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A dynamic regression approach for frequency-domain partial coherence and causality analysis of functional brain networks

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Abstract

Coherence and causality measures are often used to analyze the influence of one region on another during analysis of functional brain networks. The analysis methods usually involve a regression problem where the signal of interest is decomposed into a mixture of regressor and a residual signal. In this paper, we revisit this basic problem and present solutions that provide the minimal-entropy residuals for different types of regression filters, such as causal, instantaneously causal and noncausal filters. Using optimal prediction theory, we derive several novel frequency-domain expressions for partial coherence, causality and conditional causality analysis. In particular, our solution provides a more accurate estimation of the frequency-domain causality compared to the classical Geweke causality measure. Using synthetic examples and in vivo resting-state functional magnetic resonance imaging (rsfMRI) data from the Human Connectome Project (HCP), we show that the proposed solution is more accurate at revealing frequency-domain linear dependence among high dimensional signals.

I. Introduction

Assessing the functional connectivity of brain networks using techniques such as rsfMRI and magnetoencephalography (MEG) is a problem of significant importance in neuroscience [1], [2], [3]. A basic approach is to estimate the correlation between the measured signals from two different regions that represents the neural activity (directly as in MEG or indirectly as in fMRI) of those regions. Since the signals from the two regions of interest (ROI's) may be influenced by other external factors, a direct correlation may not reflect the true intrinsic functional connectivity of the two ROI's. Consequently, partial correlation analysis is often used to estimate functional connectivity in such scenarios [4], [5], [6]. The main idea behind partial correlation is to regress-out the influence of other external factors, such as other brain regions, from the signal of interest and subsequently compute the correlation between the intrinsic signals of interest. This concept has numerous applications and has been extended to analyze the dynamical dependence of time series data as a function of frequency [7], [8]. It is also closely related to the concept of Granger and Geweke causality and conditional causality [9], [10], [11], which quantifies the dynamical linear dependence between measurements from different brain regions [12], [13].

Moreover, oscillatory brain activity may lead to predictable patterns in imaging measures at different frequencies. Thus, frequency-domain partial coherence and causality analysis could provide more specific information about the temporal dependence of signals from different

brain regions. There are several classical methods for frequency-domain partial coherence and causality analysis approaches, which are typically computed based on the power spectral density (PSD) function of multivariate time series [14], [9], [10]. For example, the Geweke linear dependence measure (a.k.a. causality measure) [10] has been widely utilized for understanding the dynamical linear dependence between brain functional imaging measures. But, we note that the frequency-domain Geweke causality measure was not derived based on any physical principle for measuring the linear dependence between measurements from brain functional activity. Thus, it does not properly capture the expected linear dependence between signals at different frequencies, which we show mathematically and experimentally in our work.

In this paper, we revisit the partial coherence, causality and conditional causality analysis methods in a general dynamic regression framework and derive several novel frequency domain measures. In the proposed framework, the signals from regions of interest are decomposed into two terms; one term represents influences from other signals, i.e. the regressors, and the residuals are the intrinsic signals of the ROI's. Using optimal prediction theory [15], [16], [17], [18] we obtain an optimal prediction filter for such a decomposition by minimizing the entropy of the residual signal. Three different types of filters are investigated: i) strictly causal, ii) instantaneously causal, iii) noncausal filters, and separate frequency domain expressions are derived for each of these cases to compute the partial coherence, causality and conditional causality between two time series data sets. By generalizing the standard concepts of partial correlation and model fitness measures from linear regression problems, we derive several novel frequencydomain partial coherence, causality and partial causality measures. In particular, we note that the classical Geweke causality measure introduced in [10] is not a measure of model fitness. Hence, it does not accurately capture the linear dependence of signals at different frequencies. We also compared the proposed methods with exiting approaches using two synthetic examples with known causal dependence among variables and 100 rsfMRI data sets from the Human Connectome Project (HCP). In both cases, our experimental results demonstrate that the proposed frequency domain measures are better able to capture the expected frequency-domain profiles of dynamic linear dependence among the variables.

II. Theory

A. Correlation and partial correlation analysis

Correlation analysis is widely used in rsfMRI with applications in percolation and network analysis [19], [20], [21]. Here, we give a brief primer on the standard static correlation (no temporal dynamics used) and partial correlation analysis. Some of the basic concepts will be generalized for analyzing the dynamic relations between time series. Consider a n -dimensional zero-mean stationary process $\{\mathbf{u}(t)\}_{t \in \mathbb{Z}}$ with $\mathbf{u}(t) \in \mathbb{R}^n$, which represents brain functional activity measurements from n ROI's. Let $R_{uu} = \mathcal{E}(\mathbf{u}(t)\mathbf{u}(t)')$ denote the covariance matrix of $\mathbf{u}(t)$, where $'$ denotes the transpose and $\mathcal{E}(\cdot)$ denotes the expectation operator. The correlation coefficient between the i and j -th time series is given by:

$$\rho_{ij} = \frac{R_{uu,ij}}{\sqrt{R_{uu,ii}R_{uu,jj}}}.$$

The correlation coefficient above does not reflect the true intrinsic correlation between the i -th and j -th ROIs since each of these ROIs may be influenced by other ROIs or external variables. To this end, partial correlation analysis is typically used to obtain the true correlation coefficient, which allows for removing the effect of a set of control variables. For example, we consider a decomposition of $\mathbf{u}(t)$ as $\mathbf{u}(t) = [\mathbf{x}(t)' \ \mathbf{y}(t)']'$ with $\mathbf{x}(t) \in \mathbb{R}^{n_x}$, and $\mathbf{y}(t) \in \mathbb{R}^{n_y}$ with $n_y = n - n_x$. Then the corresponding decomposition of R_{uu} can be written as:

$$R_{uu} = \begin{bmatrix} R_{xx} & R_{xy} \\ R_{yx} & R_{yy} \end{bmatrix}.$$

In order to understand the linear dependence between $\mathbf{x}$ and $\mathbf{y}$, we decompose $\mathbf{x}$ as:

$$\mathbf{x}(t) = F\mathbf{y}(t) + \tilde{\mathbf{x}}(t), \quad (1)$$

where $F \in \mathbb{R}^{n_x \times n_y}$ is the optimal prediction filter minimizing the following mean-squared-error cost function:

$$\min_F \left\{ \mathcal{E}(\|\tilde{\mathbf{x}}(t)\|^2) \mid \tilde{\mathbf{x}}(t) = \mathbf{x}(t) - F\mathbf{y}(t) \right\}, \quad (2)$$

and $\tilde{\mathbf{x}}(t)$ is the residual signal which is the intrinsic information in $\mathbf{x}$ that is not explained by the regressor. As a standard result, the optimal solution of Eq. (2) is given by $F = R_{xy}R_{yy}^{-1}$, and the covariance of $\tilde{\mathbf{x}}(t)$ is given by

$$R_{xx|y} = R_{xx} - R_{xy}R_{yy}^{-1}R_{yx}. \quad (3)$$

Thus, the partial correlation coefficient between x_i and x_j is given by:

$$\bar{\rho}_{xx|y,ij} = \frac{R_{xx|y,ij}}{\sqrt{R_{xx|y,ii}R_{xx|y,jj}}}. \quad (4)$$

In a more general form, the partial correlation between $\mathbf{u}_i$ and $\mathbf{u}_j$ conditional on all the other $n-2$ variables can be directly expressed in terms of R_{uu}^{-1} as:

$$\bar{\rho}_{ij} = -\frac{R_{uu,ij}^{-1}}{\sqrt{R_{uu,ii}^{-1}R_{uu,jj}^{-1}}}. \quad (5)$$

These expressions for partial correlation have been used extensively to analyze functional brain networks using fMRI data [4], [5].

Moreover, to assess the linear dependence of $\mathbf{x}$ on $\mathbf{y}$, a standard approach is to compare the ratio between the explained variance and total variance such as the R-squared statistical measures. An analogous measure for multivariate time series is given by $1 - \det(R_{xx|y}) / \det(R_{xx})$, which reduces to the R-squared measure for scalar $\mathbf{x}$. A similar linear dependence measure has been introduced in [10] for quantifying more causal dependences between the variables, which will be explained in more detail in the following sections.

We note that the above standard methodology for computing partial correlations has several limitations in brain functional network analysis. First, the linear regression in Eq. (2) does not remove the temporal correlations of $\mathbf{x}(t)$ and $\mathbf{y}(t)$. Second, the mean-squared-error objective function in Eq. (2) does not account for autocorrelation of the residual series $\{\tilde{\mathbf{x}}(t)\}_{t \in \mathbb{Z}}$. Since the residual process $\{\tilde{\mathbf{x}}(t)\}_{t \in \mathbb{Z}}$ may have non-zero autocorrelations, i.e. $\mathcal{E}(\tilde{\mathbf{x}}(t)\tilde{\mathbf{x}}(t-k)') \neq 0$ for some $k \neq 0$, the mean squared error is not a reasonable criterion for quantifying the uncertainty of the residual processes. Consequently, in this work, we introduce a more general dynamic regression approach that overcomes the above limitations. To generalize the partial correlation and model fitness measures, we also propose several frequency-domain partial coherence and causality measures of dynamic linear dependence between the signals. The relation between the proposed measures and related existing methods will also be discussed.

B. Dynamic filters

Dynamic regression models are widely used to analyze time series data in a variety of applications [22], [23], [24]. In this section, we briefly introduce the basic concepts along with the notations used in the remainder of this paper. First, we point out that, instead of using a static filter F as in Eq. (2), we use a dynamic regression filter. For this purpose, we let z denote the shift lag operator such that $z^k \mathbf{u}(t) = \mathbf{u}(t-k)$. For a given subset $\mathbb{K} \subset \mathbb{Z}$, we define $F(z) = \sum_{k \in \mathbb{K}} F_k z^k$, where $F_k \in \mathbb{R}^{m \times (n-m)}$ and the regression for $\mathbf{x}(t)$ is as before:

$$\mathbf{x}(t) = F(z)\mathbf{y}(t) + \tilde{\mathbf{x}}(t), \quad (6)$$

with

$$F(z)\mathbf{y}(t) = \sum_{k \in \mathbb{K}} F_k \mathbf{y}(t-k).$$

Depending on the choice of $\mathbb{K}$, we can regress out the dependence of $x(t)$ on different $y(t-k)$. In the paper, we consider three situations: when $\mathbb{K}$ is a set of $\mathbb{Z}_{++}$ (positive integers), $\mathbb{Z}_+$ (non-negative integers) and $\mathbb{Z}$, respectively. The situation when $\mathbb{K} = \mathbb{Z}_{++}$ reflects of the strictly causal dependence of $x(t)$ on the past values $y(t-k)$, for $k > 0$. Similarly, for $\mathbb{K} = \mathbb{Z}_+$ the filter becomes instantaneously causal, where the instantaneous value of $y(t)$ is used for prediction. For $\mathbb{K} = \mathbb{Z}$, the filter becomes noncausal utilizing all past and future values of $y(t)$ to predict the signal $x(t)$ at each time instant t . In the rest of this paper, we use the following terminology to refer to each of these types of filters $F(z)$: *strictly causal*, *instantaneously causal*, and *noncausal* filter, respectively.

C. Power spectral density and entropy

In this section, we give a brief primer on power spectral analysis of multivariate processes which is the basis for the proposed dynamical regression framework. Consider an arbitrary non-deterministic, zero-mean, stationary time series $\{a(t)\}_{t \in \mathbb{Z}}$ with $a(t) \in \mathbb{R}^n$. For example, $a(t)$ could represent $x(t)$, $y(t)$, or $u(t)$. Let $R_{aa}(k) := \mathcal{E}(a(t)a(t-k)^T)$ for $k \in \mathbb{Z}$ denote the autocorrelation sequence of $\{a(t)\}_{t \in \mathbb{Z}}$. The autocorrelation sequence is completely determined by its power spectral density (PSD) function $S_{aa}(\theta)$, and is related by the Fourier transform:

$$R_{aa}(k) = \int_{-\pi}^{\pi} e^{-ik\theta} S_{aa}(\theta) \frac{d\theta}{2\pi}, \quad (7)$$

where $i = \sqrt{-1}$. The PSD $S_{aa}(\theta)$ is positive semidefinite for all $\theta \in [-\pi, \pi]$. Similar to the correlation coefficient, the frequency-domain coherence measure is defined as:

$$\kappa_{ij}(\theta) = \frac{S_{aa,ij}(\theta)}{\sqrt{S_{aa,ii}(\theta)S_{aa,jj}(\theta)}}, \quad (8)$$

which quantifies the similarities between the i -th and j -th signals for all frequencies θ .

If $\log(\det S_{aa}(\theta))$ is integrable on $[-\pi, \pi]$, then $S_{aa}(\theta)$ admits a spectral factorization as [15]:

$$S_{aa}(\theta) = P_a(e^{i\theta})^{-1} \Omega_{aa} P_a(e^{i\theta})^{-*},$$

where M^* denotes the conjugate transpose of matrix M , $M^* := (M^{-1})^*$, $P_a(e^{i\theta}) = P_a(z)|_{z=e^{i\theta}}$ with $P_a(z)$ given by:

$$P_a(z) = \arg \min_{P(z)} \left\{ \mathcal{E}(\|\epsilon_a(t)\|^2) | \epsilon_a(t) = P(z) \mathbf{a}(t), \quad (9) \right.$$

$$P(z) = I_{n_a} - \sum_{k>0} P_k z^k \Big\},$$

and Ω_{aa} is the corresponding optimal one-step-ahead prediction error variance, i.e. $\Omega_{aa} = \mathcal{E}(\epsilon_a(t)\epsilon_a(t)^T)$, I_{n_a} represents the identity matrix of size $n_a \times n_a$, P_k 's are all square matrices of the same size, and $P(z)$ is a square-matrix-valued function. We note an important optimality property of the solution, that is, any other feasible $P(z)$ in Eq. (9) will necessarily have a higher error-variance in the sense of positive semi-definiteness of the matrix, i.e.,

$$\int_{-\pi}^{\pi} P(e^{i\theta}) S_{aa}(\theta) P(e^{i\theta})^* \frac{d\theta}{2\pi} \geq \Omega_{aa}, \quad (10)$$

where the equality holds only if $P(z) = P_a(z)$. The one-step-ahead prediction error variance Ω_{aa} is also directly related to the PSD $S_{aa}(\theta)$ via the Szego-Kolmogorov formula [16]:

$$\det(\Omega_{aa}) = \exp \left\{ \int_{-\pi}^{\pi} \log \det(S_{aa}(\theta)) \frac{d\theta}{2\pi} \right\}. \quad (11)$$

The entropy of a time series $\{a(t)\}_{t \in \mathbb{Z}}$ is defined as [25], [26]:

$$h(a) = \int_{-\pi}^{\pi} \log \det(S_{aa}(\theta)) \frac{d\theta}{2\pi}. \quad (12)$$

Then, from Eq. (11), we get the following expression for entropy:

$$h(a) = \log \det(\Omega_{aa}). \quad (13)$$

Thus, the entropy provides a measure of the stochastic uncertainty of a time series.

D. Minimal-entropy regression

The main purpose of partial correlation analysis of functional brain network is to regress out influencing signal from control regions and to consider the residuals as the intrinsic signal of the ROI's. Thus, the information content of the intrinsic signal should be maximally retained in the regression problem. However, the minimum mean-squared-error cost function in Section II-A does not necessarily preserve this information and also does not account for the temporal correlation of the residual $\{\tilde{x}(t)\}_{t \in \mathbb{Z}}$. On the other hand, minimizing the entropy maximizes the information content of the residual. As such, we propose to minimize the

entropy of the residual signal $\tilde{x}(t)$ to estimate the intrinsic signal of the ROI's. Consequently, we propose the following entropy minimization problem with dynamical regression filters:

$$\min_{F(z)} \left\{ h(\tilde{x}) | \tilde{x}(t) = x(t) - F(z)y(t), F(z) = \sum_{k \in \mathbb{K}} F_k z^k \right\}. \quad (14)$$

We note that if the objective function in Eq. (14) is replaced by the mean-squared-error criterion, then the solution is given by the well-known Wiener filter [22], [23]. The entropy minimization problem has a different solution than that given by the Wiener filter, but it is closely related to the optimal prediction theory. In the following, we will present solutions to Eq. (14) for the three cases when the set $\mathbb{K}$ is equal to $\mathbb{Z}_{++}$, $\mathbb{Z}_+$, and $\mathbb{Z}$, respectively.

E. Optimal filters

To introduce the optimal filters, we follow Eq. (9) and let $P_u(z)$ denote the optimal one-step-ahead prediction filter of $\{u(t)\}_{t \in \mathbb{Z}}$ and

$$P_u(z)u(t) = e_u(t) \quad (15)$$

be the corresponding innovation process. Following the decomposition $u(t) = [x(t)' \ y(t)']'$, we consider the following decomposition of Eq. (15):

$$P_{11}(z)x(t) + P_{12}(z)y(t) = e_1(t), \quad (16)$$

$$P_{21}(z)x(t) + P_{22}(z)y(t) = e_2(t), \quad (17)$$

and the corresponding decomposition of the prediction error variance matrix:

$$\Omega_{uu} = \begin{bmatrix} \mathcal{E}(e_1(t)e_1^T(t)) & \mathcal{E}(e_1(t)e_2^T(t)) \\ \mathcal{E}(e_2(t)e_1^T(t)) & \mathcal{E}(e_2(t)e_2^T(t)) \end{bmatrix} = \begin{bmatrix} \Omega_{11} & \Omega_{12} \\ \Omega_{21} & \Omega_{22} \end{bmatrix}. \quad (18)$$

From Eq. (10), Ω_{uu} is the least positive semidefinite matrix that can be obtained using an optimal one-step-ahead linear prediction filter. As a sub-block of Ω_{uu} , Ω_{11} is also the least positive definite variance of $e_1(t)$ that can be obtained using any feasible $P_{11}(z)$ and $P_{12}(z)$.

1) Partial coherence for strictly causal filter: Let $F^{\text{sc}}(z)$ denote an optimal solution to Eq. (14) when $\mathbb{K} = \mathbb{Z}_{++}$. Consider the following partition

$$S_{uu}(\theta) = \begin{bmatrix} S_{xx}(\theta) & S_{xy}(\theta) \\ S_{yx}(\theta) & S_{yy}(\theta) \end{bmatrix}.$$

Then, the PSD of the residual process $\{\tilde{x}^{sc}(t)x(t) - F^{sc}(z)y(t)\}$ is given by

$$S_{xx|y}^{sc}(\theta) = \begin{bmatrix} I_{n_x} - F^{sc}(e^{i\theta}) \\ S_{yx}(\theta) \end{bmatrix} \begin{bmatrix} S_{xx}(\theta) & S_{xy}(\theta) \\ S_{yy}(\theta) \end{bmatrix}^{-1} \begin{bmatrix} I_{n_x} \\ -F^{sc}(e^{i\theta})^* \end{bmatrix}. \quad (19)$$

We assume that $S_{uu}(\theta)$ is positive definite and bounded, which implies that $(S_{xx|y}^{sc}(\theta))$ is integrable. Thus,

$S_{xx|y}^{sc}(\theta)$ admits a factorization:

$$S_{xx|y}^{sc}(\theta) = P_{\tilde{x}}^{sc}(e^{i\theta})^{-1} \Omega_{\tilde{x}\tilde{x}}^{sc} P_{\tilde{x}}^{sc}(e^{i\theta})^{-*},$$

where $P_{\tilde{x}}(z) = I_{n_x} - \sum_{k>0} P_{\tilde{x},k} z^k$ is the optimal prediction filter for $\{\tilde{x}^{sc}(t)\}_{t \in \mathbb{Z}}$. In particular, the innovation process of $\{\tilde{x}^{sc}(t)\}_{t \in \mathbb{Z}}$ is given by:

$$\begin{aligned} \epsilon_{\tilde{x}}^{sc}(t) &= P_{\tilde{x}}^{sc}(z) \tilde{x}^{sc}(t), \\ &= P_{\tilde{x}}^{sc}(z) [x(t) - F^{sc}(z)y(t)], \end{aligned} \quad (20)$$

with $\mathcal{E}(\epsilon_{\tilde{x}}^{sc}(t) \epsilon_{\tilde{x}}^{sc}(t)^T) = \Omega_{\tilde{x}\tilde{x}}^{sc}$. From the optimality of $F^{sc}(z)$ and the definition of $h(\cdot)$ in Eq. (12), $(\Omega_{\tilde{x}\tilde{x}}^{sc})$ has the smallest value (minimal entropy) among all the solutions. On the other hand, Ω_{11} in Eq. (18) is the least positive definite matrix, and hence also has the minimum determinant. Note that, $\epsilon_{\tilde{x}}^{sc}(t)$ and $\epsilon_1(t)$ represent the same innovation process. Thus, if $P_{11}(z)$ is stably invertible, we can match the coefficients of Eqs. (20) and (16) and obtain:

$$\Omega_{\tilde{x}\tilde{x}}^{sc} = \Omega_{11}, \quad (21)$$

$$P_{\tilde{x}}^{sc}(z) = P_{11}(z), \quad (22)$$

$$F^{sc}(z) = -P_{11}^{-1}(z)P_{12}(z). \quad (23)$$

Then, the PSD of $\{\tilde{x}(t)\}_{t \in \mathbb{Z}}$ is given by:

$$S_{\mathbf{xx}|y}^{\text{sc}}(\theta) = P_{11}(e^{i\theta})^{-1} \Omega_{11} P_{11}(e^{i\theta})^{-*}. \quad (24)$$

Let

$$R_{\mathbf{xx}|y}^{\text{sc}} = \mathcal{E}(\tilde{x}^{\text{sc}}(t) \tilde{x}^{\text{sc}}(t)^T) = \int_{-\pi}^{\pi} S_{\mathbf{xx}|y}^{\text{sc}}(\theta) \frac{d\theta}{2\pi}$$

denote the covariance matrix of the residual process. Similar to Eq. (4), we define the static partial correlation coefficient between components $x_i(t)$ and $x_j(t)$ of $x(t)$ after applying the strictly causal regression as:

$$\bar{\rho}_{ij}^{\text{sc}} = \frac{R_{\mathbf{xx}|y, ij}^{\text{sc}}}{\sqrt{R_{\mathbf{xx}|y, ii}^{\text{sc}} R_{\mathbf{xx}|y, jj}^{\text{sc}}}}. \quad (25)$$

Moreover, we introduce the corresponding frequency-domain partial coherence, i.e. frequency-domain analogy of partial correlation, as follows:

$$\bar{\kappa}_{\mathbf{xx}|y, ij}^{\text{sc}}(\theta) = \frac{S_{\mathbf{xx}|y, ij}^{\text{sc}}(\theta)}{\sqrt{S_{\mathbf{xx}|y, ii}^{\text{sc}}(\theta) S_{\mathbf{xx}|y, jj}^{\text{sc}}(\theta)}}. \quad (26)$$

Moreover, if an invertible scalar filter $a(z)$ is applied to all signals in $\mathbf{u}(t)$, then the $P_{ij}(z)$ in Eqs. (16) and (17) will be scaled by $a^{-1}(z)$. Then, $S_{\mathbf{xx}|y}^{\text{sc}}$ is also scaled by a scalar function.

Thus, the partial coherence function $\bar{\kappa}_{\mathbf{xx}|y, ij}^{\text{sc}}(\theta)$ is invariant if an invertible filter is applied to all the signals. This property is particularly important in rsfMRI analysis where a temporal filter is commonly used during preprocessing. Moreover, if the linear filter $a(z)$ represents the common hemodynamic response function, then the partial coherence measure is also theoretically invariant with respect to hemodynamic response.

We note that the partial correlation measure in Eq. (25) and the partial coherence measures in (26) are parts of the novel contributions of this work. In the following, we will also introduce the corresponding results for instantaneously causal and noncausal filters. While the result for instantaneously causal filters is also our contribution, the result from the noncausal filter coincides with the commonly used frequencydomain causality measure, which dates back to the work of Granger [9].

2) Partial coherence for instantaneously causal filter: For the strictly causal filter, we regress out $y(t-k)$ for $k > 0$ from $x(t)$ to obtain $\epsilon_1(t)$. On the other hand, in the residual time series $\epsilon_2(t)$, the instantaneous value of $y(t)$ is used via the optimal filter $P_{22}(z)$ (which is

of the form $I - \sum P_{22k} z^k$). Thus, to regress-out the instantaneous value of $y(t)$ from $\epsilon_1(t)$, we only need to regress out $\epsilon_2(t)$ from $\epsilon_1(t)$. Following the derivation in [10], the time series obtained after regressing out the instantaneous value of $y(t)$ is given by:

$$\tilde{\epsilon}_1(t) = \epsilon_1(t) - \Omega_{12} \Omega_{22}^{-1} \epsilon_2(t).$$

Combining the above expression with Eqs. (16) and (17), we get:

$$\begin{aligned} \tilde{\epsilon}_1(t) &= (P_{11}(z) - \Omega_{12} \Omega_{22}^{-1} P_{21}(z))x(t) \\ &+ (P_{12}(z) - \Omega_{12} \Omega_{22}^{-1} P_{22}(z))y(t), \\ &= P_{\tilde{x}}^{\text{ic}}(z)[x(t) - F^{\text{ic}}(z)y(t)], \end{aligned} \quad (27)$$

where

$$P_{\tilde{x}}^{\text{ic}}(z) = P_{11}(z) - \Omega_{12} \Omega_{22}^{-1} P_{21}(z),$$

$$F^{\text{ic}}(z) = - (P_{11}(z) - \Omega_{12} \Omega_{22}^{-1} P_{21}(z))^{-1} (P_{12}(z) - \Omega_{12} \Omega_{22}^{-1} P_{22}(z)).$$

We note that, $P_{\tilde{x}}^{\text{ic}}(z)$ is the optimal instantaneously causal filter and has the form

$I - \sum_{k>0} P_{\tilde{x}}^{\text{ic}} z^k$, whereas $F^{\text{ic}}(z)$ is the optimal instantaneously causal regression filter of the form $\sum_{k \in \mathbb{Z}_+} F_k^{\text{ic}} z^k$. Moreover, $\tilde{\epsilon}_1(t)$ is uncorrelated with $x(t-k)$ for all $k>0$ and $y(t-\ell)$ for all $\ell \geq 0$ and has the lowest entropy with variance given by:

$$\Omega_{\tilde{x}x|y}^{\text{ic}} = \Omega_{11} - \Omega_{12} \Omega_{22}^{-1} \Omega_{21}.$$

The PSD of the residual process $\{\tilde{x}^{\text{ic}}(t) = x(t) - F^{\text{ic}}(z)y(t)\}_{t \in \mathbb{Z}}$ is given by:

$$S_{\tilde{x}x|y}^{\text{ic}}(\theta) = P_{\tilde{x}}^{\text{ic}}(e^{j\theta})^{-1} \Omega_{\tilde{x}x|y}^{\text{ic}} P_{\tilde{x}}^{\text{ic}}(e^{j\theta})^{-*}.$$

The static partial correlation ρ^{ic} and the frequency-domain partial coherence $\bar{\kappa}_{\tilde{x}x|y}^{\text{ic}}(\theta)$ can be defined analogously as in Eqs. (25) and (26), respectively.

We note that the computation of $\Omega_{\tilde{x}x|y}^{\text{ic}}$ is a standard result that has been used in the context of causality analysis [10], [27]. Our contributions are the solution for the entropy minimization problem, i.e. $F^{\text{ic}}(z)$, $S_{\tilde{x}x}^{\text{ic}}(\theta)$, and the introduction of the static partial correlation measure ρ^{ic} and frequency-domain partial coherence function $\bar{\kappa}_{\tilde{x}x|y}^{\text{ic}}(\theta)$.

3) Partial coherence for a noncausal filter: Similar to the solution of Eq. (2), the optimal noncausal filter is equal to

$$F^{nc}(e^{i\theta}) = S_{xy}(\theta)S_{yy}^{-1}(\theta),$$

which lead to the following PSD of the residual process:

$$S_{xx|y}^{nc}(\theta) = S_{xx}(\theta) - S_{xy}(\theta)S_{yy}(\theta)^{-1}S_{yx}(\theta). \quad (28)$$

The corresponding static partial correlation ρ^{nc} and the frequency-domain partial coherence $\bar{\kappa}_{xx|y}^{ic}(\theta)$ can be defined similarly as in Eqs. (25) and (26), respectively.

We note that the partial coherence between $u_i(t), u_j(t)$ after regressing other influences from other signals using noncausal filter is given by

$$\bar{\kappa}_{xx|y}^{ic}(\theta) = -\frac{S_{uu,ij}^{-1}(\theta)}{\sqrt{S_{uu,ii}^{-1}(\theta)S_{uu,jj}^{-1}(\theta)}}, \quad (29)$$

which is usually referred to as the partial coherence, which dates back to [14], [9]. It has been widely used to analyze linear dependence of time series [7], [8].

F. Revisiting Geweke causality measure

Geweke and Granger causality measures are widely used approaches in studying linear dependence among multivariate stochastic processes [9], [10]. Consider the situation of strictly causal filter as an example. Let Ω_{xx} denote the optimal prediction error variance of $x(t)$ using only its past values $\{x(t-k), k > 0\}$. Let $\Omega_{xx|y}^{sc} = \Omega_{11}$ be the prediction error variance of $x(t)$ using both the past values of $\{x(t-k), k > 0\}$ and the past values $\{y(t-k), k > 0\}$ as in Eq. (21). Then, to quantify the amount of linear feedback from $y(t)$ to $x(t)$, [10] defined the following measure:

$$g_{y \rightarrow x}^{sc} = \log \frac{\det(\Omega_{xx})}{\det(\Omega_{xx|y}^{sc})}. \quad (30)$$

Moreover, $g_{y \rightarrow x}^{sc}$ can also be written in terms of the entropy function as $g_{y \rightarrow x}^{sc} = h(x) - h(\tilde{x})$. Thus, the solution of the proposed entropy minimization problem also maximizes $g_{y \rightarrow x}^{sc}$. We note that the equivalence between the $g_{y \rightarrow x}^{sc}$ and transfer entropy has been shown in [28].

A frequency-domain extension for $g_{y \rightarrow x}^{sc}$ was also introduced in [10]. To explain this expression, we denote

$$\begin{bmatrix} P_{11}(e^{i\theta}) & P_{12}(e^{i\theta}) \\ P_{21}(e^{i\theta}) & P_{22}(e^{i\theta}) \end{bmatrix}^{-1} = \begin{bmatrix} Q_{11}(e^{i\theta}) & Q_{12}(e^{i\theta}) \\ Q_{21}(e^{i\theta}) & Q_{22}(e^{i\theta}) \end{bmatrix}.$$

Then, the following identity holds:

$$\begin{bmatrix} S_{\mathbf{x}\mathbf{x}}(\theta) & S_{\mathbf{x}\mathbf{y}}(\theta) \\ S_{\mathbf{y}\mathbf{x}}(\theta) & S_{\mathbf{y}\mathbf{y}}(\theta) \end{bmatrix} = \begin{bmatrix} Q_{11}(e^{i\theta}) & Q_{12}(e^{i\theta}) \\ Q_{21}(e^{i\theta}) & Q_{22}(e^{i\theta}) \end{bmatrix} \begin{bmatrix} \Omega_{11} & \Omega_{22} \\ \Omega_{21} & \Omega_{22} \end{bmatrix} \begin{bmatrix} Q_{11}(e^{i\theta})^* & Q_{21}(e^{i\theta})^* \\ Q_{12}(e^{i\theta})^* & Q_{22}(e^{i\theta})^* \end{bmatrix}$$

To simplify notations, we define

$$\begin{aligned} \Omega_{22|1} &:= \Omega_{22} - \Omega_{21}\Omega_{11}^{-1}\Omega_{12}, \\ \hat{Q}_{11}(e^{i\theta}) &:= Q_{11}(e^{i\theta}) + Q_{12}(e^{i\theta})\Omega_{21}\Omega_{11}^{-1}. \end{aligned}$$

Following [10], $S_{\mathbf{x}\mathbf{x}}(\theta)$ can be decomposed as

$$S_{\mathbf{x}\mathbf{x}}(\theta) = \hat{Q}_{11}(e^{i\theta})\Omega_{11}\hat{Q}_{11}(e^{i\theta})^* + Q_{12}(e^{i\theta})\Omega_{22|1}Q_{12}(e^{i\theta})^*.$$

The frequency-domain Geweke causality measure (GCM) was defined in [10] as:

$$g_{\mathbf{y} \rightarrow \mathbf{x}}^{\text{GCM}}(\theta) := \log \frac{\det(S_{\mathbf{x}\mathbf{x}}(\theta))}{\det(\hat{Q}_{11}(e^{i\theta})\Omega_{11}\hat{Q}_{11}(e^{i\theta})^*)}. \quad (31)$$

The main motivation from [10] for the derivation of the denominator in $g_{\mathbf{y} \rightarrow \mathbf{x}}^{\text{GCM}}(\theta)$ in Eq. (31) was to ensure a proper normalization of $g_{\mathbf{y} \rightarrow \mathbf{x}}^{\text{GCM}}(\theta)$ so that the following equality is satisfied:

$$\int_{-\pi}^{\pi} g_{\mathbf{y} \rightarrow \mathbf{x}}^{\text{GCM}}(\theta) \frac{d\theta}{2\pi} = g_{\mathbf{y} \rightarrow \mathbf{x}}^{\text{sc}}.$$

But we note that the heuristic expression $\hat{Q}_{11}(e^{i\theta})\Omega_{11}\hat{Q}_{11}(e^{i\theta})^*$ is not equal to the PSD of the residual process $S_{\mathbf{x}\mathbf{x}|\mathbf{y}}^{\text{SC}}(\theta)$. As a result, the expression in Eq. (31) is not a frequency-domain measure of the model fitness of dynamic regression filters. Thus, $g_{\mathbf{y} \rightarrow \mathbf{x}}^{\text{GCM}}(\theta)$ may not provide the expected frequency-domain linear dependence between the time-series. As an alternative solution, we propose the following frequency-domain expression:

$$\begin{aligned}
g_{y \rightarrow x}^{\text{GCM}}(\theta) &= \log \frac{\det(S_{\mathbf{x}\mathbf{x}}(\theta))}{\det(S_{\mathbf{x}\mathbf{x}|\mathbf{y}}^{\text{sc}}(\theta))}, \\
&= \log \frac{\det(S_{\mathbf{x}\mathbf{x}}(\theta))}{\det(P_{11}(e^{i\theta})^{-1} \Omega_{11} P_{11}(e^{i\theta})^{-*})},
\end{aligned} \tag{32}$$

which is different from $g_{y \rightarrow x}^{\text{GCM}}(\theta)$, since $P_{11}(e^{i\theta})^{-1} \neq \hat{Q}_{11}(e^{i\theta})$.

We note that the proposed causality measure also satisfies

$$\int_{-\pi}^{\pi} g_{y \rightarrow x}^{\text{sc}}(\theta) \frac{d\theta}{2\pi} = g_{y \rightarrow x}^{\text{sc}}.$$

More importantly, the proposed measure $g_{y \rightarrow x}^{\text{GCM}}(\theta)$ reflects the true ratio of variances as a function of frequency. It provides information about the model fitness at different frequencies. We note that this information is not provided by $g_{y \rightarrow x}^{\text{GCM}}(\theta)$. Thus, $g_{y \rightarrow x}^{\text{sc}}(\theta)$ is a more useful measure for understanding the linear dependence between the signals.

The proposed frequency-domain causality measure in Eq.(32) can be straightforwardly extended to the case of instantaneously causal and noncausal filters, respectively. In particular we define the frequency-domain linear dependence measure with instantaneously causal filters as

$$g_{y \rightarrow x}^{\text{ic}}(\theta) = \log \frac{\det(S_{\mathbf{x}\mathbf{x}}(\theta))}{\det(S_{\mathbf{x}\mathbf{x}|\mathbf{y}}^{\text{ic}}(\theta))}.$$

Moreover $g_{y \rightarrow x}^{\text{ic}}(\theta)$ is different from the classical frequencydomain linear dependence measure in [10], [29]. But its average value

$$g_{y \rightarrow x}^{\text{ic}} = \int_{-\pi}^{\pi} g_{y \rightarrow x}^{\text{ic}}(\theta) \frac{d\theta}{2\pi} = \log \frac{\det(\Omega_{\mathbf{x}\mathbf{x}})}{\det(\Omega_{\mathbf{x}\mathbf{x}|\mathbf{y}}^{\text{ic}})}$$

is equal to the static instantaneous causality measure from [10]. Similarly, the frequency-domain linear dependence measure for noncausal filters is defined as:

$$g_{y \rightarrow x}^{\text{nc}}(\theta) = \log \frac{\det(S_{\mathbf{x}\mathbf{x}}(\theta))}{\det(S_{\mathbf{x}\mathbf{x}|\mathbf{y}}^{\text{nc}}(\theta))}.$$

Its average value is equal to $g_{y \rightarrow x}^{nc} = \log \frac{\det(\Omega_{xx})}{\det(\Omega_{xx|y}^{nc})}$ with $\Omega_{xx|y}^{nc}$ being the one-step-ahead

prediction error variance of $S_{xx|y}^{nc}(\theta)$. Finally, we note that if an invertible scalar filter, such as a bandpass filter, is applied during preprocessing for removing noise or a filter that models the hemodynamic response, is applied to all the time series data then all the proposed causality measures are invariant to such filtering, which is a property that is also held by the GCM [30].

G. On conditional linear dependence measure

Conditional linear dependence measure is a generalization of the linear dependence of two variables after regressing out influence from a third variable. Both the static and frequencydomain linear dependence measures from [10] have been generalized in [11]. A different algorithm was proposed in [31] to improve the computational efficiency of the frequencydomain measures. A multivariate extension of the conditional measure for blocks of processes was explored in [32]. Using the dynamic-regression framework developed above, we propose a different solution for frequency-domain conditional linear dependence measures.

Consider three zero-mean stationary processes $\{x(t)\}_{t \in \mathbb{Z}}$, $\{y(t)\}_{t \in \mathbb{Z}}$ and $\{z(t)\}_{t \in \mathbb{Z}}$, with the size of $x(t)$, $y(t)$ and $z(t)$ being n_x, n_y , and n_z , respectively. Analogous to Eqs. (16) and (17), we consider the following representation of the joint process $\{[x'(t), z'(t)]'\}_{t \in \mathbb{Z}}$:

$$\begin{bmatrix} A_{11}(z) & A_{12}(z) \\ A_{21}(z) & A_{22}(z) \end{bmatrix} \begin{bmatrix} x(t) \\ z(t) \end{bmatrix} = \begin{bmatrix} \epsilon_3(t) \\ \epsilon_4(t) \end{bmatrix}, \quad (33)$$

with $\begin{bmatrix} A_{11}(z) & A_{12}(z) \\ A_{21}(z) & A_{22}(z) \end{bmatrix}$ being the optimal one-step-ahead filter and the covariance matrix of the innovation process $[\epsilon_3(t)', \epsilon_4(t)']'$ given by:

$$\mathcal{E} \left(\begin{bmatrix} \epsilon_3(t) \\ \epsilon_4(t) \end{bmatrix} \begin{bmatrix} \epsilon_3(t)' & \epsilon_4(t)' \end{bmatrix} \right) = \begin{bmatrix} \Omega_{33} & \Omega_{34} \\ \Omega_{43} & \Omega_{44} \end{bmatrix}.$$

Following Eq. (24), we define

$$S_{xx|z}^{sc}(\theta) = A_{11} \left(e^{i\theta} \right)^{-1} \Omega_{33} A_{11} \left(e^{i\theta} \right)^{-*},$$

as the PSD of the minimal-entropy residual process after regressing out the past values of $z(t)$ from $x(t)$.

Similarly, we consider the following representation of the joint process $\{[x'(t), y'(t), z'(t)]'\}_{t \in \mathbb{Z}}$:

$$\begin{bmatrix} B_{11}(z) & B_{12}(z) & B_{13}(z) \\ B_{21}(z) & B_{22}(z) & B_{23}(z) \\ B_{31}(z) & B_{32}(z) & B_{33}(z) \end{bmatrix} \begin{bmatrix} x(t) \\ y(t) \\ z(t) \end{bmatrix} = \begin{bmatrix} e_5(t) \\ e_6(t) \\ e_7(t) \end{bmatrix}, \quad (34)$$

with $B_{ij}(z)$ being a sub-block of the one-step-ahead prediction filter $B(z)$. Then, we define

$$S_{xx|yz}^{\text{sc}}(\theta) = B_{11}(e^{i\theta})^{-1} \Omega_{55} B_{11}(e^{i\theta})^{-*},$$

which is equal to the PSD of the minimal-entropy residual process after regressing out the past values of both $y(t)$ and $z(t)$ from $x(t)$, where Ω_{55} is the covariance of $e_5(t)$. Thus, an approach for measuring the linear dependence between $x(t)$ and $y(t)$ conditional on $z(t)$ is to compare $S_{xx|z}^{\text{sc}}(\theta)$ and $S_{xx|yz}^{\text{sc}}(\theta)$ using the following frequency-domain measure

$$g_{y \rightarrow x|z}^{\text{sc}}(\theta) = \log \frac{\det(S_{xx|z}^{\text{sc}}(\theta))}{\det(S_{xx|yz}^{\text{sc}}(\theta))}. \quad (35)$$

We note that $g_{y \rightarrow x|z}^{\text{sc}}(\theta)$ is different from the original frequency-domain conditional linear dependence measure $g_{y \rightarrow x|z}^{\text{GCM}}(\theta)$ in [11], which is reviewed in Appendix A. But they have the same average value which is equal to

$$g_{y \rightarrow x|z}^{\text{sc}} = \int_{-\pi}^{\pi} g_{y \rightarrow x|z}^{\text{sc}}(\theta) \frac{d\theta}{2\pi} = \log \frac{\det(\Omega_{33})}{\det(\Omega_{55})}. \quad (36)$$

Similarly, we can define the conditional causal measures $g_{y \rightarrow x|z}^{\text{ic}}(\theta)$, $g_{y \rightarrow x|z}^{\text{nc}}(\theta)$ by using the PSD obtained by instantaneously causal and noncausal regression filters, respectively.

We note a theoretically interesting property of $g_{y \rightarrow x|z}^{\text{nc}}(\theta)$ from noncausal filters:

$$g_{y \rightarrow x|z}^{\text{nc}}(\theta) = g_{y \rightarrow x|z}^{\text{nc}}(\theta). \quad (37)$$

In other words, the causality measure $g_{y \rightarrow x|z}^{\text{nc}}(\theta)$ obtained by regressing out bilateral information on $z(t)$ does not provide directional information on the linear dependence between $x(t)$ and $y(t)$. The proof of Eq. (37) is provided in Appendix B.

Finally, we note that though the proposed frequency-domain causality and conditional causality measures are different from the original solutions in [10], [11], they are derived following Geweke's basic formulation, which is to compare the ratio of prediction error

variances obtained without and with regressors. There is a common alternative framework based on directed coherence (DC) [33], [34], [35], partial directed coherence (PDC) [36], [37], and a generalization of PDC for vector-valued processes [32]. These measures will not be compared with the proposed solutions since they are derived following completely different rationales.

III. Experiments

A. Synthetic examples

We compared the proposed partial coherence, causality, conditional causality measures with existing results using two synthetic examples, which are described by three-dimensional autoregressive models. The first model is given by:

$$\begin{bmatrix} u_1(t) \\ u_2(t) \\ u_3(t) \end{bmatrix} = \begin{bmatrix} 0.3 & 0.3 & 0 \\ 0.3 & 0.3 & 0 \\ 0 & 0.3 & 0.3 \end{bmatrix} \begin{bmatrix} u_1(t-1) \\ u_2(t-1) \\ u_3(t-1) \end{bmatrix} + \begin{bmatrix} \epsilon_1(t) \\ \epsilon_2(t) \\ \epsilon_3(t) \end{bmatrix} \quad (38)$$

where there is no direct interaction between $u_1(t)$ and $u_3(t)$. The second model is given by:

$$\begin{bmatrix} u_1(t) \\ u_2(t) \\ u_3(t) \end{bmatrix} = \begin{bmatrix} 0.3 & 0.3 & 0.3 \\ 0.3 & 0.3 & 0 \\ 0 & 0.3 & 0.3 \end{bmatrix} \begin{bmatrix} u_1(t-1) \\ u_2(t-1) \\ u_3(t-1) \end{bmatrix} + \begin{bmatrix} \epsilon_1(t) \\ \epsilon_2(t) \\ \epsilon_3(t) \end{bmatrix}. \quad (39)$$

A schematic diagram representation of the two dynamical systems is illustrated in the first row of Table I. The model parameters were chosen so that the PSD's have dominant energy at the low-frequency range as shown in the second row in Table I, similar to the case for in vivo BOLD signals [38]. We note that the only difference between the two models is the link between $u_1(t)$ and $u_3(t)$, which closes the loop information flow among the three variables. In both models, we assume that the covariance matrix of the three-dimensional innovation process $[\epsilon_1(t) \ \epsilon_2(t) \ \epsilon_3(t)]^T$ is equal to the identity matrix. As a result, the dynamic regression results using instantaneously causal filters are equal to the results with strictly causal filters. Thus, we will only compare the results with strictly causal and noncausal filters.

B. In vivo data

We applied the proposed method to the 100-subject data from HCP [39], where each subject had four 15-min run data provided in the standard surface space. The acquisition parameters were TE/TR=33/720 ms. The data sets have been preprocessed by the ICA-Fix method [40]. In two separate experiments, we applied the label maps from [21] to cluster the fMRI data into 7 and 17 networks, respectively. The 7 networks consist of the Visual (VS), Somatomotor (SM), Dorsal Attention (DA), Ventral Attention (VA), Limbic (LB), Frontoparietal (FP), and Default (DF) networks. For each data set, we first remove the mean value for the signal at each vertex along with regressing out the global average signal. Then,

we take the average signal from each brain region as the representative signal of the corresponding network and obtain a 7-dimensional or 17-dimensional time series. The aim of these experiments was to compare the proposed partial coherence, causality and partial causality measures with existing results.

To accomplish these goals, we first estimated the autocorrelation sequences for the 7-dimensional and 17-dimensional time series for each data set from the 4 scans of each subject. Then, we used the average value of the four autocorrelation sequences to compute a multivariate AR (autoregressive) model for each subject. The multivariate AR model was computed by solving the Yule-Walker equation as is standard in causality analysis [41]. The order of the AR model was selected as the order that minimizes the Akaike information criterion (AIC) [42]. For the 7- and 17-dimensional series, the optimal AR orders were determined as 6 and 4, respectively.

For coherence/partial coherence analysis, we computed the standard frequency-domain coherence measure $\kappa(\theta)$ between each pair of rsfMRI signals and the proposed partial coherence measures, $\kappa^{sc}(\theta)$, $\kappa^{ic}(\theta)$ and $\kappa^{nc}(\theta)$, obtained by regressing out influence from other signals using strictly causal, instantaneously causal and noncausal filters, respectively.

For causal analysis, we analyzed the linear dependence between each pair of rsfMRI signals on the other set of 5 or 15 signals using $g_{y \rightarrow x|z}^{GCM}(\theta)$, $g_{y \rightarrow x|z}^{sc}(\theta)$, $g_{y \rightarrow x|z}^{ic}(\theta)$, $g_{y \rightarrow x|z}^{nc}(\theta)$. The causality measure provides information on the fraction of variance that are explained by the dynamic filters used in the coherence/partial coherence analysis.

For conditional causality analysis, we compare the classical measure $g_{y \rightarrow x|z}^{GCM}(\theta)$ from [11] with the proposed measures $g_{y \rightarrow x|z}^{sc}(\theta)$ and $g_{y \rightarrow x|z}^{ic}(\theta)$. We note that $g_{y \rightarrow x|z}^{nc}(\theta)$ is not analyzed since it does not provide any information about the direction of linear dependence, as noted in Section II-G.

IV. Results

A. Synthetic examples

The coherence, causality, and conditional causality analysis results for the two synthetic examples are tabulated rows 3 to 5 of Table I. In the third row of Table I, we note that the coherence $\kappa_{13}(\theta)$ for the first model is nonzero, though there is no direct connection between u_1 and u_3 . But both $\kappa_{13|2}^{SC}(\theta)$ and $\kappa_{13|2}^{SC}(\theta)$ are zero, implying that both strictly causal and noncausal filters are able to completely regress out influences from u_2 on the coherence between u_1 and u_3 . All the coherence and partial coherence measures in Model 2 are nonzero. Moreover, the results from noncausal filters are different from the results using causal filters.

In the fourth row of Table I, we note that in Model 1 both the traditional causality measure $g_{3 \rightarrow 12}^{GCM}(\theta)$ and the proposed measure $g_{3 \rightarrow 12}^{sc}(\theta)$ are equal to zero, which correctly reveals the direction of information flow from u_2 to u_3 . But the same link between u_2 and u_3

also makes the measure $g_{3 \rightarrow 12}^{nc}(\theta)$ nonzero. For other 5 sets of measures in the same row, we note that both $g^{sc}(\theta)$ and $g^{nc}(\theta)$ have higher values than $g^{GCM}(\theta)$ in the low-frequency range. Since all the synthetic signals have dominant energy in the low-frequency range, the proposed measure correctly captures the real frequencydomain dependence between the signals.

The last row of Table I illustrates the conditional causality measures. We note that, in both models, if there is no direct connection from u_i to u_j for $i, j \in \{1, 2, 3\}$, then both $g_{i \rightarrow j|k}^{sc}(\theta)$ and $g_{i \rightarrow j|k}^{GCM}(\theta)$ are equal to zero. For the existing connections, $g_{i \rightarrow j|k}^{sc}(\theta)$ has much higher values than $g_{i \rightarrow j|k}^{GCM}(\theta)$ at low frequencies. The traditional measure $g_{i \rightarrow j|k}^{GCM}(\theta)$ may even take negative value at frequencies near zero. Thus, the proposed measure $g_{i \rightarrow j|k}^{sc}(\theta)$ accurately captures the dynamic linear dependence between the synthetic signals. Moreover, in both models, the noncausal-filter-based measure $g_{i \rightarrow j|k}^{nc}(\theta)$ is equal to $g_{i \rightarrow j|k}^{nc}(\theta)$ which provides a numerical validation of Eq. (37).

B. In vivo data

Figure 1 shows representative plots for partial coherence, causality and conditional causality results computed as the average over 100 HCP subjects. The first row of Fig. 1 shows the coherence and partial coherence between three pairs of networks, namely the VS-DF, DA-VA, and SM-FP networks, and the corresponding partial coherence conditional on the signals from the other 5 networks. The blue lines are the absolute values of the standard frequency-domain coherence function $\kappa(\theta)$. The absolute values of the proposed partial coherence functions based on strictly causal, instantaneously causal, and noncausal filters are shown by thick red, magenta, and green lines, respectively. For the three pairs of networks shown, the proposed frequency-domain partial coherence measures have much higher values than the (static) correlation function in the 0–0.1 Hz range, which is consistent with the frequency range of BOLD fluctuations [38]. We note that there was no temporal filter applied to remove high-frequency signals from the fMRI signals. The partial coherence functions $|\kappa^{ic}(\theta)|$ and $|\kappa^{nc}(\theta)|$ obtained using instantaneously causal and noncausal filters are much higher than the value obtained using the strictly causal filter. Moreover, $|\kappa^{ic}(\theta)|$ and $|\kappa^{nc}(\theta)|$ have very similar values, as shown in the zoomed region in the figure for the DA-VA network, which are much higher than $|\kappa^{sc}(\theta)|$. This demonstrates that the noncausal filter provides no additional information for predicting the signal at any given instant t and that the instantaneously causal filter is sufficient to use in most cases. To understand the reliability of proposed partial coherence measures, we also computed the standard deviation of $|\kappa^{sc}(\theta)|$ as illustrated by the thin red lines. In particular, the difference between the thin and thick red lines shows the standard deviation among the 100 subjects, which clearly illustrates the difference between the proposed partial coherence and the standard coherence measures. The standard deviations of the other measures are not displayed to ensure better clarity in the figures.

The second row of Fig. 1 illustrates the causality measures which provide information about the dynamic linear dependence of the 2 networks on the other 5 networks. We note that the

proposed (strictly causal) causality measure $g_{y \rightarrow x}^{sc}(\theta)$ is much higher than the Geweke causality measure $g_{y \rightarrow x}^{GCM}(\theta)$ in the 0–0.1 Hz range. Moreover, $g_{y \rightarrow x}^{ic}(\theta)$ and $g_{y \rightarrow x}^{nc}(\theta)$ have similar values which are much higher than $g_{y \rightarrow x}^{sc}(\theta)$. We can thus infer that the instantaneously causal filter is a better prediction filter than the strictly causal one and that no additional information is obtained by using a noncausal filter. Further note that, the Geweke measure $g_{y \rightarrow x}^{GCM}(\theta)$ is almost constant for all frequencies, giving no useful information for understanding frequency-domain dependence between different networks. Similar to partial coherence measures, the range of standard deviation of $g_{y \rightarrow x}^{sc}(\theta)$ is illustrated by the thin red lines.

The last two rows of the Fig. 1 illustrate the linear dependence measure between two networks conditional on signals from the other 5 networks. As in the case of causality measure, $g_{y \rightarrow x|z}^{ic}(\theta)$ and $g_{y \rightarrow x|z}^{nc}(\theta)$ have very similar values, which are significantly higher than $g_{y \rightarrow x|z}^{sc}(\theta)$. Moreover, $g_{y \rightarrow x|z}^{sc}(\theta)$ is much higher than $g_{y \rightarrow x|z}^{GCM}(\theta)$ at the 0–0.1 Hz frequency range, implying that the proposed method provides more a reasonable measure of linear dependence between BOLD signals. The standard deviations of $g_{y \rightarrow x|z}^{sc}(\theta)$ are shown by the thin red lines.

The partial coherence, causality and conditional causality measures for three pairs of representative networks from the 17-network parcellation are shown in Fig. 2. The results for N1–N17, i.e. Networks 1–17, and N3–N12 are similar to the results shown in Fig. 1. In particular, the partial coherence using strictly causal filter $|\kappa^{sc}(\theta)|$ is higher than the standard measure for partial coherence $|\kappa(\theta)|$ at low frequencies. Further, the partial coherence measures obtained using instantaneously causal and noncausal filters are much higher than the results using strictly causal filters. For N6–N7, we note that $|\kappa^{sc}(\theta)|$ is lower than $|\kappa(\theta)|$ at low frequencies, which indicates that the high correlation in $|\kappa(\theta)|$ may be caused by influences from other networks, which are regressed out by the strictly causal filter. The causality and conditional causality measures for all the three pair of networks have similar features as shown in Fig. 1. In particular, we note that the traditional measure $g_{y \rightarrow x|z}^{sc}(\theta)$ is almost equal to zero in all cases. For the conditional causality measure of $N7 \rightarrow N6$ shown in the last row panel of Fig. 2, the proposed measure $g_{y \rightarrow x|z}^{sc}(\theta)$ is also about zero, which indicates that there N7 does not dependent on the past measurements from N6 given other signals. Thus, this example shows that the proposed conditional causality measure could potentially provide information on the direction of information flow in brain functional networks.

V. Discussion and conclusion

In this paper, we revisited the partial coherence, causality and conditional causality analysis approaches in functional brain network analysis. We presented these analyses in a novel dynamic-regression framework with a minimal-entropy cost function. Using optimal prediction theory, we derived the solutions for the regression problem for different types of

regression filters. These solutions provide several novel theoretical results on partial coherence analysis and causality analysis. First, we presented several expressions for the static and frequency-domain partial coherence functions with strictly causal and instantaneously causal filters. Second, we extended the classical result from [10] and introduced several expressions for the frequency-domain causality analysis, which are able to provide information on linear dependence between signals at different frequencies. Further, we also introduced several novel expressions for frequency-domain conditional causality analysis. We note that, though the derivation of the proposed frequency-domain method is closely related to the method used in Geweke causality analysis, the theoretical expressions for the proposed causality and conditional causality measures are different from existing solutions.

We applied the proposed methods to analyze synthetic examples and in vivo rsfMRI data from 100 HCP subjects, respectively. The experimental results showed different features of these methods: 1) In both experiments, the proposed strictly-causal filters are able to regress out variance in signals at the correct frequency range and the corresponding causality measures provide more accurate information on the dynamic linear dependence between signals than the traditional Geweke causality measure. 2) In the in vivo data experiments, the instantaneously causal filter lead to significantly increased causality and partial coherence measures, and has similar performances as the noncausal filter. The significant contribution from the instantaneous values in the dynamic regression problem may be caused by the low-temporal resolution of rsfMRI, which does not provide information on short-time scale dynamic dependence between the signals. 3) It is proven that the conditional causality measure with noncausal filters do not provide information on the direction of linear dependence between the signals.

We note that a limitation of the proposed methods is the assumption about the stationarity of the time series. If nonstationarity is considered, we expect our method can be applied in a time-frequency analysis framework as in [43], which will be explored in future work. Finally, we remark that the functional connectivity analysis depends on the sampling rate of the measurements [44]. MEG and EEG measurements typically have much higher temporal resolutions than rsfMRI, and thus could potentially provide more useful information about functional brain connectivity using the proposed methods.

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Appendix

A. On the Geweke conditional linear dependence measure

For completeness, we briefly review the conditional causality measure introduced in [11], which will be compared with the proposed solution from Section II-G in Experiments. First, we take the inverse of Eq. (34) and obtain that

$$\begin{bmatrix} x(t) \\ y(t) \\ z(t) \end{bmatrix} = \begin{bmatrix} C_{11}(z) & C_{12}(z) & C_{13}(z) \\ C_{21}(z) & C_{22}(z) & C_{23}(z) \\ C_{31}(z) & C_{32}(z) & C_{33}(z) \end{bmatrix} \begin{bmatrix} \epsilon_5(t) \\ \epsilon_6(t) \\ \epsilon_7(t) \end{bmatrix}. \quad (40)$$

Next, we replace $x(t)$ and $z(t)$ in the above equation using $\epsilon_3(t)$ and $\epsilon_4(t)$ and obtain that

$$\begin{aligned} \begin{bmatrix} \epsilon_3(t) \\ y(t) \\ \epsilon_4(t) \end{bmatrix} &= \begin{bmatrix} A_{11}(z) & 0 & A_{12}(z) \\ 0 & I & 0 \\ A_{21}(z) & 0 & A_{22}(z) \end{bmatrix} \begin{bmatrix} C_{11}(z) & C_{12}(z) & C_{13}(z) \\ C_{21}(z) & C_{22}(z) & C_{23}(z) \\ C_{31}(z) & C_{32}(z) & C_{33}(z) \end{bmatrix} \begin{bmatrix} \epsilon_5(t) \\ \epsilon_6(t) \\ \epsilon_7(t) \end{bmatrix}, \quad (41) \\ &= \begin{bmatrix} D_{11}(z) & D_{12}(z) & D_{13}(z) \\ D_{21}(z) & D_{22}(z) & D_{23}(z) \\ D_{31}(z) & D_{32}(z) & D_{33}(z) \end{bmatrix} \begin{bmatrix} \epsilon_5(t) \\ \epsilon_6(t) \\ \epsilon_7(t) \end{bmatrix}. \end{aligned}$$

Then, the frequency-domain measure on the dependence of $x(t)$ on $y(t)$ conditional on the past value of $z(t)$ defined in [11] is defined as

$$g_{y \rightarrow x|z}^{\text{GCM}}(\theta) = \log \frac{\det(\Omega_{33})}{D_{11}(e^{i\theta})\Omega_{55}D_{11}(e^{i\theta})^*}.$$

The average value of $g_{y \rightarrow x|z}^{\text{GCM}}(\theta)$ over the interval $[-\pi, \pi]$ is equal to $\log \frac{\det(\Omega_{33})}{\det(\Omega_{55})}$ as in Eq(36)

B. Proof of Eq. (37)

We denote the joint PSD of $[x(t)', y(t)', z(t)']'$ as

$$\begin{bmatrix} S_{xx} & S_{xy} & S_{xz} \\ S_{yx} & S_{yy} & S_{yz} \\ S_{zx} & S_{zy} & S_{zz} \end{bmatrix},$$

where the dependence on θ is neglected to simplify notations. Following Eq. (28), we obtain the joint PSD between $x(t)$ and $y(t)$ after regressing out $z(t)$ as below:

$$\begin{bmatrix} S_{xx|z}^{\text{nc}} & S_{xy|z}^{\text{nc}} \\ S_{yx|z}^{\text{nc}} & S_{yy}^{\text{nc}} \end{bmatrix} = \begin{bmatrix} S_{xx} - S_{xz}S_{zz}^{-1}S_{zx} & S_{xy} - S_{xz}S_{zz}^{-1}S_{zy} \\ S_{yx} - S_{yz}S_{zz}^{-1}S_{zx} & S_{yy} - S_{yz}S_{zz}^{-1}S_{zy} \end{bmatrix}. \quad (42)$$

Applying Eq. (28) once more, we obtain the following PSD of $x(t)$ after regressing out both $y(t)$ and $z(t)$

$$S_{xx|yz}^{nc} = S_{xx|z}^{nc} - S_{xy|z}^{nc} (S_{yy|z}^{nc})^{-1} S_{yx|z}^{nc}. \quad (43)$$

Similarly, we have

$$S_{yy|xz}^{nc} = S_{yy|z}^{nc} - S_{yx|z}^{nc} (S_{xx|z}^{nc})^{-1} S_{xy|z}^{nc}. \quad (44)$$

From the definition of conditional causality measure, it holds that

$$\begin{aligned} g_{x \rightarrow y|z}^{sc} &= \log \frac{\det(S_{yy|z}^{nc})}{\det(S_{yy|xz}^{nc})}, \\ &= -\log \det \left(I_{n_y} - (S_{yy|z}^{nc})^{-1} S_{yx|z}^{nc} (S_{xx|z}^{nc})^{-1} S_{xy|z}^{nc} \right), \end{aligned} \quad (45)$$

$$\begin{aligned} g_{y \rightarrow x|z}^{sc} &= \log \frac{\det(S_{xx|z}^{nc})}{\det(S_{xx|yz}^{nc})}, \\ &= -\log \det \left(I_{n_x} - (S_{xx|z}^{nc})^{-1} S_{xy|z}^{nc} (S_{yy|z}^{nc})^{-1} S_{yx|z}^{nc} \right), \end{aligned} \quad (46)$$

But both of the determinants in Eqs. (45) and (46) are equal to

$$\det \begin{pmatrix} I_{n_x} & (S_{xx|z}^{nc})^{-1} S_{xy|z}^{nc} \\ (S_{yy|z}^{nc})^{-1} S_{yx|z}^{nc} & I_{n_y} \end{pmatrix}.$$

Thus, Eq. (37) is proved.

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Fig. 1:

Partial coherence, causality and conditional causality analysis results for the 7 network parcellation: The first row illustrates the partial coherence results between three representative pairs of networks after regressing out signals from the other 5 networks at different frequencies shown in the horizontal axis. The second row illustrates the causality measures which shows the linear dependence of the shown pair of networks on the other 5 networks. The last two rows show the linear dependence between the two signals conditional on signals from the other 5 networks. The thin red lines illustrate the frequency-wise

standard deviation of the corresponding measure shown by thick red lines. In all plots, the results from instantaneously causal and noncausal filters are very close to each other, as shown by the zoomed regions in the middle column panels.

Fig. 2:

Partial coherence, causality and conditional causality analysis results for the 17 network parcellation: The first row illustrates the partial coherence results between three representative pairs of networks after regressing out signals from the other 15 networks at different frequencies shown in the horizontal axis. The second row illustrates the causality measures which shows the linear dependence of the shown pair of networks on the other 15 networks. The last two rows show the linear dependence between the two signals conditional on signals from the other 15 networks. The thin red lines illustrate the frequency-wise

standard deviation of the corresponding measure shown by thick red lines. In all plots, the results from instantaneously causal and noncausal filters are very close to each other, as shown by the zoomed regions in the middle column panels.

Table I:

Illustration of the system diagram, power spectra of the two synthetic examples and their (partial) coherence, causality and conditional causality measures.