Detecting Nonlinear Granger Causality via the kernelization of Partial Directed Coherence

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Abstract

Though by now classic for inferring causal relations between time series, linear vector autoregressive models fail to capture certain types of nonlinear coupling. Here we explore a new concept kernel-nonlinear-Partial Directed Coherence and its ability to overcome those limitations, via a simulated example of its asymptotic behaviour.

Keywords: Nonlinear-Granger causality; Partial Directed Coherence; Inference; Detection; Kernel Processing.

1 Introduction

Thanks to the well understood properties of linear vector autoregressive (VAR) models, convergence and asymptotics among them (Lütkepohl, 2005), they have long been the methods of choice for inferring Granger causality (Granger, 1969) even when nonlinear time series are under investigation (Schelter et al., 2006) despite their proven inability to portray polynomial couplings of even power (Massaroppe et al., 2011). Alternatives exist, both parametric (Faes et al., 2008; He et al., 2014; Pereda et al., 2005) and nonparametric (Hlaváčková-Schindler et al., 2007; Marinazzo et al., 2008; Paluš et al., 2001), they share the weakness of requiring many data points for proper convergence or, sometimes, require explicit prior knowledge of the coupling structure. Additional shortcomings stem from having to deal with many parameters and/or the minimization of nonconvex functionals.

Here we examine a new parametric approach, termed kernel-nonlinear-Partial Directed Coherence (Kannan and Tangirala, 2014) based on computing the partial directed coherence (PDC) (Baccalá and Sameshima, 2001) of properly ‘kernelized’ data. The present approach differs from Kannan and Tangirala (2014) in two important ways: (a) the use of polynomial kernels instead of the gaussian kernel adopted by the latter and (b) in the use of implicit kernel mapping generalizing Kumar and Jawahar (2007) to the multivariate time series case.

After a brief recap (Section 2), simulation of a simple model borrowed from Massaroppe et al. (2011) illustrates the potential viability (Section 3) of applying our recently developed asymptotic causality detection criteria (Baccalá et al., 2013; Takahashi et al., 2010) to this new form of PDC. We end with a brief discussion (Section 4).

2 The Method

To extend partial directed coherence (PDC) (Baccalá and Sameshima, 2001) to capture more general couplings, we propose to represent the observed data $x_i(n) \ (1 \leq i \leq N)$ through a Kernel Vector Autoregressive ($k$VAR) model

$$
\phi[x(n)] = \sum_{r=1}^{p} A^\phi(r) \phi[x(n-r)] + \phi^\phi(n), \{ \phi^\phi(n) \}_{n \in \mathbb{Z}} \sim \text{i.i.d.} \text{WN}(0, \Sigma_{\phi^\phi}),
$$

(1)
where $\phi(\cdot)$ stands for a mapping (Parzen, 1959) taking the data from its input space $\mathcal{X}$ to a suitably defined feature space $\mathbf{F}$, by choosing $\phi(\cdot)$ so that $\mathbb{E}\{\phi[x_i(n)]\phi[x_i(n - k)]\} = \mathbb{E}\{\kappa[x_i(n), x_i(n - k)]\}$ where $\kappa(\cdot)$ is a Mercer kernel.

This leads naturally to the definition of kernel-nonlinear-PDC as

$$
\kappa\pi_{ij}(f) = \frac{\overline{A}_{ij}(f)}{\sqrt{\Sigma_{ii}^{\phi}}} \left( \frac{\sigma_{ii}^{\phi}}{\kappa_{ij}^{\phi}} \right),
$$

where

$$
\overline{A}_{ij}(f) = \delta_{ij} - \sum_{l=1}^{p} a_{ij}^\phi(l)e^{-i2\pi f l}, \quad (i^2 = -1),
$$

with $a_{ij}^\phi(l)$ representing adequately fit kVAR model coefficients, while $\pi_{ij}^\phi(f)$ represent the columns of the $[\overline{A}_{ij}(f)]$ matrix.

To fit (1) we extend the univariate model fitting approach from Kumar and Jawahar (2007) to the multivariate case by rewriting it as:

$$
\Phi_i = A^\phi(XJ)^T + \Theta_i^\phi
$$

where

$$
\Phi_i = (\phi[x(1)], \ldots, \phi[x(N)]) \quad (K \times N), \quad A^\phi = (A^\phi(1), \ldots, A^\phi(p)) \quad (K \times Kp),
$$

$$
X(n) = \begin{bmatrix}
\phi[x(n)] \\
\vdots \\
\phi[x(n - p + 1)]
\end{bmatrix} \quad (Kp \times 1), \quad J_i = \begin{bmatrix}
0_{(i-Kp-1)\times Kp} \\
I_p \\
0_{(N-i-1)\times Kp}
\end{bmatrix},
$$

which upon the application of the vec operator

$$
\varphi_i = \text{vec}(\Phi_i) \quad (KN \times 1), \quad \alpha^\phi = \text{vec}(A^\phi) \quad (K^2p \times 1), \quad \theta_i^\phi = \text{vec}(\Theta_i^\phi) \quad (KN \times 1),
$$

leads to

$$
\varphi_i = (XJ_i \otimes I_K)\alpha^\phi + \theta_i^\phi,
$$

whose least squares solution

$$
\hat{\alpha}^\phi = \left( \sum_{i=p+1}^{N} J_i^T X^T X J_i \right)^{-1} \left( \sum_{i=p+1}^{N} J_i^T X^T \varphi_i \right) = \left( \sum_{i=p+1}^{N} J_i^T K J_i \right)^{-1} \left( \sum_{i=p+1}^{N} J_i^T K \varphi_i \right),
$$

where $K = X^T X$ is the block-Kernel matrix and the matrix $X^T \varphi_i$ equals $K$’s $i$-th column $= K^i$.

In computing $K$, the usual kernel centering procedure (Kumar and Jawahar, 2007; Shawe-Taylor and Cristianini, 2004) was adopted together with proper ridge regression stabilization procedures, with $\lambda = 10^{-6}$. Model orders were estimated using a suitably adapted Hannan-Quinn criterion.

Note that (4,7) generalize the univariate time series formulations of Kallas et al. (2013); Kumar and Jawahar (2007), while (2) employs the information theoretical formulation of PDC (Takahashi et al., 2010), which more closely portrays the notion of information flow between series (Baccalá and Sameshima, 2014a,b).

### 3 Numerical Illustration

To gauge approach performance we simulated the following system:

$$
\begin{bmatrix}
x_1(n) \\
x_2(n)
\end{bmatrix} = \begin{bmatrix}
2R \cos(2\pi f_0) & 0 \\
0 & \xi
\end{bmatrix} \begin{bmatrix}
x_1(n-1) \\
x_2(n-1)
\end{bmatrix} + \begin{bmatrix}
-R^2 & 0 \\
0 & 0
\end{bmatrix} \begin{bmatrix}
x_1(n-2) \\
x_2(n-2)
\end{bmatrix} + \begin{bmatrix}
0 & 0 \\
c & 0
\end{bmatrix} \begin{bmatrix}
x_1^2(n-1) \\
x_2^2(n-1)
\end{bmatrix} + \begin{bmatrix}
w_1(n) \\
w_2(n)
\end{bmatrix},
$$

with $R = 0.99$ chosen to produce a sharp resonance at $f_0 = 0.1$ and for $\xi = -0.9$, where $w_i(n)$ are independent zero mean and unit variance innovations. The quadratic coupling constant $c$ was in turn allowed
to take different values (\{0.10, 0.50, 1.00\}) and realization lengths \(N\) in \{100, 250, 500, 750, 1000\} taken after sufficiently long burn-in times as in Massaroppe et al. (2011), which also shows a sample run of this example and its allied result of linear PDC’s inability to capture coupling without prior kernelization.

Figure 1 shows the result of applying the detection criteria described in Baccalá et al. (2013) to the computed \(\text{knPDC}\) of a typical realization under a bi-quadratic kernel, showing that it is possible detect the effect \(\phi[x_1(n)] \rightarrow \phi[x_2(n)]\) at \(f = f_0 = 0.1\). Threshold computations were made based on the covariance structure from the data before kernelization.

![Figure 1: knPDC for a sample run of (9) under \(\kappa(x, y) = (x^\top y)^4\) capable of capturing the right direction \((\phi[x_1(n)] \rightarrow \phi[x_2(n)]\)) of connectivity in the feature space \((c = 1.00\) and \(N = 750\)) at confidence level of \(\alpha = 0.01\).](image)

Figure 2 contrasts knPDC ensemble behaviour with that predicted, based on the sample run result of Figure 1 at \(f = f_0 = 0.1\). Figure 3 portrays the actual ensemble data distribution against the best fits to a normal distribution \((\phi[x_1(n)] \rightarrow \phi[x_2(n)]\)) and an \(\alpha \chi^2\) distribution \((a = 0.05, \nu = 1.08\) for \(\phi[x_2(n)] \rightarrow \phi[x_1(n)]\)). Both Figures 2 and 3 point to a slightly high predicted \(\text{FP}\) rate at \(N = 750\) which is confirmed by Table 1 results where one immediately sees the \(\text{FP}\) convergence to 1% as \(N\) increases.

To investigate Baccalá et al. (2013)’s detection capabilities we performed a Monte Carlo simulation comprising 10,000 repetitions whose distribution behaviour is exemplified in Figure 3 for \(c = 1.00\) and \(N = 750\). More details for other parameters are shown on Table 1 for both quadratic and bi-quadratic kernels.

- **Table 1**: Details for other parameters are shown for both quadratic and bi-quadratic kernels.
Figure 3: Ensemble asymptotic behaviour of applying the criteria from Baccalá et al. (2013), at $f = f_0 = 0.1$ using $\kappa(x, y) = \langle x, y \rangle^4$ ($N = 750$ and $c = 1.00$), showing the approximate normal behaviour for the existing connection $\phi[x_1(n)] \rightarrow \phi[x_2(n)]$, against the distribution of the non-existing $\phi[x_2(n)] \rightarrow \phi[x_1(n)]$, compared to the expected $\chi^2$ distribution that best fits the data ($a = 0.05, \nu = 1.08$).

Table 1: Observed knPDC true positive (TP) and false positive (FP) detection rates under quadratic and bi-quadratic homogenous polynomial kernels of orders $d = 2$ and $4$, respectively, for the connections $\phi[x_1(n)] \rightarrow \phi[x_2(n)]$ and $\phi[x_2(n)] \rightarrow \phi[x_1(n)]$ ($f = f_0 = 0.1$).
4 Discussion

After introducing a generalized form of PDC and how to compute the required time series coupling model (8), we used an example to investigate the possibility that connectivity detection criteria developed for treating linear VAR models (Baccalá et al., 2013) could still be nonetheless be useful, even if only as an approximate guideline. Our simulations in the example point to reasonably good performance, approaching the expected FP rate as $N \to \infty$.

The choice of (9) was in part dictated by the possibility of making ready comparisons with results in Massaroppe et al. (2011) whose approach was based on preprocessing the data into time varying estimates of the time series approximate entropy (Pincus, 2008) and whose relationships were then investigated using linear models. Whereas that methodology managed to capture quadratic connections, in all counts, the present one outperforms the latter by dispensing with the need for approximate entropy reconstruction parameters whose values proved responsible for the large degrees of sensitivity inherent to the latter method’s results.

Our current efforts are geared towards expanding this investigation to systems whose dynamics goes beyond that of the narrow bandwidth represented by (9) and towards rigorously establishing connectivity criteria based for connectivity detection including time domain criteria as in Baccalá et al. (1998), which applied Wald type likelihood tests.

An important open issue regards kernel choice. Our preliminary evidence suggests that polyspectral analysis can be useful in this regard (Nikias and Petropulu, 1993).

Finally it is interesting to mention that bivariate causality representations involving nonlinear systems have appeared before (Marinazzo et al., 2014, 2008) though they are more akin to what we called influentiability in Baccalá and Sameshima (2014a,b) rather than to causality, because of the data partialization capability of vector autoregressive modeling.

For the present case, the optimal kernel is the (bi-)quadratic one, due to the conditions of the coupling, as (perhaps) expected. Therefore, this points to studying the present technique specially in cases of models in larger dimensions. Exploratory data analysis of further examples is under way, as is the use of kernels other than homogenous polynomials.

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References


