Information Flows? A Critique of Transfer Entropies

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Information Flows?
A Critique of Transfer Entropies

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A central task in analyzing complex dynamics is to determine the loci of information storage and the communication topology of information flows within a system. Over the last decade and a half, diagnostics for the latter have come to be dominated by the *transfer entropy*. Via straightforward examples, we show that it and a derivative quantity, the *causation entropy*, do not, in fact, quantify the flow of information. At one and the same time they can overestimate flow or underestimate influence. We isolate why this is the case and propose several avenues to alternate measures for information flow. We also address an auxiliary consequence: The proliferation of networks as a now-common theoretical model for large-scale systems, in concert with the use of transfer-like entropies, has shoehorned dyadic relationships into our structural interpretation of the organization and behavior of complex systems. This interpretation thus fails to include the effects of *polyadic* dependencies. The net result is that much of the sophisticated organization of complex systems may go undetected.

Keywords: stochastic process, transfer entropy, causation entropy, partial information decomposition, network science

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An important task in understanding a complex system is determining its information dynamics and information architecture—what mechanisms generate information, where is that information stored, and how is it transmitted within a system? While this pursuit goes back perhaps as far as Shannon's foundational work on communication [1], in many ways it was Kolmogorov [2–4] who highlighted the transmission of information from the micro- to the macroscales as central to the behavior of complex systems. Later, Lin showed that "information flow" is key to understanding network controllability [5] and Shaw speculated that such flows between information sources and sinks is a necessary descriptive framework for spatially extended chaotic systems—an alternative to narratives based on tracking energy flows [6, Sec. 14].

A common thread in these works is quantifying the flow of information. To facilitate our discussion, let's first consider an intuitive definition: Information flow from process X to process Y is the existence of information that is *currently* in Y, the "cause" of which can be *solely* attributed to X's *past*. If information can be solely attributed in such a manner, we refer to it as *localized*. This notion of localized flow mirrors the intuitive general definitions of "causal" flow proposed by Granger [7] and, before that, Wiener [8].

Ostensibly to measure information flow—and notably much later than the above efforts—Schreiber introduced the transfer entropy [9] as the information shared between X's past and the present Y_t, conditioning on information from Y's past. Perhaps not surprisingly, given the broad and pressing need to probe the organization of modern life's increasingly complex systems, the transfer entropy's use has been substantial—over the last decade and a half, its introduction alone garnered an average of 100 citations per year.

The primary goal of the following is to show that the transfer entropy does not, in fact, measure information flow, specifically in that it attributes an information source to influences that are not localizable and so not flows. We draw out the interpretational errors, some quite subtle, that result—including overestimating flow, underestimating influence, and more generally misidentifying structure when modeling complex systems as networks with edges given by transfer entropies.

Identifying shortcomings in the transfer entropy is not new. Smirnov [10] pointed out three: Two relate to how it responds to using undersampled empirical distributions and are therefore not conceptual issues with the measure. The third, however, was its inability to differentiate indirect influences from direct influences. This weakness motivated Sun and Bollt to propose the causation entropy [11]. While their measure does allow differentiating between direct and indirect effects via the addition of a third hidden variable, it too ascribes an information source to unlocalizable influences.

Our exposition reviews the notation and information theory needed and then considers two rather similar examples—one involving influences between two processes and the other, influences among three. They make operational what we mean by "localized", "flow", and "influence", leading to the conclusion that the transfer entropy fails to capture information flow. We close by discussing a distinctive philosophy underlying our critique and then turn to possible resolutions and to concerns about modeling practice in network science.

Background Following standard notation [12], we denote random variables with capital letters and their associated outcomes using lower case. For example, the observation of a coin flip might be denoted X, while the coin actually landing Heads or Tails would be x. Emphasizing temporal processes, we subscript a random variable with a time index; *e.g.*, the random variable representing a coin flip at time t is denoted X_t. We denote a temporally contiguous block of random variables (a time series) using a Python slice-like notation $X_{i:j} = X_i X_{i+1} \ldots X_{j-1}$, where the final index is exclusive. When X_t is distributed according to $\Pr(X_t)$, we denote this as $X_t \sim \Pr(X_t)$. We assume familiarity with basic information measures, specifically the Shannon entropy $\mathrm{H}[X]$, mutual information $\mathrm{I}[X : Y]$, and their conditional forms $\mathrm{H}[X \mid Z]$ and $\mathrm{I}[X : Y \mid Z]$ [12].

The *transfer entropy* $\mathrm{T}_{X \to Y}$ from time series X to time series Y is the information shared between X's past and Y's present, given knowledge of Y's past [9]:

$$\mathrm{T}_{X \to Y} = \mathrm{I}[Y_t : X_{0:t} \mid Y_{0:t}] \ . \qquad (1)$$

Intuitively, this quantifies how much better one predicts Y_t using both $X_{0:t}$ and $Y_{0:t}$ over using $Y_{0:t}$ alone. A nonzero value of the transfer entropy certainly implies a kind of influence of X on Y. Our questions are: Is this influence necessarily via information flow? Is it necessarily direct?

Addressing the last question, the *causation entropy* $\mathcal{C}_{X \to Y \mid (Y,Z)}$ is similar to the transfer entropy, but conditions on the past of a third (or more) time series [11]:

$$\mathcal{C}_{X \to Y \mid (Y,Z)} = \mathrm{I}[Y_t : X_{0:t} \mid Y_{0:t}, Z_{0:t}] \ . \qquad (2)$$

(It is also known as the *conditional transfer entropy*.) The primary improvement over $\mathrm{T}_{X \to Y}$ is the causation entropy's ability to determine if a dependency is indirect (*i.e.*, mediated by the third process Z) or not. Consider, for example, the following system $X \to Z \to Y$: variable X influences Z and Z in turn influences Y. Here, any influence that X has on Y must pass through Z. In this case, the transfer entropy $\mathrm{T}_{X \to Y} > 0$ bit even though X does not directly influence Y. The causation entropy $\mathcal{C}_{X \to Y \mid (Y,Z)} = 0$ bit, however, due to conditioning on Z.

Many concerns and pitfalls in applying information measures comes not in their definition, estimation, or derivation of associated properties. Rather, many arise in *interpreting* results. Properly interpreting the meaning of a measure can be the most subtle and important task we face when using measures to analyze a system's structure, as we will now demonstrate. Furthermore, while these examples may seem pathological, they were chosen for their transparency and simplicity; similar failures arise in Gaussian systems [13] signifying that the issue at hand is widespread.

Example: Two Time Series Consider two time series, say X and Y, given by the probability laws:

$$X_t \sim \begin{cases} 0 & \text{with probability } 1/2 \\ 1 & \text{with probability } 1/2 \end{cases} ,$$

$$Y_0 \sim \begin{cases} 0 & \text{with probability } 1/2 \\ 1 & \text{with probability } 1/2 \end{cases} , \text{ and}$$

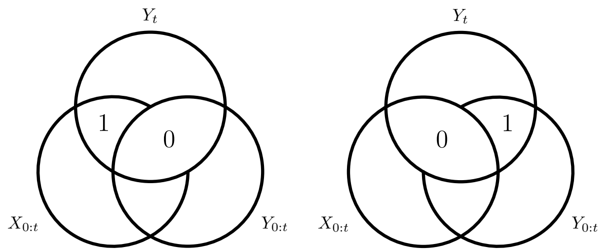
$$Y_t = X_{t-1} \oplus Y_{t-1} \ ;$$

that is, X_t and Y_0 are independent and take values 0 and 1 with equal probability, and y_t is the *Exclusive Or* of the prior values x_{t-1} and y_{t-1}. By a straightforward calculation we find that $\mathrm{T}_{X \to Y} = 1$ bit. Does this mean that one bit of information is being *transferred* from X to Y at each time step? Let's take a closer look.

We first observe that the amount of information in Y_t is $\mathrm{H}[Y_t] = 1$ bit. Therefore, the uncertainty in Y_t can be reduced by at most 1 bit. Furthermore, the information shared by Y_t and the prior behavior of the two time series is $\mathrm{I}[Y_t : (X_{0:t}, Y_{0:t})] = 1$ bit. And so, the 1 bit of Y_t's uncertainty in fact can be removed by the prior observations of both time series.

How much does $Y_{0:t}$ alone help us predict Y_t? We quantify this using mutual information. Since $\mathrm{I}[Y_t : Y_{0:t}] = 0$ bit, the variables are independent: $Y_{0:t}$ alone does not help in predicting Y_t. However, knowing $Y_{0:t}$, how much does $X_{0:t}$ help in predicting Y_t? The conditional mutual information $\mathrm{I}[Y_t : X_{0:t} \mid Y_{0:t}] = 1$ bit—the transfer entropy we just computed—quantifies this. This situation is graphically analyzed via the *I-Diagram* [14] in Fig. 1a.

To obtain a more complete picture of the information dynamics under consideration, let's reverse the order in which the time series are queried. The mutual information



(a) $Y_{0:t}$ alone does not predict Y_t. (The -shaped region $\mathrm{I}[Y_{0:t} : Y_t] = 0\,\mathrm{bit}$.) However, when used in conjunction with $X_{0:t}$, they completely predict its value. (The -shaped region $\mathrm{I}[X_{0:t} : Y_t \mid Y_{0:t}] = 1\,\mathrm{bit}$.)

(b) X's past $X_{0:t}$ alone does not aid in predicting Y_t. (The -shaped region $\mathrm{I}[X_{0:t} : Y_t] = 0\,\mathrm{bit}$.) However, given knowledge of $X_{0:t}$, then $Y_{0:t}$ can predict Y_t. (The -shaped region $\mathrm{I}[Y_{0:t} : Y_t \mid X_{0:t}] = 1\,\mathrm{bit}$.)

FIG. 1. Two complementary ways to view the information shared between $X_{0:t}, Y_{0:t}$, and Y_t. In each I-Diagram, a circle represents a random variable whose area measures the random variable's entropy. Overlapping regions are information that is shared. The transfer entropy is a conditional mutual information; a region where two random variables overlap, but that falls outside the random variable being conditioned on.

$\mathrm{I}[Y_t : X_{0:t}] = 0\,\mathrm{bit}$ tells us that the X time series alone does not help predict Y_t. However, the conditional mutual information $\mathrm{I}[Y_t : Y_{0:t} \mid X_{0:t}] = 1\,\mathrm{bit}$. And so, from this point of view it is Y's past that helps predict Y_t, contradicting the preceding analysis. This complementary situation is presented diagrammatically in Fig. 1b.

How can we rectify the seemingly inconsistent conclusions drawn by these two lines of reasoning? The answer is quite straightforward: the 1 bit of information about Y_t does not come from *either* time series individually, but rather from *both* of them simultaneously. (In fact, the I-Diagrams are naturally consistent, once one recognizes that the *co-information* [15], the inner-most information atom, is $\mathrm{I}[Y_t : X_{0:t} : Y_{0:t}] = -1\,\mathrm{bit}$.)

In short, the 1 bit of reduction in uncertainty $\mathrm{H}[Y_t]$ should not be *localized* to either time series. The transfer entropy, however, erroneously localizes this information to $X_{0:t}$. In light of this, the transfer entropy *overestimates* information flow.

This example shows that the transfer entropy can be positive due not to information flow, but rather to nonlocalizable influence—in this case, a *conditional dependence* between variables. This suggests that, though inappropriate for measuring information flow, the transfer entropy may be a viable measure of such influence. Our next example illustrates that this too is incorrect.

Example: Three Time Series Our second example parallels the first. Before, we considered the case where *one* of two time series is determined by the past of *both*, we now consider the case where *two* time series determine a *third*, again via an Exclusive Or operation. Their probability laws are:

$$X_t \sim \begin{cases} 0 & \text{with probability } 1/2 \\ 1 & \text{with probability } 1/2 \end{cases} ,$$

$$Y_t \sim \begin{cases} 0 & \text{with probability } 1/2 \\ 1 & \text{with probability } 1/2 \end{cases} , \text{ and}$$

$$Z_t = X_{t-1} \oplus Y_{t-1} ,$$

in which z_0's value is irrelevant. Unlike the prior example, the transfer entropy from either X or Y to Z is zero: $\mathrm{T}_{X \to Z} = \mathrm{T}_{Y \to Z} = 0\,\mathrm{bit}$, and it therefore *underestimates* influence that is present. Furthermore, the relevant pairwise mutual informations all vanish: $\mathrm{I}[Z_t : X_{0:t}] = \mathrm{I}[Z_t : Y_{0:t}] = \mathrm{I}[Z_t : Z_{0:t}] = 0\,\mathrm{bit}$. The time series are pairwise independent.

Given that we are probing the influences between three time series, it is natural now to consider the behavior of the causation entropy. In this case, we have $\mathcal{C}_{X \to Z|(Y,Z)} = \mathcal{C}_{Y \to Z|(X,Z)} = 1\,\mathrm{bit}$, indicating that given the past behavior of Z and X (or Y), the past of Y (or X) can be used to predict the behavior of Z_t. Like before, this 1 bit of information cannot be localized to either X or Y and so it is inaccurate to ascribe the 1 bit of information in Z_t to either X or Y alone. In this way, the causation entropy also erroneously localizes the 1 bit of joint influence. While the causation entropy succeeds here as a measure of nonlocalizable influence, as a measure of information flow, it overestimates. These information quantities are displayed in the I-Diagram in Fig. 2.

Discussion We see that transfer-like entropies can both overestimate information flow (first example) and underestimate influence (second example). The primary misunderstanding of these quantities stems from a mischaracterization of the conditional mutual information. Most basically, probabilistic conditioning is not a "subtractive" operation: $\mathrm{I}[X : Y \mid Z]$ is not the information shared by X and Y once the influences of Z have been removed. Rather, it is the information shared by X and Y *taking into account* Z. This is not a game of mere semantics: Conditioning can *increase* the information shared between two processes: $\mathrm{I}[X : Y] < \mathrm{I}[X : Y \mid Z]$. This cannot happen if conditioning merely removed influence: conditional dependence includes *additional* dependence that occurs in the presence of a third variable [16]. Measuring information flow—as we have defined it—requires a method of *localizing* information. Since simple conditioning can fail to localize information, the transfer

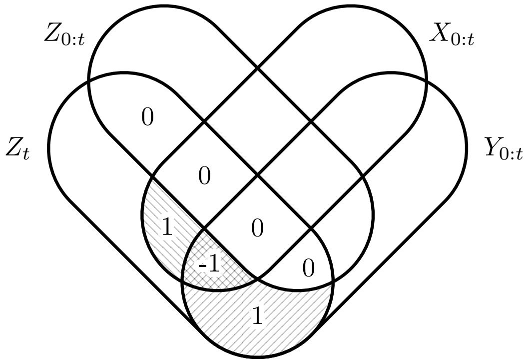


FIG. 2. I-Diagram depicting both transfer entropies and causation entropies for three times series X, Y, and Z. $\mathrm{T}_{X\to Z} = 0$ bit corresponds to the two regions shaded with south-east sloping lines and $\mathrm{T}_{Y\to Z} = 0$ bit, the two regions shaded with north-east sloping lines. $\mathcal{C}_{X\to Z|(Y,Z)} = 1$ bit is the region containing only south-east sloping lines and, similarly, $\mathcal{C}_{Y\to Z|(X,Z)} = 1$ bit is the region containing only north-east sloping lines.

entropy, causation entropy, and other measures utilizing the conditional mutual information can fail as measures of information flow.

Another way to understand conditional dependence is through the *partial information decomposition* [17]. Within this framework, the mutual information between two random variables X_1 and X_2 (call them *inputs*) and a third random variable Y (the *output*) is decomposed into four mutually exclusive components: $\mathrm{I}[(X_1, X_2) : Y] = R + U_1 + U_2 + S$. R quantifies how the inputs *redundantly* inform the output Y, U_1 and U_2 quantify how each provides *unique* information to Y, and finally S quantifies how the inputs together *synergistically* inform the output. In this decomposition, the mutual information between one input and the output is equal to what uniquely comes from that input plus what is redundantly provided by both inputs; $\mathrm{I}[X_1 : Y] = R + U_1$, for example. However, the mutual information between that input and the output conditioned on the other input is equal to what uniquely comes from that one input, plus what is synergistically provided by both inputs: $\mathrm{I}[X_1 : Y \mid X_2] = U_1 + S$. In other words, conditioning removes the redundant information, but adds the synergistic information. Here, conditional dependencies manifest themselves as synergy.

Treating $X_{0:t}$ and $Y_{0:t}$ as inputs and Y_t as output, the partial information decomposition identifies the transfer entropy $\mathrm{T}_{X\to Y}$ as the sum of the unique information from $X_{0:t}$ plus the synergistic information from both $X_{0:t}$ and $Y_{0:t}$ together. It seems natural, and has been previously proposed [13, 18], to associate only this unique information with information flow. The transfer entropy, however, conflates unique information and synergistic information leading to inconsistencies, such as analyzed in the examples. Similar conclusions follow for the causation entropy; however, due to the additional variable, the analysis is more involved.

Though there is as yet no broadly accepted quantification of unique information [19], if one were able to accurately measure it, it may prove to be a viable measure of information flow. It is notable that Stramaglia *et al.*, building on Ref. [20], considered how total synergy and redundancy of a collection of variables influence each other [21].

Other quantifications of information flow between time series have been proposed. The *directed information* [22] is essentially a sum of transfer entropies and so inherits the same flaws. Furthermore, both the transfer entropy and directed information have been shown to be generalizations of *Granger causality* [7, 23–25], itself purportedly a measure of "predictive causality" [26]. Ay and Polani proposed a measure of information flow based on active intervention in which an outside agent modifies the system in question by removing components [27]. We conjecture that all these measures suffer for the same reasons—conflation of dyadic and polyadic relationships.

Conclusions and Consequences Although the examples were intentionally straightforward, the consequences appear far-reaching. Let's consider network science [28] which, over the same decade and a half period since the introduction of the transfer entropy, has developed into a vast and vibrant field, with significant successes in many application areas. Standard (graph-based) networks are composed of *nodes*, representing system observables, and *edges*, representing relationships between them. As commonly practiced, such networks represent dyadic (binary) relationships between nodes [29]—article co-authorship, power transmission between substations, and the like. It would seem, then, that much of the popularity of using the transfer entropy to analyze large-scale complex systems is that it is an information measure specifically adapted to quantifying dyadic relationships. Such a tool goes hand-in-hand with standard network modeling.

As the examples emphasized, though, observables may be related by polyadic relationships that cannot be naturally represented on a standard network as commonly practiced. For example, all three variables in our second example are pairwise independent. A standard network representing dependence between them therefore consists of three disconnected nodes, thus failing to capture the dependence between variables that is, in fact, present. As a start to repair this deficit, it would be more appropriate to represent such a complex system as a *hypergraph* [30, 31].

Continuing this line of thought, if one believes that a standard network is an accurate model of a complex system, then one implicitly assumes that polyadic relationships are either not important or do not exist. Said this way, it is clear that when modeling a complex system, one must test for this lack of polyadic relationship first. With this assumption generally unspoken, though, it is not surprising that a nonzero value of the transfer entropy leads analysts to interpret it as information flow. Within that narrow view, indeed, how else could one time series influence another if all interactions are dyadic? Restated, when a system is modeled as a standard network, all relationships are assumed to be dyadic. One is therefore naturally inclined to explain all observed dependencies as being dyadic. The cost, of course, is either a greatly impoverished or a spuriously embellished view of organization in the world. As such, modeling a complex system by way of a graph with edges determined by transfer or causation entropies is intrinsically flawed.

Many of the preceding issues are difficult to analyze since at present notions of "influence" are not sufficiently precise and, even when they are as with the use of information diagrams and measures and the partial information decomposition, there is a combinatorial explosion in possible types of dependence relationships. Said differently, what one needs is a more explicit, even more elementary, structural view of how one process can be transformed to another. Paralleling the canonical ϵ-machine minimal sufficient statistic representation of stationary processes, two of us (NB and JPC) recently introduced a minimal optimal transformation of one process into another, the ϵ-transducer [32]. This provides a structural representation for the minimal optimal predictor of one process about another. The corresponding analysis, hinted at above in Figs. 1 and 2, identifies new informational atoms beyond those of the transfer entropies [33].

In short, the transfer entropy can both overestimate information flow (first example) and underestimate influence (second example). These effects are compounded when viewing complex systems as standard networks since the latter further misconstrue polyadic relationships. While we do not object to the transfer entropy as a measure of the reduction in uncertainty about one time series given another, we do find its mechanistic interpretation as information *flow* or *transfer* to be incorrect. In fact, this is true for any related measures—such as the causation entropy—that are based on conditional mutual information between observed variables. In light of these interpretational concerns, it seems that several recent works that rely heavily on transfer-like entropies—ranging from cellular automata [34] and information thermodynamics [35] to cell regulatory networks [36] and consciousness [37]—will benefit from a close reexamination.

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