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Direct or indirect? Graphical models for neural oscillators

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Abstract

Univariate and bivariate time series analysis techniques have enabled new insights into neural processes. However, these techniques are not feasible to distinguish direct and indirect interrelations in multivariate systems. To this aim multivariate times series techniques are presented and investigated by means of simulated as well as physiological time series. Pitfalls and limitations of these techniques are discussed.

Keywords: Multivariate time series analysis; Graphical models; Coherence; Partial coherence; Partial directed coherence; Essential tremor

1. Introduction

Time series analysis techniques such as synchronization analysis [14] or cross-spectral analysis [4,18] are established to analyze bivariate data sets. If more than two signals are available, investigations based on pairwise combinations of the recorded data sets are still the most often applied procedure. However, multivariate data contain more information than those inferable from multiple bivariate examinations. Moreover, pairwise analysis of multivariate data may yield misleading results.

If for example one process influences two other, originally mutually independent processes, an influence between these two processes is also detected by bivariate analysis techniques. In this case, the influence is mediated by the common process. When increasing the number of processes, more complex interrelation structures can arise.

Therefore, time series analysis techniques that allow to elucidate such interrelation structures are desired. For cross-spectral analysis, several methods exist enabling to distinguish direct and indirect interrelations. Partial coherence has been introduced as the multivariate counterpart of coherence [3]. Graphical models applying partial coherence provide a proper methodology to estimate partial coherence and visualize its results [5].

As coherence and partial coherence are symmetric measures, an inference of directions of influences is impossible. Information contained in phase spectra or partial phase spectra are in general difficult to interpret. Coherence and partial coherence, respectively, have to be significant for a broad range of frequencies to draw reliable conclusions about phase relations and therefore direction of influences, which is rarely given for empirical time series [13].

Recently, partial directed coherence has been introduced to deduce directions of interrelations in

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multivariate data sets [1]. Based on modeling the multivariate time series by vector autoregressive processes, partial directed coherence enables differentiation of direct and indirect interrelations. Directed graphical models summarize the network of influences estimated by partial directed coherence analysis [6].

Within this paper, coherence, partial coherence, and partial directed coherence as well as the methodology of graphical models are discussed. We investigate abilities and limitations by means of simulated time series. As an example, an application to physiological time series recorded from a patient suffering from essential tremor is presented.

2. Methods

Within this section, coherence, partial coherence, and partial directed coherence are summarized with respect to their corresponding graphical models.

2.1. Cross-spectral analysis

To analyze relationships between two processes cross-spectral analysis has been introduced. Coherence

$$\mathrm{Coh}_{XY}(\omega) = \frac{|S_{XY}(\omega)|}{\sqrt{S_{XX}(\omega)S_{YY}(\omega)}} \in [0,1]$$

measures the linear relationship between processes X and Y, where $S_{XX}(\omega)$ and $S_{YY}(\omega)$ denote the auto-spectra of the processes, and $S_{XY}(\omega)$ the cross-spectrum between processes X and Y. Coherence assumes values close to one if a linear filter exists between processes X and Y. Values close to zero are present, if there is no interrelation between the processes described by linear filters [4].

As the cross-spectrum is a complex valued measure, the phase spectrum $\Phi_{XY}(\omega)$ can be defined as the argument of the cross-spectrum

$$S_{XY}(\omega) = |S_{XY}(\omega)|\mathrm{e}^{i\Phi_{XY}(\omega)}$$

via its polar representation. Time delays between the processes as well as filter properties can be estimated using the information contained in the phase spectrum $\Phi_{XY}(\omega)$. A pure time delay d between X and Y would result in a linear phase relation $\Phi_{XY}(\omega) = d\omega$.

In case of finite time series coherence and phase spectra can be estimated by applying these equations with the estimators for the cross- and auto-spectra. Auto- and cross-spectra themselves can be estimated through various techniques. Often used techniques are, for example, averaging periodograms calculated for equally sized sections of the time series [8,9] or smoothing periodograms [17]. To decide about the significance of estimated coherence a critical value

$$s = \sqrt{1 - \alpha^{\frac{2}{v-2}}}$$

has been derived for a significance level α, where v is the equivalent number of degrees of freedom and depends on the estimation procedure of $S_{XX}(\omega)$, $S_{YY}(\omega)$, and $S_{XY}(\omega)$ [2]. For the technique based on cutting the time series into equally seized sections, the equivalent number of degrees of freedom is $v = 2L$, where L is the number of disjoint sections. For smoothing the periodogram the equivalent number of degrees of freedom is $v = 2/\sum_{i=1}^{h} w_i^2$, where w denotes the smoothing function evaluated at discrete w_i and h is the width of the smoothing function.

Similarly, α-confidence intervals

$$\Phi(\omega) \pm \kappa_\alpha \sqrt{\frac{1}{v}\left[\frac{1}{\mathrm{Coh}^2(\omega)} - 1\right]}$$

for the phase $\Phi(\omega)$ can be derived, where κ_α is the α-quantile of the standard Gaussian distribution [2]. Since v is fixed by the estimation procedure, no reliable phase spectra can be estimated, if $\mathrm{Coh}^2(\omega)$ is small compared to one.

2.2. Partial coherence

Partial coherence has been introduced to differentiate direct and indirect interrelations [5,3]. The underlying idea is to subtract linear influences from other processes to obtain the partial cross-spectrum

$$S_{XY|Z}(\omega) = S_{XY}(\omega) - S_{XZ}(\omega)S_{ZZ}^{-1}(\omega)S_{ZY}(\omega)$$

between X and Y given all the linear information of the remaining processes Z, that might be vector valued. Analogously, $S_{XX|Z}(\omega)$ denotes the partial auto-spectrum leading to the definition of partial coherence

$$\mathrm{Coh}_{XY|Z}(\omega) = \frac{\left|S_{XY|Z}(\omega)\right|}{\sqrt{S_{XX|Z}(\omega)S_{YY|Z}(\omega)}} \in [0,1]$$

and partial phase spectrum $\Phi_{XY|Z}(\omega)$

$$S_{XY|Z}(\omega) = \left|S_{XY|Z}(\omega)\right|\mathrm{e}^{\mathrm{i}\Phi_{XY|Z}(\omega)}.$$

For partial coherence the critical value

$$s = \sqrt{1 - \alpha^{\frac{2}{v-2L-2}}}$$

can be calculated depending on the dimension L of Z and v the equivalent number of degrees of freedom [18].

2.3. Partial directed coherence

Estimating the elements $a_{kj,r}$ (k, $j = 1,\ldots,n$, $r = 1,\ldots,p$) of the coefficient matrices $\mathbf{a}_r$ of a n-dimensional vector autoregressive process of model order p (VAR[p])

$$\begin{pmatrix} X_1(t) \\ \vdots \\ X_n(t) \end{pmatrix} = \sum_{r=1}^{p} \mathbf{a}_r \begin{pmatrix} X_1(t-r) \\ \vdots \\ X_n(t-r) \end{pmatrix} + \begin{pmatrix} \varepsilon_1(t) \\ \vdots \\ \varepsilon_n(t) \end{pmatrix}$$

is the basic step of partial directed coherence analysis, where ε_i is Gaussian distributed with covariance matrix Σ. Therefor, a n-dimensional VAR[p]-process is fitted to the empirical time series. Fourier transformation of the coefficient matrices

$$A_{kj}(\omega) = \delta_{kj} - \sum_{r=1}^{p} a_{kj,r} e^{-i\omega r}$$

where $\delta_{kj} = 1$ if $k = j$ and $\delta_{kj} = 0$ if $k \neq j$, leads to the definition of partial directed coherence

$$\pi_{i\leftarrow j}(\omega) = \frac{|A_{ij}(\omega)|}{\sqrt{\sum_k A^*_{kj}(\omega) A_{kj}(\omega)}}$$

with $(\cdot)^*$ denoting complex conjugation. Partial directed coherence $\pi_{i\leftarrow j}$ is normalized between 0 and 1 and indicates an influence from process X_j onto process X_i, if it is non-zero. For finite time series a significance level has recently been introduced [16]. A significant direction of interrelation detected by partial directed coherence analysis has to be interpreted in terms of Granger causality, i.e. that there is no reaction without a cause [7]. However, there can be influencing processes which are not measured. In this case a conclusion to causality is impossible.

2.4. Graphical models

Graphical models serve as a proper methodology to visualize and to enlighten multivariate interrelation structures. In Fig. 1 three different graphs are shown for an exemplary, five-dimensional system. All processes, denoted as the vertices in the graphs are connected by edges representing significant pairwise coherences (a), partial coherences (b), and partial directed coherences (c). If, for example, a partial coherence between X_1 and X_2 is non-significant, processes X_1 and X_2 are interpreted as not mutually influencing each other linearly and directly. Thus, an edge in the corresponding graphical model is missing between X_1 and X_2, if and only if $\mathrm{Coh}_{X_1X_2|Z}(\omega) = 0$. For directed graphical models applying partial directed coherence edges are substituted by arrows indicating the direction of the interrelation.

In the graph deduced from bivariate coherence analysis, all possible edges are present. In the graphical model applying partial coherence, the edges between processes X_1 and X_3, X_2 and X_3, as well as X_3 and X_4 are missing. These missing edges represent indirect interrelations between the corresponding processes, which cannot be detected by pairwise coherence analysis. For example, the edge between process X_1 and X_3 in (a) is mediated by process X_5, which can be inferred from the graph applying partial coherence (b). X_5 mediates all influence between X_3 and the remaining processes. This property is defined as separation. In conclusion, a system corresponding to the graph in Fig. 1(b) analyzed by pairwise coherence would lead to the graph in Fig. 1(a). In addition, the direction of the interrelation is contained in the directed graph in Fig. 1(c).

3. Results

In the following, the differences of the three introduced time series analysis techniques are illustrated by means of simulated data and in an application to physiological data sets recorded from one patient suffering from essential tremor.

3.1. Application to simulated time series

Coherence analysis, partial coherence as well as partial directed coherence are illustrated in application to the following five-dimensional VAR[4]-process

$$\begin{aligned}
X_1(t) &= 0.4X_1(t-1) - 0.5X_1(t-2) + 0.4X_5(t-1) + \eta_1(t)\\
X_2(t) &= 0.4X_2(t-1) - 0.3X_1(t-4) + 0.4X_5(t-2) + \eta_2(t)\\
X_3(t) &= 0.5X_3(t-1) - 0.7X_3(t-2) - 0.3X_5(t-3) + \eta_3(t)\\
X_4(t) &= 0.8X_4(t-3) + 0.4X_1(t-2) + 0.3X_2(t-2) + \eta_4(t)\\
X_5(t) &= 0.7X_5(t-1) - 0.5X_5(t-2) - 0.4X_4(t-1) + \eta_5(t)\\
\eta_i &\sim \mathcal{N}(0,1), \quad i = 1,\ldots,5.
\end{aligned}$$

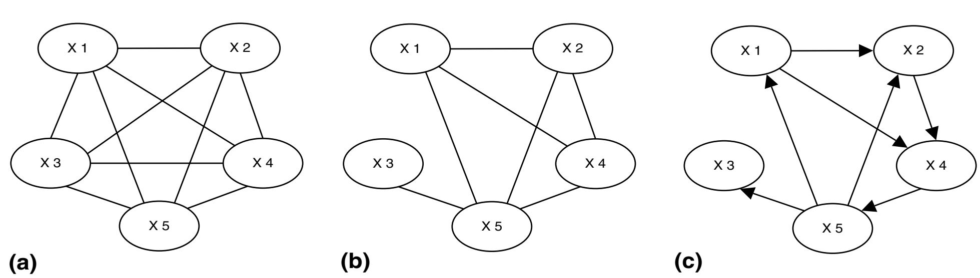

Fig. 1. Graphical models for an illustrative, five-dimensional process. (a) All edges are present denoting the presence of significant coherences between each pairwise combination of processes denoted by the vertices, (b) some edges are missing due to results from partial coherence analysis and (c) direction of interrelations between the processes are indicated by arrows in the directed graph, obtained by partial directed coherence analysis.

On the diagonal of Fig. 2, the spectra of the five processes are shown. Above the diagonal pairwise estimated coherence is shown, while below the diagonal partial coherence is presented. The graph concluded from the bivariate coherence analysis is the same as the one already used as an example in Fig. 1(a). Results of partial coherence analysis are summarized in the graphical model in Fig. 1(b). The partial coherence graph is in agreement with the simulated influences within the VAR[4]-process, as edges between processes X_1 and X_3, X_2 and X_3, as well as between processes X_3 and X_4 are missing.

The simulated VAR[4]-processes, however, contains more information than obtained from the partial coherence graph. For instance, process X_5 is influencing process X_1, while there is no direct influence from process X_1 onto process X_5. The influence between processes X_1 and X_5 is, thus, asymmetric. Partial directed coherence analysis (Fig. 3) reflects these asymmetric influences. Again, the corresponding graph is shown in Fig. 1(c).

For this analysis, the correct model order is chosen for the fitted VAR[p]-process. On the diagonal the spectra are presented, while the off-diagonal elements represent the partial directed coherences. Directed influences could thus be detected from process X_1 onto the processes X_2 and X_4, from process X_2 onto process X_4, from process X_4 onto process X_5, and finally from process X_5 onto processes X_1, X_2, and X_3.

A comparison between the graphical model summarizing these results and the simulated process illustrates, that interrelations of the simulated VAR-process can be reproduced correctly. Process X_5 is not only separating process X_3 from the remaining processes, but process X_5 is projecting the informations contained in processes X_1, X_2, X_4, and X_5 itself onto process X_3. No influence from process X_3 enters any other process.

A parametric approach such as partial directed coherence has some pitfalls and limitations. For example the number of parameters and, thus, the order of the fitted VAR[p] has to be small compared to the number of data points, otherwise a reliable parameter estimation is impossible. Furthermore, the variance of the noise in the estimated VAR model has to be equal to the identity matrix. In Fig. 4 an example is shown in which the variance of the stochastic, driving noise of the second process is 2500 times higher than the variance of the stochastic, driving noise of the remaining two processes. The corresponding graph summarizes the simulated interrelations in the system (a). Partial directed

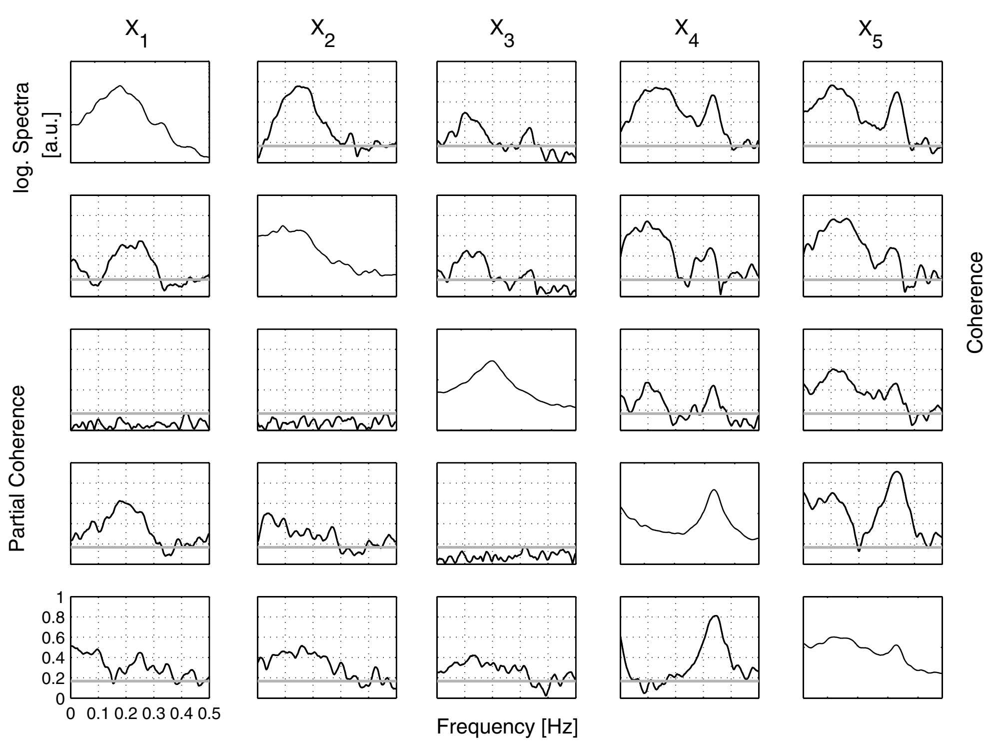

Fig. 2. Coherence and partial coherence for a simulated five-dimensional VAR[4]-process. In the upper right corner bivariate coherences are shown. In the lower left corner, partial coherences are shown. The significance level is denoted as the horizontal, gray line. On the diagonal the spectra of the processes are shown. For bivariate coherence each pair of processes is coherent, for example coherence between process X_1 and X_3 (1st row/3rd column). In contrast, partial coherence is non-significant between process X_1 and X_3 (3rd row/1st column), X_2 and X_3 (3rd row/2nd column), as well as X_3 and X_4 (4th row/3rd column). This illustrates that there is no direct interrelation between those processes.

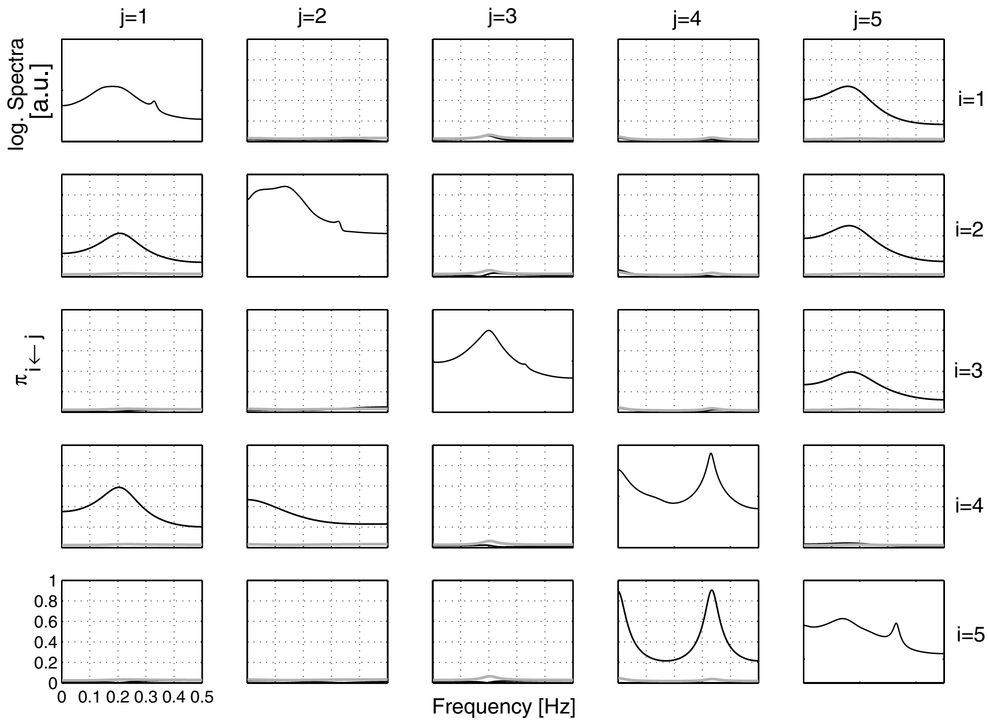

Fig. 3. Partial directed coherence for the simulated five-dimensional VAR[4]-process (off-diagonal). The significance level is the gray, almost horizontal line. On the diagonal the spectra are shown. While coherence and partial coherence (Fig. 2) do not allow for inferring directed influences, partial directed coherence indicates a directed interrelation structure in the system. For example, process X_1 is influencing X_2 (2nd row/1st column), while process X_2 is not influencing X_1 (1st row/2nd column). Partial directed coherences reproduce the simulated system correctly.

coherence applied to this system detects spurious interrelations from process X_1 and X_3 onto process X_2 (Fig. 4(b)), as the differences in the variance of the stochastic, driving noise terms yield high errors on the parameter estimations. A renormalization of the covariance matrix Σ of the noise in the estimated VAR model and subsequent application of partial directed coherence leads to the results presented in Fig. 4(c). Only the valid influences are significantly different from zero.

As partial directed coherence is developed to detect and visualize directed influences in linear autoregressive processes, it is not obvious that partial directed coherence can be generalized to other classes of dynamic systems, especially non-linear systems.

To illustrate that partial directed coherence is feasible to detect directed interrelations even in non-linear systems, partial directed coherence is applied to coupled, stochastic Roessler oscillators [15].

$$\begin{pmatrix} \dot{X}_j \\ \dot{Y}_j \\ \dot{Z}_j \end{pmatrix} = \begin{pmatrix} -\omega_j Y_j - Z_j + \left[\sum_i \varepsilon_{ji}(X_i - X_j)\right] + \sigma_j \eta_j \\ \omega_j X_j + a Y_j \\ b + (X_j - c) Z_j \end{pmatrix}$$
$$i, j = 1, 2, 3, 4.$$

The parameters of the four oscillators are $\sigma_j = 1$, $\omega_1 = 1.03$, $\omega_2 = 0.97$, $\omega_3 = 1.09$, $\omega_4 = 0.91$, $a = 0.15$, $b = 0.2$, $c = 10$, and η_j is Gaussian distributed white noise. Only $\varepsilon_{13} = 0.05$, $\varepsilon_{23} = 0.05$, $\varepsilon_{32} = 0.05$, and $\varepsilon_{24} = 0.05$ are different from zero. For the estimation of interrelations between the four oscillators, partial directed coherence is applied only to the X-components of the simulated system.

Using a sufficiently large order of the VAR[p]-process of $p = 200$, the coupling scheme is reproduced correctly by partial directed coherence (Fig. 5). The large model order is required by the non-linearities in the Roessler system. In general, in case of an unknown system the order of the fitted VAR[p]-process should be chosen rather oversized than undersized. If the number of parameters is too small, especially smaller than the time lags between the processes, a correct conclusion to the underlying structure of causal influences is impossible. Note that the significance level increases with the order of the fitted processes, preventing erroneous conclusions.

3.2. Application to essential tremor

So far, the discussed multivariate analysis techniques have been applied to simulated time series. To illustrate their performance in physiological applications, an example of a patient suffering from essential tremor is presented.

For unilaterally activated tremor, tremor correlated cortical activity to the contralateral tremor side has been revealed by magnetoencephalography (MEG) and

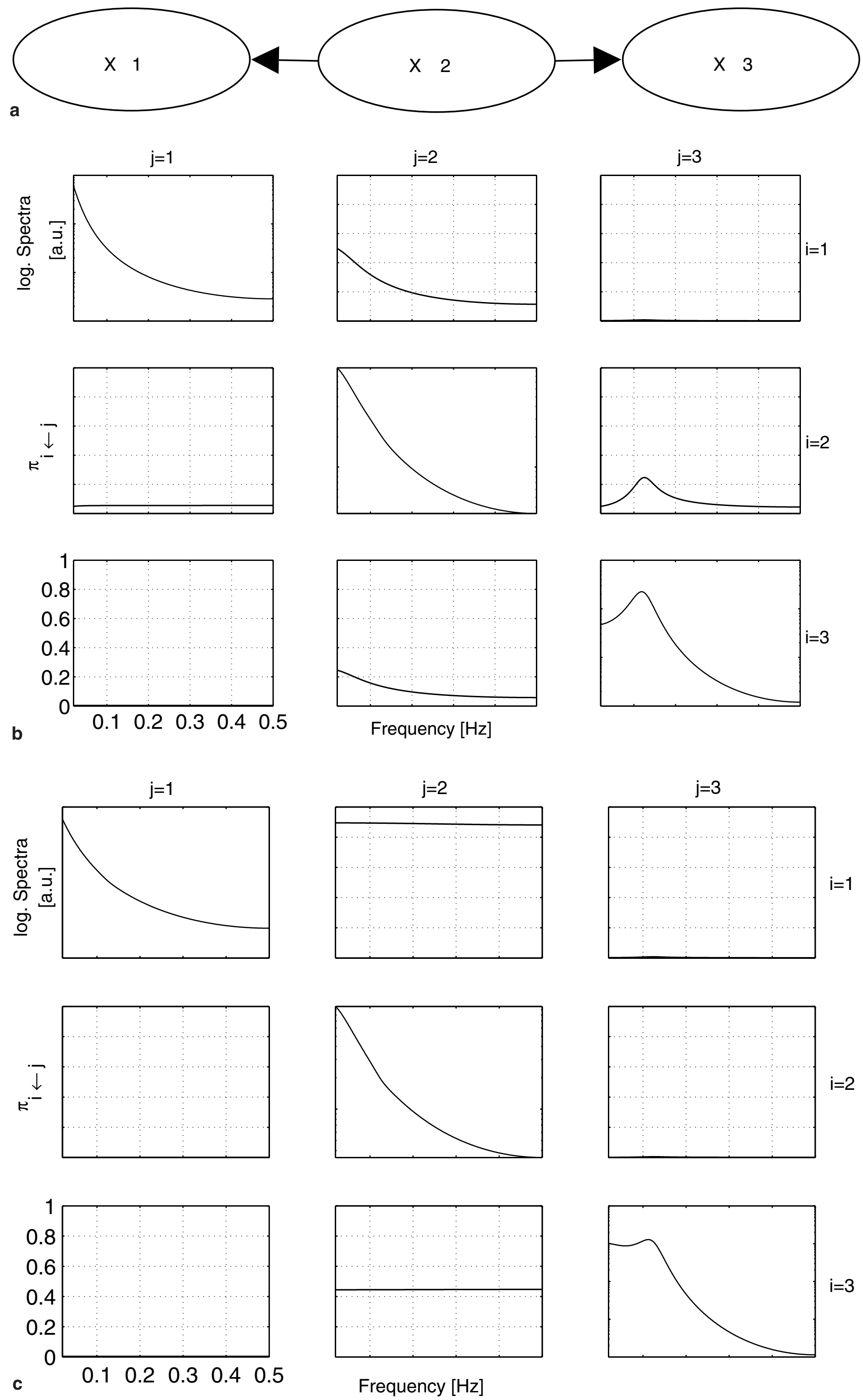

Fig. 4. Partial directed coherence for a three-dimensional example of a VAR[2]-process. The variance of the stochastic, driving noise influence of the second process is 2500 times higher than that of the remaining two. The simulated directed interrelations in the three-dimensional VAR-model are shown in the graph (a). Spurious directed interrelations are found from process X_1 onto process X_2 and from process X_3 onto process X_2 caused by the different variances of the stochastic noise influences (b). VAR-parameters show larger errors in this cases. (c) Partial directed coherence for the same three-dimensional VAR[2]-process, but the variance of the stochastic noise influence of the second process is renormalized to one as for the remaining two processes. The simulated causal connections are re-estimated from the time series. There is only a causal influence from process X_2 onto process X_1 and onto process X_3.

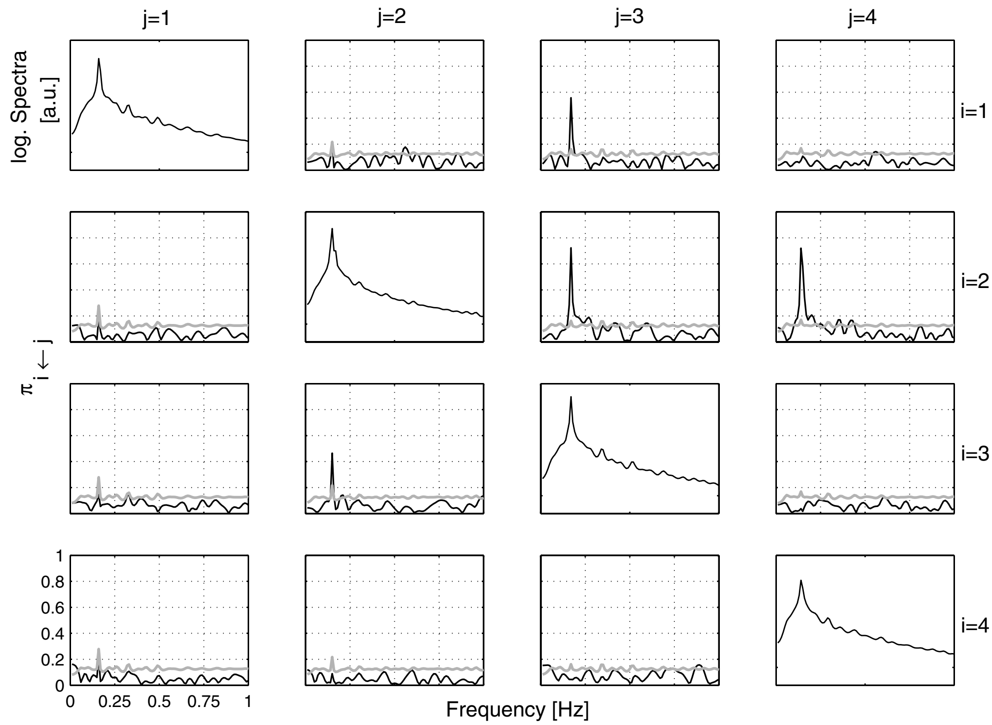

Fig. 5. Results of partial directed coherence analysis for a four-dimensional, stochastic Roessler system. Directed influences are present from process X_2 onto process X_3, from process X_3 onto process X_1 and onto X_2, as well as from process X_4 onto process X_2. The significance level indicated by the almost horizontal, gray line is frequency dependent and may show small peaks at the oscillation frequency of the corresponding Roessler oscillators. This leads for example to the fact that there is no significant influence from process X_1 onto X_3 even if there is a peak in the corresponding partial directed coherence spectrum.

electroencephalography (EEG) for Parkinson tremor [19,10] and by electroencephalography for essential tremor [11]. In bilaterally activated essential tremor, however, a more complex interrelation structure has been observed by simultaneous electroencephalographic recordings from the scalp and electromyographic (EMG) recordings from the extensor muscles [12]. In addition to contralateral coherences, also ipsilateral coherences between the sensori-motor cortex and the muscles have been detected.

For this investigation, eight patients were seated in a comfortable chair having their forearms supported while their hands were outstretched to activate tremor. Data were sampled at 1000 Hz. The EEG data as well as the EMG data were preprocessed applying a low-pass filter of 200 Hz to avoid aliasing. Furthermore, the EMG was high-pass filtered above 30 Hz to avoid movement artifacts and was rectified afterward. The EEG was high pass filtered above 0.5 Hz to avoid baseline fluctuations.

Scalp electrodes over the left and right sensori-motor cortex and the EMG of the left and right wrist extensor are analyzed. The results are shown for one representative patient. Coherence as well as partial coherence analysis are presented in Fig. 6. For bivariate coherence analysis, the right EMG is coherent with the left and right EEG and the left EMG is coherent with the right EEG. The ipsilateral connection between the right EMG and the right EEG (Fig. 6 1st row/4th column) is rather unlikely to be valid from a physiological point of view. As partial coherence analysis demonstrates for this patient (Fig. 6), the ipsilateral connection between the right EMG and the right EEG is not direct and most likely mediated by an inter-hemispheric coupling (Fig. 6 4th row/1st column).

Directions of the interrelations are determined using partial directed coherence analysis (Fig. 7). Both directions from the cortex to the muscles and vice versa are observed. A significant influence from the right EEG onto the left EMG, from the left EMG onto the right EEG, from the left EEG onto the right EMG, and from the right EMG onto the left EEG is detected. Especially, the partial directed coherence from the right EMG to the left EEG is rather large.

4. Discussion

Bivariate analysis techniques, like coherence and synchronization analysis, are limited by the impossibility to distinguish direct and indirect interrelations between processes in higher dimensional systems. Graphical models applying partial coherence have been introduced to elucidate more complex interrelation structures. As it is usually impossible to determine the direction of

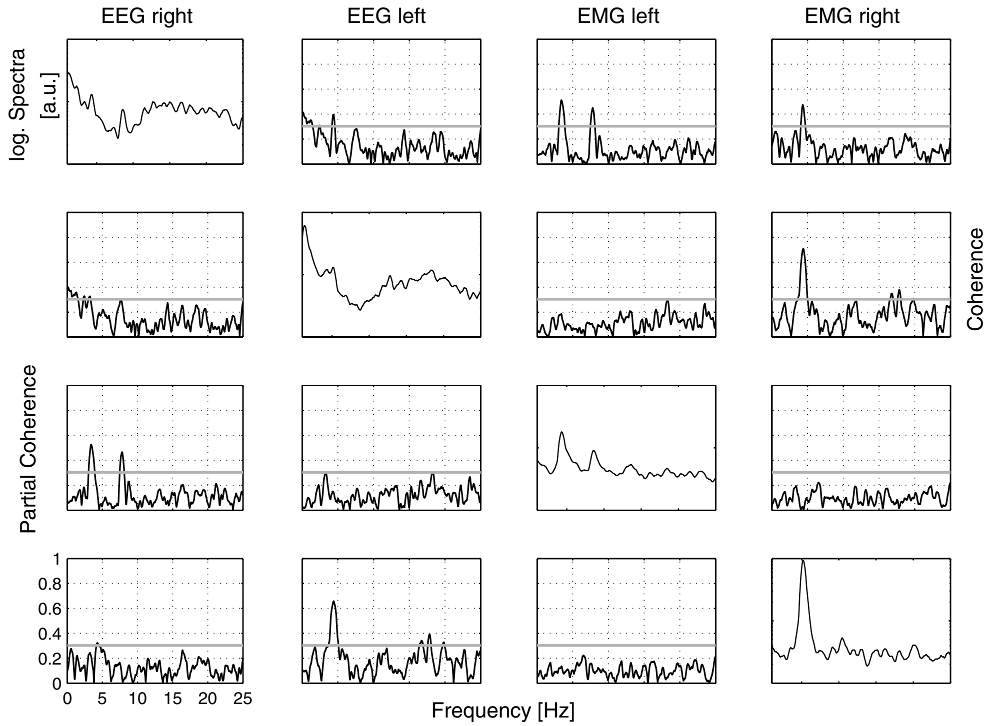

Fig. 6. Spectra, coherence, and partial coherence between EEGs over the left and right sensori-motor cortex and EMGs from the left and right wrist extensor for a patient suffering from essential tremor. Significant coherence and partial coherences are detected between the EEGs and the corresponding contralateral tremor side. The ipsilateral significant coherence between the right EEG and right EMG is mediated most likely by an inter-hemispheric coupling, as it vanishes using partial coherence analysis.

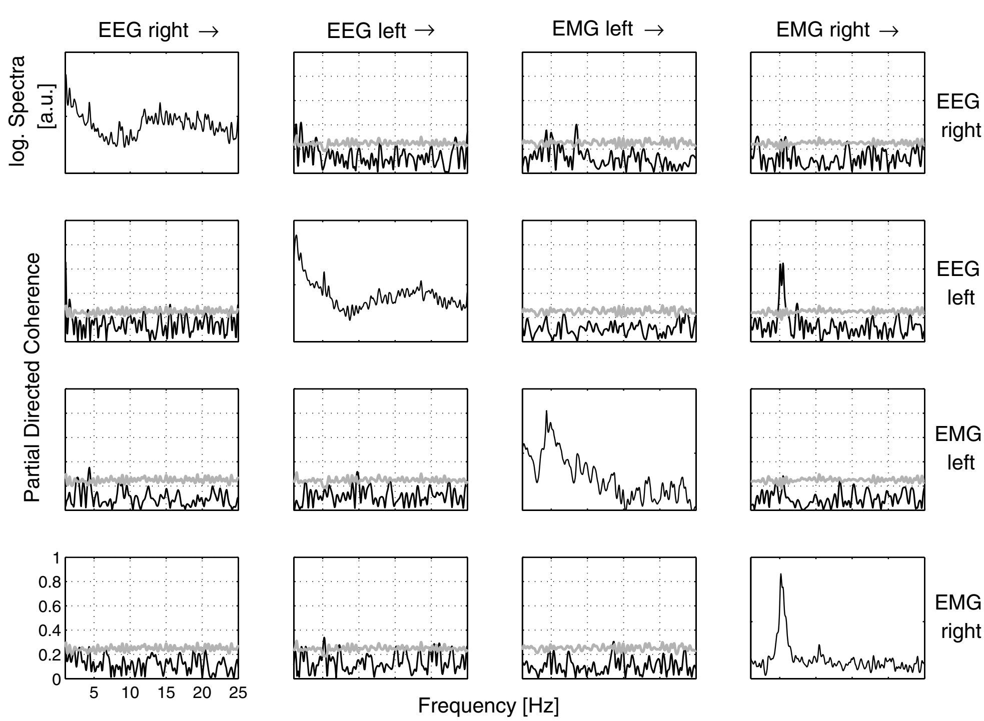

Fig. 7. Partial directed coherence analysis for the patient suffering from essential tremor. The significance level is indicated by the gray line. A significant influence from the right EEG onto the left EMG (3rd row/1st column), from the left EMG onto the right EEG (1st row/3rd column), from the left EEG onto the right EMG (4th row/2nd column), and from the right EMG onto the left EEG (2nd row/4th column) is detected. Concerning mediated influences, the results are in agreement with results from partial coherence analysis.

influences by cross-spectral analysis techniques, a parametric approach has recently been proposed, the partial directed coherence. Partial directed coherences enable to infer directed influences in multivariate systems. However, they do not always allow for real causal inference, as for example unobserved processes might have an influence.

The abilities of coherence, partial coherence, and partial directed coherence have been demonstrated by means of simulated time series. Complex interrelation structures could be correctly reestimated from simulated time series. Even for an example of a non-linear system, conclusions about the underlying interrelations have been feasible.

Since partial directed coherence is a parametric approach, further pitfalls arise. Estimations of the necessary order p of the VAR[p] is rather difficult. A comparison of spectra from the parametric and non-parametric approach can yield a hint for the appropriate model order p. A significance level has recently been derived [16], allowing to decide whether a partial directed coherence value at the investigated frequency is significantly different from zero. Especially, for higher orders of p that introduce more variability to partial directed coherences, the significance level prevents erroneous conclusions about the interrelation structure. Finally, as shown in this paper large variations of the covariance matrix of the stochastic noise might lead to wrong conclusions about the underlying interdependence structure. High partial directed coherence values are not necessarily indicating a dominant influence between the corresponding processes. Valid influences are usually underestimated in this circumstance, too. A renormalization of the covariance matrix of the driving noise in the fitted VAR-model is, thus, strongly recommended to achieve comparable values for any partial directed coherence spectrum.

In an application to bilaterally activated essential tremor, an unexpected ipsilateral interrelation detected by coherence analysis could be unmasked as an indirect interrelation by partial coherence and partial directed coherence analysis. It has recently been shown, that the ipsilateral connection is most likely mediated by an interhemispheric coupling [12]. Furthermore, partial directed coherence analysis has enabled deeper insights into the directions of interrelations. The partial directed coherence from the right EMG to the left EEG is rather large (Fig. 7). Basically, this is caused by the fact that the signal-to-noise ratio for the right EMG is the highest. Moreover, partial directed coherence is normalized by the Fourier transform of the coefficients of the outgoing process. High partial directed coherences indicate that a rather large fraction of the EMG is reflected in the EEG. In contrast, if a signal like the EEG is contaminated by a huge amount of non-tremor related influences, the fraction of the signal related to tremor is rather small leading to comparably small partial directed coherence values. In conclusion, it could be shown that the cortex imposes its oscillatory activity on the contralateral muscles via the corticospinal tract and that additionally muscle activity is reflected to the contralateral cortex via proprioceptive afferences.

5. Conclusion

Graphical models applying partial coherence and partial directed coherence allow for deeper insights into multivariate systems. The abilities of these multivariate analysis techniques have been shown by means of simulated as well as physiological time series. In the application to essential tremor the knowledge about the physiology underlying tremor has been extended compared to results originating from bivariate coherence analysis.

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