demonstrated by the reported multichannel EEG application, bPDC analysis is particularly useful for the assessment of directional interactions between specified brain rhythms in neurophysiological settings where multiple signals are simultaneously collected from each investigated brain region of interest. As a final remark, we note that the proposed bPDC is based on the assumption of strict causality, which presupposes absence of zero-lag correlations between the observed processes and needs to be tested through proper check of uncorrelation of the model residuals [Faes et al., 2012]. Future research will be aimed at providing a more general form of the bPDC in order to incorporate zero-lag effects, in line with a similar extension recently proposed for the traditional PDC [Faes and Nollo, 2010].

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