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Short communication

A critical note on the definition of phase–amplitude cross-frequency coupling

Tolga Esat Özkurt[a,b,*], Alfons Schnitzler[a]

[a] Institute of Clinical Neuroscience and Medical Psychology, Heinrich Heine University, Düsseldorf, Germany
[b] Department of Electronics and Communications Engineering, Istanbul Technical University, Istanbul, Turkey

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ABSTRACT

Recent studies have observed the ubiquity of phase–amplitude coupling (PAC) phenomenon in human and animal brain recordings. While various methods were performed to quantify it, a rigorous analytical definition of PAC is lacking. This paper yields an analytical definition and accordingly offers theoretical insights into some of the current methods. A direct PAC estimator based on the given definition is presented and shown theoretically to be superior to some of the previous methods such as general linear model (GLM) estimator. It is also shown that the proposed PAC estimator is equivalent to GLM estimator when a constant term is removed from its formulation. The validity of the derivations is demonstrated with simulated data of varying noise levels and local field potentials recorded from the subthalamic nucleus of a Parkinson's disease patient.

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1. Introduction

Phase–amplitude coupling (PAC) between low and high frequency components of electrophysiological signals has received great interest in neuroscience (Jensen and Colgin, 2007; Jerbi and Bertrand, 2009; Canolty and Knight, 2010). Many diverse estimation methods were suggested and utilized to measure this phenomenon (Bruns and Eckhorn, 2004; Mormann et al., 2005; Canolty et al., 2006; Tort et al., 2008; Lakatos et al., 2008; Osipova et al., 2008; Cohen, 2008). Some of these methods were also evaluated and their performances were numerically compared in various studies (Penny et al., 2008; Tort et al., 2010; Onslow et al., 2011). However, a formal analytical definition of PAC is still lacking.

These methods were designed intuitively to capture and measure PAC, but we believe the usual strategy hitherto is standing on its head by asserting the methods without a proper prior definition of PAC itself as a universal phenomenon. A recent study by He et al. (2010) already gives clues of this universality as it addresses PAC in other man-made and natural processes such as Dow–Jones index and seismic waves.

From a signal processing point of view, the natural way would be first to define a universal PAC function and then consider appropriate methods that would capture the most accurate estimate possible. In this second step, the estimation method would mainly depend on the statistical properties and type of the data set being analyzed. Hence, our approach in this study aims to invert the research path taken so far by providing a rigorous analytical definition of PAC and then proceeding to consider the appropriate estimators for the quantification of it.

In this respect, we present a direct PAC estimator stemming from this definition and relate it theoretically to general linear model (GLM) estimator (Penny et al., 2008), modulation index (MI) with and without statistics (Canolty et al., 2006). We also discuss some other widely used estimators such as envelope-to-signal correlation (ESC) (Bruns and Eckhorn, 2004) and cross-frequency coherence (CFC) (Osipova et al., 2008) following the same context.

Throughout this paper estimates (not the true values) are denoted with a triangular hat ^ while E, *, superscript T and := stand for expectation operator, convolution operator, transpose and symbol of "defined as", respectively.

2. Theory

2.1. Definition of PAC function

Let $a_H(n)$ be the amplitudes of a narrowband random vector $z_H(n)$ and let $\varphi_L(n)$ be the phases of narrowband random vector $z_L(n)$, where $z_H(n)$ and $z_L(n)$ are bandpass filtered complex analytic representations from a common random signal or two separate signals such that

$$\begin{aligned} z_L(n) &= |z_L(n)|e^{i\varphi_L(n)} \\ z_H(n) &= |z_H(n)|e^{i\varphi_H(n)} \end{aligned} \quad (1)$$

$$a_L(n) := |z_L(n)|, \qquad a_H(n) := |z_H(n)|$$

* Corresponding author at: Istanbul Technical University, Faculty of Electrical and Electronics Engineering, Signal Processing Laboratory, 80626 Maslak Istanbul, Turkey. Tel.: +90 536 583 80 82; fax: +90 212 285 35 65.
E-mail address: tolgaozkurt@gmail.com (T.E. Özkurt).

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where

$$z_L(n) := z(n) * h_L(n) + i\mathbf{H}\{z(n) * h_L(n)\}$$
$$z_H(n) := z(n) * h_H(n) + i\mathbf{H}\{z(n) * h_H(n)\}$$
$$H_L(\omega) := \begin{cases} 1, & \omega_L - \Delta\omega_L \le \omega \le \omega_L + \Delta\omega_L \\ 0, & \text{otherwise} \end{cases} \tag{2}$$
$$H_H(\omega) := \begin{cases} 1, & \omega_H - \Delta\omega_H \le \omega \le \omega_H + \Delta\omega_H \\ 0, & \text{otherwise} \end{cases}$$
$$\omega_H > \omega_L + \Delta\omega_L + \Delta\omega_H$$

with $h_L(n)$ and $h_H(n)$ being the impulse functions of the filters $H_L(\omega)$ and $H_H(\omega)$, respectively. Here $\Delta\omega_L$ and $\Delta\omega_H$ denote the bandwidths of the filters and $\mathbf{H}$ denotes the Hilbert transform. Please note that complex analytic signals contain no negative frequency components and can be constructed with the Hilbert transform of real-valued bandpass filtered signals (Smith, 2007).

Then we define PAC function as

$$\rho(z, \omega_L, \omega_H) := \frac{|E\{a_H e^{i\varphi_L}\}|}{\sqrt{E\{|a_H|^2\}E\{|e^{i\varphi_L}|^2\}}}$$

simplifying to

$$\rho(z, \omega_L, \omega_H) := \frac{|E\{a_H e^{i\varphi_L}\}|}{\sqrt{E\{a_H{}^2\}}} \tag{3}$$

Following the definition of coherence function (Carter et al., 1973), the PAC function has similar boundaries of $0 \le \rho(z, \omega_L, \omega_H) \le 1$.

Please note that the definition provided above should be considered only for "monophasic" situations, i.e., phase–amplitude probability density function has only one peak, if it ever has. For multiphasic cases, our definition can easily be generalized by constraining φ_L within a step of interval and integrating them over. However, the limit of this study is kept only to monophasic cases, where the considered estimators will not take into account any phase related distribution or asymmetry in the phase dimension of coupling such as the entropy based measures suggested by Tort et al. (2010).

2.2. Direct PAC estimate

It is the most straightforward estimate evaluating the statistical expectation as averaging over realizations of an ensemble

$$\hat{\rho}_D := \frac{1}{\sqrt{N}} \frac{\left|\sum_{n=1}^{N} a_H(n) e^{i\varphi_L(n)}\right|}{\sqrt{\sum_{n=1}^{N} a_H(n)^2}} \tag{4}$$

Since it has a similar structure to the coherence, its bias must also tend to zero as the data length N increases or when the PAC estimate approaches to unity, as Nuttall and Carter (1976) showed for the case of magnitude-squared coherence estimate.

2.3. Relation to the other estimators

Eq. (4) implies the similarity of the direct PAC estimator with a popular PAC measure known as "modulation index" (MI) (Canolty et al., 2006)

$$\hat{\rho}_{MI} = \left|\sum_{n=1}^{N} a_H(n) e^{i\varphi_L(n)}\right| \tag{5}$$

excepting a subtle difference of the factor in its denominator, i.e., direct estimation additionally involves a normalization factor being equivalent to the power of amplitude vector $a_H(n)$.

In the following, we will show that other well-known estimators such as "general linear model" (GLM) (Penny et al., 2008) gives in fact no better accuracy than the direct PAC estimator. GLM as a PAC estimator was suggested by Penny et al. (2008) and was claimed to be the most preferable when compared to the others such as $\hat{\rho}_{MI}$, envelope-to-signal correlation (ESC) and phase locking value (PLV) based methods.

On the light of the PAC definition (3), we will demonstrate on the contrary that direct estimation given by Eq. (4) relates very closely to GLM and it is expected to give more accurate estimates than GLM and the others mentioned.

2.4. What does GLM measure amount to?

GLM estimates the PAC strength by linearly regressing the amplitude vector (Penny et al., 2008)

$$a_H = X\beta + \varepsilon \tag{6}$$

with a least-squared approximation. Here $X := [\cos\varphi_L \quad \sin\varphi_L \quad 1]$ is a vector of cosines, sines and unities, $\beta = [\beta_1 \quad \beta_2 \quad \beta_3]^T$ is regression coefficient vector and ε is the residual vector. The GLM estimate is given as

$$\hat{\rho}_{GLM} = \sqrt{\frac{\sum_{n=1}^{N} a_H(n)^2 - \sum_{n=1}^{N} \varepsilon(n)^2}{\sum_{n=1}^{N} a_H(n)^2}} \tag{7}$$

One can rewrite the GLM definition as

$$\rho_{GLM} = \sqrt{\frac{P(a_H) - P(\varepsilon)}{P(a_H)}} \tag{8}$$

where $P(x) := E\{x^T x\}$ refers to the power. Since the amplitude vector power can be expressed in terms of regression coefficients and the residue

$$\begin{aligned} P(a_H) &= E\left\{a_H{}^T a_H\right\} = E\{(\beta^T X^T + \varepsilon^T)(X\beta + \varepsilon)\} \\ &= E\{\beta^T X^T X \beta\} + E\{\varepsilon^T \varepsilon\} = 2E\{\beta^T \beta\} + P(\varepsilon) \end{aligned} \tag{9}$$

Then GLM function will reduce to

$$\rho_{GLM} = \sqrt{\frac{2E\{\beta^T\beta\}}{P(a_H)}}$$

$$\rho_{GLM} \sim \sqrt{\frac{E\{\beta^T\beta\}}{P(a_H)}} \tag{10}$$

when (9) is replaced into (8). Accordingly, these equations indicate the relation between GLM estimate and the regression coefficients as

$$\hat{\rho}_{GLM} := \sqrt{\frac{\beta_1{}^2 + \beta_2{}^2 + \beta_3{}^2}{\sum_{n=1}^{N} a_H(n)^2}} =: \hat{\rho}_{\beta GLM}$$

$$\hat{\rho}_{GLM} := \sqrt{\frac{\beta_1{}^2 + \beta_2{}^2 + \beta_3{}^2}{\sum_{n=1}^{N} a_H(n)^2}} =: \hat{\rho}_{\beta GLM} \tag{11}$$

Eq. (11) will help us relate the direct PAC estimator to the GLM estimator.

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