An overview of the quantitative causality analysis and causal graph reconstruction based on a rigorous formalism of information flow

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Abstract

Inference of causal relations from data now has become an important field in artificial intelligence. During the past 16 years, causality analysis has been developed independently in physics from first principles, and, moreover, in a quantitative sense. This short note presents a brief summary of this line of work, including part of the theory and several representative applications.

Keywords: Quantitative causality, information flow, causal graph, correlation, dynamical system, normalization, self loop

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I. INTRODUCTION

The recent rush in artificial intelligence has stimulated enormous interest in causal inference, particularly after the connection of independent causal mechanisms to semi-supervised learning, thanks to Schölkopf et al. (2012). Historically causal inference has been formulated as a problem of statistical testing; see Granger (1969) and Pearl (2009) for the classics. In parallel, it has also been investigated as a physical problem. Researches along this line include Schreiber (2000) or Paluš et al. (2001), and Liang and Kleeman (2005). Particularly, the latter is the first one formulated on a rigorous footing within the framework of dynamical systems, which yields an explicit solution in closed form, allowing for quantifying and normalizing with ease the causality between dynamical events. This short note presents a summary of this line of work, including the theory and several representative applications.

II. A GENTLE STROLL THROUGH PART OF THE THEORY

Although causality has long been studied ever since Granger’s seminal work, its “mathematization is a relatively recent development,” said Peters et al. (2017). On the other hand, Liang (2016) argued that causality is actually “a real physical notion that can be rigorously derived ab initio.” This line of work begins with Liang and Kleeman (2005), where a discovery about the information flow with two-dimensional deterministic systems was presented. A comprehensive study with generic systems has been fulfilled recently, with explicit formulas attained in closed forms; see Liang (2008) and Liang (2016). These formulas have been validated with benchmark systems such as baker transformation, Hénon map, Kaplan-Yorke map, Rössler system, to name a few. They have also been applied to real world problems in the diverse disciplines such as climate science, meteorology, turbulence, neuroscience, financial economics, etc. The following is a brief introduction of the theory.

Consider a dynamical system, which may be either a discrete-time mapping or a continuous-time system. For easy presentation, hereafter only the results with the latter are shown. (The former requires the aid of the Frobenius-Perron operator; see Liang (2016).) Let

$$d\mathbf{X} = \mathbf{F}(\mathbf{X}, t)dt + \mathbf{B}(\mathbf{X}, t)d\mathbf{W}, \quad (1)$$

be a $d$-dimensional continuous-time stochastic system for $\mathbf{X} = (X_1, ..., X_d)$, where $\mathbf{F} = (F_1, ..., F_d)$ may be arbitrary nonlinear functions of $\mathbf{X}$ and $t$, $\mathbf{W}$ is a vector of standard Wiener processes, and $\mathbf{B} = (b_{ij})$ is the matrix of perturbation amplitudes which may also be any functions of $\mathbf{X}$ and $t$. Assume that $\mathbf{F}$ and $\mathbf{B}$ are both differentiable with respect to $\mathbf{X}$ and $t$. Now define the rate of information flow, or simply information flow, from a component $X_j$ to another component $X_i$ as the contribution of entropy from $X_j$ per unit time in increasing the marginal entropy of $X_i$. We then have the following theorem (Liang, 2016):

**Theorem 1** For the system [1], the rate of information flowing from $X_j$ to $X_i$ (in nats per unit time) is

$$T_{j\rightarrow i} = -E \left[ \frac{1}{\rho_i} \int_{\mathbb{R}^{d-2}} \frac{\partial (F_i \rho_j)}{\partial x_i} d\mathbf{x}_{\bar{i}} \right] + \frac{1}{2} E \left[ \frac{1}{\rho_i} \int_{\mathbb{R}^{d-2}} \frac{\partial^2 (g_{ii} \rho_j)}{\partial x_i^2} d\mathbf{x}_{\bar{i}} \right],$$

where $\rho_i$ and $\rho_j$ are the marginal densities of $X_i$ and $X_j$, respectively.
\[\int \nabla \left( F_i \rho_j \right) \nabla \rho_j = \int \nabla \left( \nabla \cdot \left( g_{ii} \rho_j \left( x \right) \right) \right) \nabla x, \tag{2}\]

where \( \nabla x_{ij} \) signifies \( dx_1...dx_{i-1}dx_{i+1}...dx_{j-1}dx_{j+1}...dx_n \), \( E \) stands for mathematical expectation, \( g_{ii} = \sum_{k=1}^{n} b_{ik} b_{ik} \), \( \rho_i = \rho_i \left( x_i \right) \) is the marginal probability density function (pdf) of \( X_i \), \( \rho_j | i \) is the pdf of \( X_j \) conditioned on \( X_i \), and \( \rho_j \) is the pdf of \( x_j \).

Equation (2) has a nice property, which forms the basis of the information flow-based causality analysis (Liang, 2008). Without loss of generality, here the subscripts 1 and 2 are substituted by \( i \) and \( j \); same below.

**Theorem 2** If in (1) neither \( F_1 \) nor \( g_{11} \) depends on \( X_2 \), then \( T_{2 \rightarrow 1} = 0 \).

The algorithm for the information flow-based causal inference is as follows: If \( T_{j \rightarrow i} = 0 \), then \( X_j \) is not causal to \( X_i \); otherwise it is causal, and the absolute value measures the magnitude of the causality from \( X_j \) to \( X_i \).

Another property regards the invariance upon coordinate transformation, indicating that the obtained information flow is an intrinsic property in nature (Liang, 2018).

**Theorem 3** \( T_{2 \rightarrow 1} \) is invariant under arbitrary nonlinear transformation of \( (X_3, X_4, ..., X_d) \).

As shown in Liang (2021) (and other publications), this is very important in causal graph reconstruction. It together with Theorem 2 makes it promising toward a solution of the problem of latent confounding.

For linear systems, the formula in (2) can be simplified.

**Theorem 4** In (1), if \( F(X) = f + AX \), and the matrix \( B \) is constant, then

\[ T_{j \rightarrow i} = a_{ij} \frac{\sigma_{ij}}{\sigma_{ii}}, \tag{3} \]

where \( a_{ij} \) is the \((i, j)\)th entry of \( A \) and \( \sigma_{ij} \) the population covariance between \( X_i \) and \( X_j \).

Notice if \( X_i \) and \( X_j \) are not correlated, then \( \sigma_{ij} = 0 \), which yields a zero causality: \( T_{j \rightarrow i} = 0 \). But conversely it is not true. We hence have the following corollary:

**Corollary 1** In the linear sense, causation implies correlation, but not vice versa.

In an explicit expression, this corollary fixes the debate on causation vs. correlation ever since George Berkeley (1710).

In the case with only time series (no dynamical system is given), we have the following result (Liang, 2021):

**Theorem 5** Given \( d \) time series \( X_1, X_2, ..., X_d \), under the assumption of a linear model with additive noise, the maximum likelihood estimator (mle) of (2) for \( T_{2 \rightarrow 1} \) is

\[ \hat{T}_{2 \rightarrow 1} = \frac{1}{\det C} \cdot \sum_{j=1}^{d} \Delta_{2j} C_{j,d1} \cdot \frac{C_{12}}{C_{11}}, \tag{4} \]

where \( C_{ij} \) is the sample covariance between \( X_i \) and \( X_j \), \( \Delta_{ij} \) the cofactors of the matrix \( C = (C_{ij}) \), and \( C_{i,dj} \) the sample covariance between \( X_i \) and a series derived from \( X_j \) using the Euler forward differencing scheme: \( \hat{X}_{j,n} = (X_{j,n+k} - X_{j,n})/(k\Delta t) \), with \( k \geq 1 \) some integer.
Eq. (4) is rather concise in form, involving only the common statistics, i.e., sample covariances. The transparent formula makes causality analysis, which otherwise would be complicated, very easy and computationally efficient. Note, however, that Eq. (4) cannot replace (2); it is just the maximum likelihood estimator (mle) of the latter. One needs to test the statistical significance before making a causal inference based on the estimator $\hat{T}_{2\rightarrow 1}$.

If what are given are not time series, but independent, identically distributed (i.i.d.) panel data, it has been shown that $\hat{T}_{2\rightarrow 1}$ has the same form as (4); see Rong and Liang (2021).

Besides the information flow between two components, say $X_1$ and $X_2$, it is also possible to estimate the influence of one component, say $X_1$, on itself. Following the convention since Liang and Kleeman (2005), write it as $dH_1^* / dt$.

**Theorem 6** Under a linear assumption, the mle of $dH_1^* / dt$ is

$$
\left( \frac{dH_1^*}{dt} \right) = \frac{1}{\det C} \cdot \sum_{j=1}^{d} \Delta_{1j} C_{j,1} dt.
$$

(5)

This result, first obtained in Liang (2014), provides an efficient approach to identifying self loops in a causal graph (cf. Hyttinen et al., 2012).

Statistical significance tests can be performed for the estimators. This is done with the aid of a Fisher information matrix. See Liang (2014) and Liang (2021) for details.

Causality in this sense can be normalized in order to reveal the relative importance of a causal relation. See Liang (2015) for details. Note that recently there has some similar developments along this line, e.g., Røysland (2012), Moij et al. (2013), and Mogensen et al. (2018). We want to mention that the above formalism appears 7-13 years earlier, and, to our best knowledge, it is the first one studying causality within the framework of dynamical systems.

### III. SOME REPRESENTATIVE APPLICATIONS

The above rigorous formalism has been successfully put to application to many real world problems such as tropical cyclone genesis prediction (Bai et al., 2018), near-wall turbulence (Liang and Lozano-Durán, 2016), global climate change (Stips et al., 2016), financial analysis (Lu et al., 2020; Liang, 2015), soil moisture-precipitation interaction (Hagan et al., 2018), neuroscience problems (Hristopulos et al., 2019), El Niño (Liang et al., 2021), to name a few. Among these we want to particularly mention the study by Stips et al. (2016) on CO$_2$ emission vs. global warming. They found that CO$_2$ emission does drive the recent global warming during the past century, and the causal relation is one-way. However, on a time scale of 1000 years or up, this one-way causality is is completely reversed, becoming a causality from air temperature to carbon dioxide. In other words, on the paleoclimate scale, it is global warming that drives the CO$_2$ emission! This remarkable result is consistent with that inferred from the recent ice-core data from Antarctica.

Another interesting application (Liang, 2015) regards the relation between the two corporations IBM and GE, using the time series of US stocks downloaded from YAHOO! finance. Overall the causality between the two is insignificant, but if a running time causality analysis is performed, there appears a strong, almost one-way causality from IBM to GE in 70’s, starting from 1971. This abrupt one-way causality out of blue reveals to us an old story about
“Seven Dwarfs and a Giant”: In 50-60’s, GE was believed to be the biggest computer user outside the U.S. Federal Government; to avoid relying on IBM the computer “Giant”, it together with six other companies (“Seven Dwarfs”) began to build mainframes. GE itself of course is a giant, but in the computer market, it is just a “Dwarf”. Since it could not beat IBM, in 1970, it sold its computer division. As a result, starting from 1971, it had to rely on IBM again. This is the story behind the jump in $T_{IBM\rightarrow GE}$ from 1970 to 1971. While the story has almost gone to oblivion, this finding, which is solely based on a simple causality analysis of two time series with Eq. (4), is really remarkable.

Figure 1: El Niño prediction has become a benchmark problem for the testing of machine learning algorithms. The present wisdom is that El Niño may be predicted at a lead time of 1-2 years. Shown here are 1000 predictions (pink) of the El Niño Modoki index (EMI) as described in the text. Overlaid are the observed EMI (blue), the mean of the realizations (cyan). The light shading marks the period for validation, while the darker shading marks the prediction period. (From Liang et al., 2021.)

The latest application on the prediction of El Niño Modoki, or Central-Pacific type El Niño, is also a remarkable one. El Niño is a climate mode that has been linked to many hazards globewide, e.g., flooding, drought, wild fires, heat waves, etc. Its accurate forecasting is of great importance to many sectors of our society such as agriculture, energy, hydrology, to name several. With its societal importance and the elegant setting, El Niño prediction has become a testbed for AI algorithms.

Currently the wisdom for El Niño prediction is that it may be predictable at a lead time of 1-2 years. However, there still exists much uncertainty; an example is the 2014-16 “Monster El Niño,” almost all projections fell off the mark. Among the El Niño varieties, it is believed that El Niño Modoki is particularly difficult to predict.

A striking breakthrough has just been made. Liang et al. (2021) took advantage of the quantitative nature of the above information flow-based causality analysis, and identified a delayed causal pattern, i.e., the structure of the information flow from the solar activity to the sea surface temperature, very similar to the El Niño Modoki mode. They then conjectured that, based on the series of sunspot numbers, El Niño Modoki should be predictable. This is indeed the case, and, remarkably, the prediction can be at a lead time of as long as 10 years or up! This remarkable progress, among others, is a result of the rigorously formulated quantitative causality analysis.
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