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Information theoretic interpretation of frequency domain connectivity measures

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Abstract In order to provide adequate multivariate measures of information flow between neural structures, modified expressions of partial directed coherence (PDC) and directed transfer function (DTF), two popular multivariate connectivity measures employed in neuroscience, are introduced and their formal relationship to mutual information rates are proved.

Keywords Information flow · Partial directed coherence · Directed transfer function · Mutual information rate · Granger causality

1 Introduction

Over the last decade, Neuroscience has been witnessing an important paradigm shift owing to the fast advancement of multichannel data acquisition technology. This process has been marked by the growing realization that the brain's inner workings can only be grasped through a detailed description of how brain areas interact functionally in a scenario that has come to be generally referred as the study of brain connectivity and which stands in sharp contrast to former longstanding efforts mostly directed at merely identifying which brain areas were involved in specific functions.

As such, many techniques have been proposed to address this problem, specially because of the need to process and make sense of many simultaneously acquired brain activity signals, (Kaminski and Blinowska 1991; Sommer and Wichert 2003; Astolfi et al. 2007). Among the available methods, we introduced and developed the idea of partial directed coherence (PDC) (Baccalá and Sameshima 2001a,b) which consists of a means of dissecting the frequency domain relationship between pairs of signals from among a set of $K \geq 2$ simultaneously observed time series.

The main characteristic of PDC is that it decomposes the interaction of each pair of time series within the set into directional components while deducting the possibly shrouding effect of the remaining $K - 2$ series. It has, for instance, been possible to show that PDC is related to the notion of Granger causality which corresponds to the ability of pinpointing the level of attainable improvement in predicting a time series $x_i(n)$ when the past of another time series $x_j(n)$ is known ($i \neq j$) (Granger 1969).

In fact, multivariate Granger causality tests as described in Lütkepohl (1993) map directly onto statistical tests for PDC nullity. Like Granger causality, and as opposed to ordinary coherence (Priestley 1981), PDC is a directional quantity; this fact leads to the idea of "directed" connectivity that allows one to expressly test for the presence of feedback and to the idea that PDC is somehow associated with the direction of information flow.

The appeal of associating PDC with information flow has been strong; we have used it ourselves (Baccalá and Sameshima 2001a,b). Yet, this suggestion has until now remained vague and to some extent almost apocryphal. The aim of this article is to correct this state of affairs by making

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the relationship between PDC and information flow at once formally explicit and precise.

On a par with PDC, is the no less important notion of directed transfer function (DTF) by Kaminski and Blinowska (1991), whose information theoretic interpretation is also addressed here.

By providing further details and full proofs, this article expands on our previous publication (Takahashi et al. 2010) and is organized as follows: in Sect. 2, we provide some explicit information theoretic background leaving the main result to Sect. 3 followed by illustrations and comments in Sects. 4 and 5, respectively. Detailed proofs are covered in the Appendix.

2 Background

The relationship between two discrete time stochastic processes $x = \{x(k)\}_{k\in\mathbb{Z}}$ and $y = \{y(k)\}_{k\in\mathbb{Z}}$ is assessed via their mutual information rate, MIR(x, y), by comparing their joint probability density with the product of their marginals:

$$\text{MIR}(x, y) = \lim_{m \to \infty} \frac{1}{m+1}$$
$$\times \mathbb{E}\left[\log \frac{d\mathbb{P}(x(1), \ldots, x(m), y(1), \ldots, y(m))}{d\mathbb{P}(x(1), \ldots, x(m))d\mathbb{P}(y(1), \ldots, y(m))}\right], \quad (1)$$

where $\mathbb{E}[\cdot]$ is the expectation with respect to the joint measure of x and y, and $d\mathbb{P}$ denotes the appropriate probability density. An immediate consequence of (1) is that independence between x and y implies MIR nullity.

The main classic result for jointly Gaussian stationary processes, due to Gelfand and Yaglom (1959), relates (1) to the coherence between the processes via

$$\text{MIR}(x, y) = -\frac{1}{4\pi} \int_{-\pi}^{\pi} \log(1 - |C_{xy}(\omega)|^2) d\omega, \quad (2)$$

where the coherence in (2) is given by

$$C_{xy}(\omega) = \frac{S_{xy}(\omega)}{\sqrt{S_{xx}(\omega)S_{yy}(\omega)}}, \quad (3)$$

with $S_{xx}(\omega)$ and $S_{yy}(\omega)$ standing for the autospectra and $S_{xy}(\omega)$ for the cross-spectrum, respectively.

The important consequence of this result is that the integrand in (2) may be interpreted as the frequency decomposition of MIR(x, y).

In view of this result, the following questions arise: does a similar result hold for PDC? How and in what sense?

Before addressing these problems, consider the zero mean stationary vector process $\mathbf{x}(n) = [x_1(n) \ldots x_K(n)]^T$ representable by multivariate autoregressive model

$$\mathbf{x}(n) = \sum_{l=1}^{+\infty} \mathbf{A}(l)\mathbf{x}(n-l) + \mathbf{w}(n), \quad (4)$$

where $\mathbf{w}(n) = [w_1(n) \ldots w_K(n)]^T$ stand for zero mean stationary innovation processes with positive definite covariance matrix $\boldsymbol{\Sigma}_\mathbf{w} = \mathbb{E}\left[\mathbf{w}(n)\mathbf{w}^T(n)\right]$.

A sufficient condition for the existence of representation (4) is that the spectral density matrix associated with the process $\{\mathbf{x}(n)\}_{n\in\mathbb{Z}}$ be uniformly bounded from below and above and be invertible at all frequencies (Hannan 1970). From the coefficients $a_{ij}(l)$ of $\mathbf{A}(l)$ we may write

$$\bar{A}_{ij}(\omega) = \begin{cases} 1 - \sum_{l=1}^{+\infty} a_{ij}(l)e^{-\mathbf{j}\omega l}, & \text{if } i = j \\ -\sum_{l=1}^{+\infty} a_{ij}(l)e^{-\mathbf{j}\omega l}, & \text{otherwise} \end{cases} \quad (5)$$

where $\mathbf{j} = \sqrt{-1}$ for $\omega \in [-\pi, \pi)$.

Also let $\bar{\mathbf{a}}_j(\omega) = [\bar{A}_{1j}(\omega) \ldots \bar{A}_{Kj}(\omega)]^T$ and consider the quantity, henceforth termed *information* PDC (ιPDC) from j to i,

$$\iota\pi_{ij}(\omega) = \frac{\bar{A}_{ij}(\omega)\sigma_{ii}^{-1/2}}{\sqrt{\bar{\mathbf{a}}_j^H(\omega)\boldsymbol{\Sigma}_\mathbf{w}^{-1}\bar{\mathbf{a}}_j(\omega)}}, \quad (6)$$

where $\sigma_{ii} = \mathbb{E}\left[w_i^2(n)\right]$ and which simplifies to the originally defined PDC when $\boldsymbol{\Sigma}_\mathbf{w}$ equals the identity matrix. Note also that the generalized PDC (gPDC) from Baccalá et al. (2007) is obtained if $\boldsymbol{\Sigma}_\mathbf{w}$ is a diagonal matrix whose elements are not necessarily the same.

Before stating the main result, note that to our knowledge, mention of (6), as in Baccalá et al. (2006), has not appeared in the literature with any explicit association with information theoretic ideas.

3 Results

3.1 PDC

Theorem 1 *Let the K-variate wide sense stationary time series* $\mathbf{x}(n) = [x_1(n) \ldots x_K(n)]^T$ *satisfy* (4), *then*

$$\iota\pi_{ij}(\omega) = C_{w_i\eta_j}(\omega), \quad (7)$$

where $\eta_j(n) = x_j(n) - \mathbb{E}[x_j(n)|\{x_l(m), \ l \neq j, \ m \in \mathbb{Z}\}]$ *which is known as the partialized process associated to* x_j *given the remaining time series.*

Corollary 1 *Let the K-variate Gaussian stationary time series* $\mathbf{x}(n) = [x_1(n) \ldots x_K(n)]^T$ *satisfy* (4), *then*

$$\text{MIR}(w_i, \eta_j) = -\frac{1}{4\pi} \int_{-\pi}^{\pi} \log(1 - |\iota\pi_{ij}(\omega)|^2) d\omega. \quad (8)$$

To obtain the process η_k, remember that it constitutes the residue of the projection of x_k onto the past, the future and the present of the remaining processes. Hence its autospectrum is given by

$$S_{\eta_k \eta_k}(\omega) = S_{x_k x_k}(\omega) - \mathbf{s}_{x_k \mathbf{x}^k}(\omega) \mathbf{S}_{\mathbf{x}^k \mathbf{x}^k}^{-1}(\omega) \mathbf{s}_{\mathbf{x}^k x_k}(\omega), \qquad (9)$$

for $\mathbf{x}^k = [x_{l_1} \ldots x_{l_{K-1}}]^T$, $\{l_1, \ldots, l_{K-1}\} = \{1, \ldots, K\} \setminus \{k\}$ where $\mathbf{s}_{x_k \mathbf{x}^k}(\omega)$ is the $K-1$-dimensional vector whose entries are the cross spectra between x_k and the remaining $K-1$ processes, whereas $\mathbf{S}_{\mathbf{x}^k \mathbf{x}^k}(\omega)$ is the spectral density matrix of $\mathbf{x}^k$. The spectrum $S_{\eta_k \eta_k}(\omega)$ is also known in the literature as the partial spectrum of x_k given $\mathbf{x}^k$ (Priestley 1981).

Note that

$$\mathbf{g}_k(\omega) = \mathbf{s}_{x_k \mathbf{x}^k}(\omega) \mathbf{S}_{\mathbf{x}^k \mathbf{x}^k}^{-1}(\omega) \qquad (10)$$

constitutes an optimum Wiener filter whose role in producing η_k is to deduct the influence of the other variables from x_k to single out that contribution that is only its own.

Theorem 1 shows that PDC from x_j to x_i measures the amount of information common to the η_j partial process and the w_i innovation. The proof is left to the Appendix but its main idea is to prove (7) so that (8) follows by use of (2) to produce $\text{MIR}(w_i, \eta_j)$.

3.2 DTF

Every stationary process $\{\mathbf{x}(n)\}_{n \in \mathbb{Z}}$ with autoregressive representation (4) also has the following moving average representation

$$\mathbf{x}(n) = \sum_{l=0}^{+\infty} \mathbf{H}(l) \mathbf{w}(n-l), \qquad (11)$$

where the innovation process $\mathbf{w}$ is the same as that of (4).

In connection to the $h_{ij}(l)$ coefficients of $\mathbf{H}(l)$, consider the matrix $\bar{\mathbf{H}}(\omega)$ with entries

$$\bar{H}_{ij}(\omega) = \sum_{l=0}^{+\infty} h_{ij}(l) e^{-\mathbf{j}\omega l}, \qquad (12)$$

and let $\bar{\mathbf{h}}_j(\omega) = [\bar{H}_{j1}(\omega) \ldots \bar{H}_{jK}(\omega)]^T$ whence follows the definition of *information* DTF (ιDTF) from j to i as

$$\iota\gamma_{ij}(\omega) = \frac{\bar{H}_{ij}(\omega) \rho_{jj}^{1/2}}{\sqrt{\bar{\mathbf{h}}_j^H(\omega) \boldsymbol{\Sigma}_{\mathbf{w}} \bar{\mathbf{h}}_j(\omega)}}, \qquad (13)$$

where ρ_{jj} is the variance of the partialized innovation process $\zeta_j(n) = w_j(n) - \mathbb{E}[w_j(n)/\{w_l(n), \ l \neq j\}]$ given explicitly by

$$\rho_{jj} = \sigma_{jj} - \sigma_{j\cdot} \boldsymbol{\Sigma}_{\cdot\cdot}^{-1} \sigma_{j\cdot}^T,$$

where $\sigma_{j\cdot}$ is the vector of covariances for innovations $\mathbf{w}^j(n) = [w_{l_1}(n) \ldots w_{l_{K-1}}(n)]^T$ where $\{l_1, \ldots, l_{K-1}\} = \{1, \ldots, K\} \setminus \{j\}$ and $\boldsymbol{\Sigma}_{\cdot\cdot}$ is the covariance matrix of $\mathbf{w}^j(n)$.

When $\boldsymbol{\Sigma}_{\mathbf{w}}$ is the identity matrix, (13) reduces to the original DTF from Kaminski and Blinowska (1991). Also when $\boldsymbol{\Sigma}_{\mathbf{w}}$ is a diagonal matrix with distinct elements (13) reduces to directed coherence as defined in Baccalá et al. (1999).

For this new quantity, a result analogous to Theorem 1 holds.

Theorem 2 *Let the K-variate wide sense stationary time series $\mathbf{x}(n) = [x_1(n) \ldots x_K(n)]^T$ satisfy (11), then*

$$\iota\gamma_{ij}(\omega) = C_{x_i \zeta_j}(\omega), \qquad (14)$$

where ζ_j is the previously defined partialized innovation process.

Corollary 2 *Let the K-variate Gaussian stationary time series $\mathbf{x}(n) = [x_1(n) \ldots x_K(n)]^T$ satisfy (11), then*

$$\text{MIR}(x_i, \zeta_j) = -\frac{1}{4\pi} \int_{-\pi}^{\pi} \log(1 - |\iota\gamma_{ij}(\omega)|^2) d\omega. \qquad (15)$$

An important remark is that (7)/(14) hold for wide-sense stationary processes, respectively, with a autoregressive/ moving average representations and that the Gaussianity requirement is unnecessary for their validity.

Also the integrands in (8) and (15) are readily interpretable as mutual information rates at each frequency.

4 Illustrative example

Through the following simple accretive example, It is possible to explicitly expose the nature of (7):

$$\begin{bmatrix} x_1(n) \\ x_2(n) \end{bmatrix} = \begin{bmatrix} 0 & 0 \\ \alpha & 0 \end{bmatrix} \begin{bmatrix} x_1(n-1) \\ x_2(n-1) \end{bmatrix} + \begin{bmatrix} w_1(n) \\ w_2(n) \end{bmatrix}, \qquad (16)$$

where $\mathbb{E}[w_i(n) w_j(m)] = \delta_{nm} \delta_{ij}$, for $m, n \in \mathbb{Z}$ and $i, j \in \{1, 2\}$ with δ_{pq} standing for the usual Kronecker delta symbol.

Clearly, $\iota\pi_{12}(\omega) = 0$ and

$$\iota\pi_{21}(\omega) = \frac{-\alpha e^{-\mathbf{j}\omega}}{\sqrt{1 + \alpha^2}}.$$

To obtain $C_{w_1 \eta_2}(\omega)$ using the fact that

$$\mathbf{s}_{21}(\omega) \mathbf{S}_{11}^{-1}(\omega) = \alpha e^{-\mathbf{j}\omega}$$

implies $\eta_2(n) = x_2(n) - \alpha x_1(n-1) = w_2(n)$ so that $C_{w_1 \eta_2}(\omega) = 0$, and hence $\iota\pi_{12}(\omega) = C_{w_1 \eta_2}(\omega)$.

Now to compute $C_{w_2 \eta_1}(\omega)$, one must use the spectral density matrix of $[x_1 \ x_2]^T$ given by

$$\begin{bmatrix} S_{x_1 x_1}(\omega) & S_{x_1 x_2}(\omega) \\ S_{x_2 x_1}(\omega) & S_{x_2 x_2}(\omega) \end{bmatrix} = \begin{bmatrix} 1 & \alpha e^{\mathbf{j}\omega} \\ \alpha e^{-\mathbf{j}\omega} & 1 + \alpha^2 \end{bmatrix},$$

leading to the optimum filter

$$\mathbf{G}_1(\omega) = \mathbf{s}_{12}(\omega)\mathbf{S}_{22}^{-1}(\omega) = \frac{\alpha}{1+\alpha^2}e^{\mathbf{j}\omega}$$

for $\mathbb{E}[x_1(n)/\{x_2(m),\ m \in \mathbb{Z}\}]$. It is noncausal and produces $\frac{\alpha}{1+\alpha^2}x_2(n+1)$ so that

$$\eta_1(n) = x_1(n) - \frac{\alpha}{1+\alpha^2}x_2(n+1).$$

Since $x_1(n) = w_1(n)$ and $x_2(n) = \alpha w_1(n-1) + w_2(n)$,

$$\eta_1(n) = w_1(n)\frac{1}{1+\alpha^2} - w_2(n+1)\frac{\alpha}{1+\alpha^2},$$

which leads to

$$S_{w_2\eta_1}(\omega) = \frac{-\alpha e^{-\mathbf{j}\omega}}{1+\alpha^2}$$

and

$$S_{\eta_1}(\omega) = \frac{1}{1+\alpha^2}$$
$$S_{w_2}(\omega) = 1,$$

showing that

$$C_{w_2\eta_1}(\omega) = \frac{-\alpha e^{-\mathbf{j}\omega}}{\sqrt{1+\alpha^2}}$$

confirms that $\iota\pi_{21}(\omega) = C_{w_2\eta_1}(\omega)$ via direct computation of the Fourier transforms of the covariance/cross-covariance functions involving w_2 and η_1.

It is easy to verify that $\zeta_i(n) = w_i(n)$ so that direct computations also confirm ιPDC and ιDTF equality in the $K = 2$ case (Baccalá and Sameshima 2001b) when $\mathbf{\Sigma}$ is the identity matrix.

Let model (16) be enlarged by including a third observed variable

$$x_3(n) = \beta x_2(n-1) + w_3(n), \tag{17}$$

where $w_3(n)$ is zero mean unit variance Gaussian and orthogonal to $w_1(n)$ and $w_2(n)$ for all lags. This new equation means that the signal x_1 has an indirect path to x_3 via x_2 but no direct means of reaching x_3.

For this augmented model, the following joint moving average representation holds

$$\begin{bmatrix} x_1(n) \\ x_2(n) \\ x_3(n) \end{bmatrix} = \begin{bmatrix} w_1(n) \\ w_2(n) \\ w_3(n) \end{bmatrix} + \begin{bmatrix} 0 & 0 & 0 \\ \alpha & 0 & 0 \\ 0 & \beta & 0 \end{bmatrix} \begin{bmatrix} w_1(n-1) \\ w_2(n-1) \\ w_3(n-1) \end{bmatrix}$$
$$+ \begin{bmatrix} 0 & 0 & 0 \\ 0 & 0 & 0 \\ \alpha\beta & 0 & 0 \end{bmatrix} \begin{bmatrix} w_1(n-2) \\ w_2(n-2) \\ w_3(n-2) \end{bmatrix},$$

which produces

$$\iota\gamma_{21}(\omega) = \frac{\alpha e^{-\mathbf{j}\omega}}{\sqrt{1+\alpha^2}},$$
$$\iota\gamma_{32}(\omega) = \frac{\beta e^{-\mathbf{j}\omega}}{\sqrt{1+\beta^2+\alpha^2\beta^2}},$$
$$\iota\gamma_{31}(\omega) = \frac{\alpha\beta e^{-2\mathbf{j}\omega}}{\sqrt{1+\beta^2+\alpha^2\beta^2}}, \tag{18}$$

and $\iota\gamma_{kl} = 0$ for $l > k$ by direct computation using (13). To verify (14), one obtains $\zeta_i = w_i$ since the w_i innovations are uncorrelated leading to

$$S_{x_2\zeta_1}(\omega) = \alpha, \qquad S_{x_3\zeta_2}(\omega) = \beta e^{-\mathbf{j}\omega},$$
$$S_{x_3\zeta_1}(\omega) = \alpha\beta e^{-2\mathbf{j}\omega}, \qquad S_{x_2x_2}(\omega) = 1+\alpha^2,$$
$$S_{x_3x_3}(\omega) = 1+\beta^2+\alpha^2\beta^2, \quad S_{\zeta_1\zeta_1}(\omega) = 1 = S_{\zeta_2\zeta_2}(\omega),$$

wherefrom $\iota\gamma_{21}(\omega) = C_{x_2\zeta_1}(\omega)$, $\iota\gamma_{32}(\omega) = C_{x_3\zeta_2}(\omega)$, and $\iota\gamma_{31}(\omega) = C_{x_3\zeta_1}(\omega)$.

One may compute this model's PDCs

$$\iota\pi_{21}(\omega) = \frac{-\alpha e^{-\mathbf{j}\omega}}{\sqrt{1+\alpha^2}},$$
$$\iota\pi_{32}(\omega) = \frac{-\beta e^{-\mathbf{j}\omega}}{\sqrt{1+\beta^2}},$$
$$\iota\pi_{31}(\omega) = 0,$$

either via (6), or via Theorem 1.

This exposes the fact that the augmented model's direct interaction is represented by PDC, whereas DTF from x_1 to x_3 (18) is zero if either α or β is zero. This means that a signal pathway leaving x_1 reaches x_3 so that DTF therefore represents the net directed effect of x_1 onto x_3 as in fact previously noted in Baccalá and Sameshima (2001a).

5 Discussion

In their *information* forms, both PDC and DTF represent true coherences and thus constitute complete alternative descriptions of the dynamic relations involving the observed vector time series $\mathbf{x}(n)$ and $\mathbf{w}(n)$, the innovations vector process, or its orthogonalized version $\mathbf{\zeta}(n)$, which summarize the stochastic novelty after stripping all mutual correlations present in $\mathbf{x}(n)$.

DTF can be thought of as a forward description for it depicts how $\mathbf{\zeta}(n)$ affect the $\mathbf{x}(n)$ observations, whereas PDC describes how $\mathbf{w}(n)$ relates to $\mathbf{\eta}(n)$ which is obtained by the mutual partialization of the components of $\mathbf{x}(n)$. Thus, $\eta_i(n)$ essentially excludes those redundancies in $x_i(n)$ that can be attributed to the other $x_j(n)$ ($j \neq i$). This redundancy extraction by direct analogy with linear algebraic procedures gives rise to $\{\eta_j, j = 1, \ldots, K\}$ as a *dual* (also frequently

termed *reciprocal*) basis to the $\{x_i, i = 1, \ldots, K\}$ basis as its elements η_i are orthogonal to all x_j for $i \neq j$. It is in this precise sense that PDC's description is dual to DTF's—they map the innovations onto dual representations of the observed dynamics.

A question that may come to mind is: how can DTF (PDC) being related to mutual information, a recognizably reciprocal quantity, are able to describe unreciprocal aspects of the interaction between time series? The answer lies in that they relate the x_i (η_i) to innovations ζ_j (w_j) so that permuting i and j describes the relationship between distinct inner component subprocesses. As such, for example, in the case of PDC, $\mathrm{MIR}(w_i, \eta_j)$ (for $|\iota\pi_{ij}(\omega)|^2$) and $\mathrm{MIR}(w_j, \eta_i)$ (for $|\iota\pi_{ji}(\omega)|^2$) are not equal in general as opposed to

$$\mathrm{MIR}(w_i, \eta_j) = \mathrm{MIR}(\eta_j, w_i) \tag{19}$$

whose equality always holds because $|\iota\pi_{ij}(\omega)|^2 = |\iota\pi_{ij}^*(\omega)|^2$ where $*$ denotes complex conjugation. In other words, index permutation in PDC entails comparing different underlying intrinsic component processes. A similar result holds for DTF.

Another point is why PDC/DTF are related to Granger causality. This is so because the inherent decorrelation $\mathbb{E}\left[w_i(n)w_j(m)\right] = 0$ for all i, j provided that $n \neq m$ introduces the necessary time asymmetry to allow their causal interpretations. Also observe that by definition of innovation, time asymmetry is an automatic consequence of $w_i(n)$'s uncorrelation to $\eta_j(k)$ for $k < n$. The same holds for $\zeta_j(n)$ which is uncorrelated with $x_i(k)$ for $k \leq n$.

Though left to the Appendix, the proof of Theorem 1 reveals an interesting aspect, namely Eq. 26 that allows interpreting $\bar{A}_{ij}(\omega)$ (5) as a transfer function from η_j to w_i. This observation sheds light on Schelter et al. (2009)'s employment of a studentized version of $\bar{A}_{ij}(\omega)$ in characterizing the relationship between $\mathbf{x}(n)$ components. Similar observations hold for the $\bar{H}_{ij}(\omega)$, whose magnitude has been used by Blinowska et al. (2010).

PDC and DTF are not alone as attempts to describe information flow between multivariate time series. To discuss these ideas, one must also mention the efforts of Geweke (1982) and Hosoya (1991). Though delving into detailed and specific comparative aspects of their proposals vis-à-vis those described herein is beyond our intended scope and is planned for future publications, it is perhaps reassuring to note when just time series pairs are considered ($K = 2$) all of the latter frequency domain measures coalesce into one and the same measure.

As a matter of fact, for $K = 2$, it is possible to show that

$$|\iota\pi_{ij}(\omega)|^2 = |\iota\gamma_{ij}(\omega)|^2 = 1 - e^{-\mathrm{f}_{j\to i}(\omega)} = 1 - e^{-\mathrm{M}_{j\to i}(\omega)} \tag{20}$$

for ($i, j \in \{1, 2\}$), where $\mathrm{f}_{j\to i}(\omega)$ and $\mathrm{M}_{j\to i}(\omega)$ describe, respectively, Geweke's and Hosoya's frequency domain
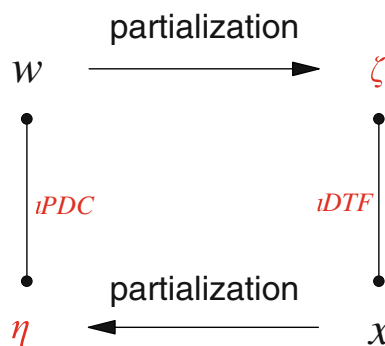
Fig. 1 The diagram summarizes the relationship between the various descriptive processes associated with the original observations $\mathbf{x}$ including the innovations process $\mathbf{w}$ and their respective partialized versions $\boldsymbol{\eta}$ and $\boldsymbol{\zeta}$. The mutual information rate relationships are described by ιPDC for ($\boldsymbol{\eta}$,$\mathbf{w}$) and ιDTF for ($\boldsymbol{\zeta}$,$\mathbf{x}$). Information flow sources are indexed among the greek type face vector components and the information receiving structures are chosen among the components of the latin type face processes

causal measures in their own notation (the arrow shows the direction information flow). Furthermore, when it comes to testing for the null hypothesis of Granger causality when $K = 2$, it is straightforward to verify the equivalence of the following statements:

1. There is no Granger causality from x_j to x_i.
2. $\mathrm{MIR}(x_i, \zeta_j) = 0$.
3. $\mathrm{MIR}(w_i, \eta_j) = 0$.
4. $|\iota\pi_{ij}(\omega)|^2 = 0, \ \forall\omega \in [-\pi, \pi)$.
5. $|\iota\gamma_{ij}(\omega)|^2 = 0, \ \forall\omega \in [-\pi, \pi)$.
6. $\mathrm{f}_{j\to i}(\omega) = 0, \ \forall\omega \in [-\pi, \pi)$.
7. $\mathrm{M}_{j\to i}(\omega) = 0, \ \forall\omega \in [-\pi, \pi)$.
8. $\bar{A}_{ij}(\omega) = 0, \ \forall\omega \in [-\pi, \pi)$.
9. $\bar{H}_{ij}(\omega) = 0, \ \forall\omega \in [-\pi, \pi)$.

Which of the above statements is more convenient depends on criteria like knowledge of precise asymptotic statistics and test power. In fact, precise results of this kind for the general $K > 2$ case, that also include asymptotic confidence intervals, are known for $|\iota\pi_{ij}(\omega)|^2$ and are being prepared for submission.

Though time domain considerations are strictly outside our scope, they are required to fully understand the difference between the various measures (Takahashi 2009) and underlie the difficulties of generalizing Geweke's and Hosoya's proposals to $K > 2$ as attempted, respectively, in Geweke (1984) and Hosoya (2001) while keeping a consistent interpretation of information flow in association with Granger causality.

A summary of the relationships between the underlying processes addressed in this article is portrayed in Fig. 1.

Finally, it should be noted that iPDC, as herein defined, provides an absolute signal scale invariant measure of

direct connectivity strength between observed time series as opposed to either PDC or gPDC that provide only relative coupling assessments.

6 Conclusion

New properly weighted multivariate directed dependence measures between stochastic processes that generalize PDC and DTF have been introduced and their relationship to mutual information has been spelled out in terms of more fundamental adequately partialized processes. These results enlighten the relationship of formerly available connectivity measures and the notion of information flow. Theorem 1 is a novel result. For bivariate time series, results similar to Theorem 2 have appeared several times in the literature in association with Geweke's measure of directed dependence Geweke (1982). The ιDTF introduced herein is novel and constitutes a proper generalization of Geweke's result for the multivariate setting while ιPDC's result (also novel) is its dual.

The present results not only introduce a unified framework to understand connectivity measures, but also open new generalization perspectives in nonlinear interaction cases for which information theory seems to be the natural study toolset.

A Appendix

A.1 Proof of Theorem 1 and Corollary 1

Before proving Theorem 1 consider the following lemma:

Lemma 1 *Let $\mathbf{S_x}(\omega)$ be the power spectral density matrix of the stationary K-variate time series $\mathbf{x}(n)$ obeying (4). Then*

$$\bar{\mathbf{a}}_j(\omega)^H \Sigma_{\mathbf{w}}^{-1} \bar{\mathbf{a}}_j(\omega) = \mathbf{S}_{\eta_j \eta_j}^{-1}(\omega). \tag{21}$$

holds.

Proof One may rewrite (5) in matrix form as

$$\bar{\mathbf{A}}(\omega) = \mathbf{I} - \sum_{l=1}^{+\infty} \mathbf{A}(l) e^{-\mathbf{j}\omega l}, \tag{22}$$

where $\mathbf{I}$ is the $K \times K$ identity matrix.

Because (4) holds, the inverse of the $\mathbf{x}$ may be written as

$$\mathbf{S_x}^{-1}(\omega) = \bar{\mathbf{A}}(\omega)^H \Sigma_{\mathbf{w}}^{-1} \bar{\mathbf{A}}(\omega). \tag{23}$$

each of whose elements $[\cdot]_{jj}$

$$\left[\mathbf{S_x}^{-1}(\omega) \right]_{jj} = \left(S_{x_j x_j}(\omega) - \mathbf{s}_{x_j \mathbf{x}^j}(\omega) \mathbf{S}_{\mathbf{x}^j \mathbf{x}^j}^{-1}(\omega) \mathbf{s}_{\mathbf{x}^j x_j}(\omega) \right)^{-1},$$

follows from the partitioned matrix inversion formula (see e.g. the appendix in Lütkepohl (1993)) which equals

$$S_{\eta_j \eta_j}^{-1}(\omega) = \bar{\mathbf{a}}_j^H(\omega) \Sigma_{\mathbf{w}}^{-1} \bar{\mathbf{a}}_j(\omega) \tag{24}$$

by direct computation of $\left[\mathbf{S_x}(\omega)^{-1} \right]_{jj}$ from (23). $\quad\square$

Lemma 1 allows rewriting (6) as

$$\iota\pi_{ij}(\omega) = \bar{A}_{ij}(\omega) \sigma_{ii}^{-1/2} \sqrt{S_{\eta_j \eta_j}(\omega)}.$$

Hence to prove Theorem 1 all one must show is that

$$\begin{aligned} C_{w_i \eta_j}(\omega) &\triangleq \frac{S_{w_i \eta_j}(\omega)}{\sqrt{S_{w_i w_i}(\omega) S_{\eta_j \eta_j}(\omega)}} \\ &= \bar{A}_{ij}(\omega) \sigma_{ii}^{-1/2} \sqrt{S_{\eta_j \eta_j}(\omega)}. \end{aligned} \tag{25}$$

Since

$$S_{w_i w_i}(\omega) = \sigma_{ii},$$

proving (25) reduces to showing

$$\bar{A}_{ij}(\omega) = \frac{S_{w_i \eta_j}(\omega)}{S_{\eta_j \eta_j}(\omega)}. \tag{26}$$

By straightforward computation with help of (10)

$$S_{w_i \eta_j}(\omega) = \sum_{l=1}^{K} \bar{A}_{il}(\omega) \left\{ S_{x_l x_j}(\omega) - \mathbf{s}_{x_j \mathbf{x}^j}(\omega) \mathbf{S}_{\mathbf{x}^j \mathbf{x}^j}^{-1}(\omega) \mathbf{s}_{x_l \mathbf{x}^j}(\omega) \right\}.$$

whose right-hand side can be broken as

$$\bar{A}_{ij}(\omega) S_{\eta_j \eta_j}(\omega) + \\ \sum_{\substack{l=1 \\ l \neq j}}^{K} \bar{A}_{il}(\omega) \left\{ S_{x_l x_j}(\omega) - \mathbf{s}_{x_j \mathbf{x}^j}(\omega) \mathbf{S}_{\mathbf{x}^j \mathbf{x}^j}^{-1}(\omega) \mathbf{s}_{x_l \mathbf{x}^j}(\omega) \right\}. \tag{27}$$

which simplifies to

$$S_{w_i \eta_j}(\omega) = \bar{A}_{ij}(\omega) S_{\eta_j \eta_j}(\omega)$$

as the partialized process η_j is orthogonal to $\mathbf{x}^j$ by construction, i.e.

$$S_{x_l x_j}(\omega) - \mathbf{s}_{x_j \mathbf{x}^j}(\omega) \mathbf{S}_{\mathbf{x}^j \mathbf{x}^j}^{-1}(\omega) \mathbf{s}_{x_l \mathbf{x}^j}(\omega) = 0, \quad \forall l \neq j, \quad \omega \in [-\pi, \pi]. \tag{28}$$

thereby concluding the proof.

When w_i and η_j are stationary Gaussian, Corollary 1 is a direct consequence of applying the following.

Theorem 3 (Gelfand and Yaglom 1959) *Let x and y be jointly Gaussian stationary time series. Assume that*

$$\mathbb{E}[w_x(n) w_y(n)]^2 < \mathbb{E}[w_x^2(n)] \mathbb{E}[w_y^2(n)],$$

where $w_x(n)$ and $w_y(n)$ are the innovations associated to x and y. Then the following equality holds:

$$MIR(x, y) = -\frac{1}{4\pi} \int_{-\pi}^{\pi} \log(1 - |C_{xy}(\omega)|^2)d\omega, \qquad (29)$$

when w_i and η_j are both jointly stationary Gaussian.

A.2 Proof of Theorem 2 and Corollary 2

To prove Theorem 2 recall that by definition

$$C_{x_i \zeta_j}(\omega) = \frac{S_{x_i \zeta_j}(\omega)}{\sqrt{S_{x_i x_i}(\omega) S_{\zeta_j \zeta_j}(\omega)}}.$$

and that

$$S_{\zeta_j \zeta_j}(\omega) = \rho_{jj}.$$

Therefore, it suffices to show that

$$\frac{\bar{H}_{ij}(\omega)}{\sqrt{\bar{\mathbf{h}}_j^H(\omega) \boldsymbol{\Sigma}_{\mathbf{w}} \bar{\mathbf{h}}_j(\omega)}} = \frac{S_{x_i \zeta_j}(\omega)}{\sqrt{S_{x_i x_i}(\omega)}}. \qquad (30)$$

By the existence of the moving average representation (11)

$$S_{x_i x_i}(\omega) = \bar{\mathbf{h}}_j^H(\omega) \boldsymbol{\Sigma}_{\mathbf{w}} \bar{\mathbf{h}}_j(\omega). \qquad (31)$$

Also, by the existence of moving average representation (11) and the orthogonality of the partialized innovation process ζ_j with respect to the innovations w_l, $l \neq j$, it follows that

$$S_{x_i \zeta_j}(\omega) = \bar{H}_{ij}(\omega).$$

and this concludes the proof.

Corollary 2 follows immediately from Theorems 2 and 3.

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