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Frequency Domain Connectivity: an Information Theoretic Perspective

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Abstract— **This paper addresses the relationship between Partial Directed Coherence (PDC) and Directed Transfer Function (DTF), popular multivariate connectivity measures employed in neuroscience, and information flow as quantified by mutual information rate.**

I. INTRODUCTION

Neuroscience has witnessed an important paradigm change over the last decade or so. Associated with the rapid advancement in multichannel data acquisition technology, there has been a growing realization that the inner workings of the brain can only be grasped by a detailed description of how brain areas interact functionally. This came to be generally referred as the study of brain connectivity. This new scenario stands in sharp contrast to former longstanding approaches whereby the goal was that of merely identifying which brain areas were involved in specific functions.

Thus, a large array of 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 [1], [2], [3], [4]. Among the available methods, we introduced and developed the idea of *partial directed coherence* (PDC)[5], [6] 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 in 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 (GC) 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 $(i \neq j)$ [7].

In fact, multivariate Granger causality tests as described in [8] map directly onto statistical tests for PDC nullity. Like Granger causality, and as opposed to ordinary coherence [9], PDC is a directional quantity; this fact lead 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.

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The appeal of associating PDC with information flow has been strong, as we have used it ourselves [5], [6]. This suggestion has nonetheless remained vague and to some extent almost apocryphal. The aim of this paper is correct this state of affairs by making 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 [1], whose information theoretic interpretation is also addressed here for the sake of completeness.

This paper is organized as follows: in Sec. II we provide some explicit information theoretic background leaving the main result to Sec. III followed by illustrations and comments in Sec. IV and V respectively.

II. 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 $\mathrm{MIR}(x, y)$ by means of comparing their joint probability density with the product of their marginals:

$$\mathrm{MIR}(x,y) = \lim_{m\to\infty} \frac{1}{m+1}\mathbb{E}\left[\log \frac{\mathrm{d}\mathbb{P}(x(1),\dots,x(m),y(1),\dots,y(m))}{\mathrm{d}\mathbb{P}(x(1),\dots,x(m))\mathrm{d}\mathbb{P}(y(1),\dots,y(m))}\right] \tag{1}$$

where $\mathbb{E}[\cdot]$ is the expectation with respect to the joint measure of x and y and where $\mathrm{d}\mathbb{P}$ 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 [10], relates (1) to the coherence between the processes via

$$\mathrm{MIR}(x,y) = -\frac{1}{4\pi}\int_{-\pi}^{\pi} \log(1 - |\mathrm{C}_{xy}(\omega)|^2)d\omega, \tag{2}$$

where the coherence is given by

$$\mathrm{C}_{xy}(\omega) = \frac{S_{xy}(\omega)}{\sqrt{S_{xx}(\omega)S_{yy}(\omega)}}, \tag{3}$$

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 $\mathrm{MIR}(x, y)$.

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

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

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

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. From the coefficients $a_{ij}(l)$ of $\mathbf{A}(l)$ we may write

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

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

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

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

where $\sigma_{jj} = \mathbb{E}\left[w_j^2(n)\right]$ and which simplifies to the originally defined PDC when $\mathbf{\Sigma_w}$ equals the identity matrix. Note also that the generalized PDC (gPDC) from [11] is obtained if $\mathbf{\Sigma_w}$ is a diagonal matrix whose elements are distinct.

Before stating the main result, note that to our knowledge, mention of (6) [12] has not appeared in the literature with any explicit association with information theoretic ideas.

III. RESULTS

A. PDC

Theorem 1: Let the K-dimensional Gaussian stationary time series $\mathbf{x}(n) = [x_1(n) \ldots x_K(n)]^T$ satisfying (4), then

$$\iota\pi_{ij}(\omega) = \mathbf{C}_{w_i\eta_j}(\omega), \tag{7}$$

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_i given the remaining time series. Moreover,

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

To obtain the process η_k, it is worth remembering 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

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

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 $\mathbf{s}_{x_k\mathbf{x}^k}(\lambda)$ is the $K-1$-dimensional vector whose entries are the cross spectra between x_k and the remaining $K-1$ processes, and $\mathbf{S}_{\mathbf{x}^k\mathbf{x}^k}(\lambda)$ 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 $\mathbf{x}^k$ [9].

Note that

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

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 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. Its formal proof is omitted due to space limitations but can be found in [13]. The main idea behind it is to prove (7) so that (8) follows by use of (2) to produce MIR(w_i, η_j).

B. DTF

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

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

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

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

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

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

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

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

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

When $\mathbf{\Sigma_w}$ is the identity matrix, (13) reduces to the original DTF [1]. Also when $\mathbf{\Sigma_w}$ is a diagonal matrix with distinct elements (13) reduces to directed coherence (DC) as defined in [14].

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

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

$$\iota\gamma_{ij}(\omega) = \mathbf{C}_{x_i\zeta_j}(\omega), \tag{14}$$

where ζ_j is the previously defined partialized innovation process.

Because (14) is the coherence between Gaussian processes,

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

also holds.

The proof of Theorem 2 may be found in [13].

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. The Theorems refer to Gaussian processes for simplicity and because the validity of identities (8) and (15) rest on this assumption.

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

IV. ILLUSTRATIVE EXAMPLE

Via 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 $\mathbb{E}[w_i(n)w_j(m)] = \delta_{n,m}\delta_{i,j}$, for $m, n \in \mathbb{Z}$ and $i, j \in \{1, 2\}$.

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

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

To obtain $\mathbf{C}_{w_1\eta_2}(\omega)$ 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 $\mathbf{C}_{w_1\eta_2}(\omega) = 0$, and hence $\iota\pi_{12}(\omega) = \mathbf{C}_{w_1\eta_2}(\omega)$.

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

$$\begin{bmatrix} S_{x_1x_1}(\omega) & S_{x_1x_2}(\omega) \\ S_{x_2x_1}(\omega) & S_{x_2x_2}(\omega) \end{bmatrix} = \begin{bmatrix} 1 & \alpha e^{\mathbf{j}\omega} \\ \alpha e^{-\mathbf{j}\omega} & 1+\alpha^2 \end{bmatrix},$$

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 iPDC and iDTF equality in the $K = 2$ case (see [5]) when $\mathbf{\Sigma}$ is the identity matrix.

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

$$x_3(n) = \beta x_2(n-1) + w_3(n) \qquad (17)$$

where $w_3(n)$ is zero mean unit variance Gaussian and orthogonal to the other $w_k(n)$, $1 \le k \le 2$ 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

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

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

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

wherefrom $\iota\gamma_{21}(\omega) = \mathrm{C}_{x_2\zeta_1}(\omega)$, $\iota\gamma_{32}(\omega) = \mathrm{C}_{x_3\zeta_2}(\omega)$ and $\iota\gamma_{31}(\omega) = \mathrm{C}_{x_3\zeta_1}(\omega)$ using (14).

One may compute this model's PDCs

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

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 only zero if either α or β is zero which 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 [6].

V. FINAL COMMENTS

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 [15]. The iDTF introduced herein is novel and constitutes a proper generalization of Geweke's result for the multivariate setting while iPDC´s result is its dual. Observe that previous attempts to use Geweke's approach in the multivariate setting [16] have been fruitless in providing clear information theoretical interpretations.

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.

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