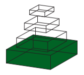
frontiers in
ROBOTICS AND AI

METHODS ARTICLE
published: 02 December 2014
doi: 10.3389/frobt.2014.00011



JIDT: an information-theoretic toolkit for studying the dynamics of complex systems

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Complex systems are increasingly being viewed as distributed information processing systems, particularly in the domains of computational neuroscience, bioinformatics, and artificial life. This trend has resulted in a strong uptake in the use of (Shannon) information-theoretic measures to analyze the dynamics of complex systems in these fields. We introduce the Java Information Dynamics Toolkit (JIDT): a Google code project, which provides a standalone (GNU GPL v3 licensed) open-source code implementation for empirical estimation of information-theoretic measures from time-series data. While the toolkit provides classic information-theoretic measures (e.g., entropy, mutual information, and conditional mutual information), it ultimately focuses on implementing higher-level measures for information dynamics. That is, JIDT focuses on quantifying information storage, transfer, and modification, and the dynamics of these operations in space and time. For this purpose, it includes implementations of the transfer entropy and active information storage, their multivariate extensions and local or pointwise variants. JIDT provides implementations for both discrete and continuous-valued data for each measure, including various types of estimator for continuous data (e.g., Gaussian, box-kernel, and Kraskov–Stögbauer–Grassberger), which can be swapped at run-time due to Java's object-oriented polymorphism. Furthermore, while written in Java, the toolkit can be used directly in MATLAB, GNU Octave, Python, and other environments. We present the principles behind the code design, and provide several examples to guide users.

Keywords: information transfer, information storage, complex systems, complex networks, information theory, transfer entropy, Java, MATLAB

1. INTRODUCTION

Information theory was originally introduced by Shannon (1948) to quantify fundamental limits on signal processing operations and reliable communication of data (Cover and Thomas, 1991; MacKay, 2003). More recently, it is increasingly being utilized for the design and analysis of complex self-organized systems (Prokopenko et al., 2009). *Complex systems* science (Mitchell, 2009) is the study of large collections of entities (of some type), where the global system behavior is a non-trivial result of the local interactions of the individuals, e.g., emergent consciousness from neurons, emergent cell behavior from gene regulatory networks and flocks determining their collective heading. The application of information theory to complex systems can be traced to the increasingly popular perspective that commonalities between complex systems may be found "in the way they handle information" (Gell-Mann, 1994). Certainly, there have been many interesting insights gained from the application of traditional information-theoretic measures such as entropy and mutual information to study complex systems, for example, proposals of candidate complexity measures (Tononi et al., 1994; Adami, 2002), characterizing order-chaos phase transitions (Miramontes, 1995; Solé and Valverde, 2001; Prokopenko et al., 2005, 2011), and measures of network structure (Solé and Valverde, 2004; Piraveenan et al., 2009).

More specifically though, researchers are increasingly viewing the global behavior of complex systems as emerging from the *distributed information processing*, or *distributed computation*, between the individual elements of the system (Langton, 1990; Mitchell, 1998; Fernández and Solé, 2006; Wang et al., 2012; Lizier, 2013), e.g., collective information processing by neurons (Gong and van Leeuwen, 2009). Computation in complex systems is examined in terms of: how information is transferred in the interaction between elements, how it is stored by elements, and how these information sources are non-trivially combined. We refer to the study of these operations of *information storage, transfer, and modification*, and in particular, how they unfold in space and time, as *information dynamics* (Lizier, 2013; Lizier et al., 2014).

Information theory is the natural domain to quantify these operations of information processing, and we have seen a number of measures recently introduced for this purpose, including the well-known transfer entropy (Schreiber, 2000), as well as active information storage (Lizier et al., 2012b) and predictive information (Bialek et al., 2001; Crutchfield and Feldman, 2003). Natural affinity aside, information theory offers several distinct

advantages as a measure of information processing in dynamics[1], including its model-free nature (requiring only access to probability distributions of the dynamics), ability to handle stochastic dynamics, and capture non-linear relationships, its abstract nature, generality, and mathematical soundness.

In particular, this type of information-theoretic analysis has gained a strong following in computational neuroscience, where the transfer entropy has been widely applied (Honey et al., 2007; Vakorin et al., 2009; Faes et al., 2011; Ito et al., 2011; Liao et al., 2011; Lizier et al., 2011a; Vicente et al., 2011; Marinazzo et al., 2012; Stetter et al., 2012; Stramaglia et al., 2012; Mäki-Marttunen et al., 2013; Wibral et al., 2014b,c) (for example, for effective network inference), and measures of information storage are gaining traction (Faes and Porta, 2014; Gómez et al., 2014; Wibral et al., 2014a). Similarly, such information-theoretic analysis is popular in studies of canonical complex systems (Lizier et al., 2008c, 2010, 2012b; Mahoney et al., 2011; Wang et al., 2012; Barnett et al., 2013), dynamics of complex networks (Lizier et al., 2008b, 2011c, 2012a; Damiani et al., 2010; Damiani and Lecca, 2011; Sandoval, 2014), social media (Bauer et al., 2013; Oka and Ikegami, 2013; Steeg and Galstyan, 2013), and in artificial life and modular robotics both for analysis (Lungarella and Sporns, 2006; Prokopenko et al., 2006b; Williams and Beer, 2010a; Lizier et al., 2011b; Boedecker et al., 2012; Nakajima et al., 2012; Walker et al., 2012; Nakajima and Haruna, 2013; Obst et al., 2013; Cliff et al., 2014) and design (Prokopenko et al., 2006a; Ay et al., 2008; Klyubin et al., 2008; Lizier et al., 2008a; Obst et al., 2010; Dasgupta et al., 2013) of embodied cognitive systems (in particular, see the "Guided Self-Organization" series of workshops, e.g., (Prokopenko, 2009)).

This paper introduces *JIDT* – the *Java Information Dynamics Toolkit* – which provides a standalone implementation of information-theoretic measures of dynamics of complex systems. JIDT is open-source, licensed under GNU General Public License v3, and available for download via Google code at http://code.google.com/p/information-dynamics-toolkit/. JIDT is designed to facilitate *general-purpose* empirical estimation of information-theoretic measures from time-series data, by providing easy to use, portable implementations of measures of information transfer, storage, shared information, and entropy.

We begin by describing the various information-theoretic measures, which are implemented in JIDT in Section 2.1 and Section S.1 in Supplementary Material, including the basic entropy and (conditional) mutual information (Cover and Thomas, 1991; MacKay, 2003), as well as the active information storage (Lizier et al., 2012b), the transfer entropy (Schreiber, 2000), and its conditional/multivariate forms (Lizier et al., 2008c, 2010). We also describe how one can compute *local* or *pointwise* values of these information-theoretic measures at specific observations of time-series processes, so as to construct their *dynamics* in time. We continue to then describe the various estimator types, which are implemented for each of these measures in Section 2.2 and Section S.2 in Supplementary Material (i.e., for discrete or binned data, and Gaussian, box-kernel, and Kraskov–Stögbauer–Grassberger estimators). Readers familiar with these measures and their estimation may wish to skip these sections. We also summarize the capabilities of similar information-theoretic toolkits in Section 2.3 (focusing on those implementing the transfer entropy).

We then turn our attention to providing a detailed introduction of JIDT in Section 3, focusing on the current version 1.0 distribution. We begin by highlighting the unique features of JIDT in comparison to related toolkits, in particular, in providing *local* information-theoretic measurements of dynamics; implementing conditional, and other multivariate transfer entropy measures; and including implementations of other related measures including the active information storage. We describe the (almost 0) installation process for JIDT in Section 3.1: JIDT is standalone software, requiring no prior installation of other software (except a Java Virtual Machine), and no explicit compiling or building. We describe the contents of the JIDT distribution in Section 3.2, and then in Section 3.3 outline, which estimators are implemented for each information-theoretic measure. We then describe the principles behind the design of the toolkit in Section 3.4, including our object-oriented approach in defining interfaces for each measure, then providing multiple implementations (one for each estimator type). Sections 3.5 and 3.7 then describe how the code has been tested, how the user can (re-)build it, and what extra documentation is available (principally the project wiki and Javadocs).

Finally, and most importantly, Section 4 outlines several demonstrative examples supplied with the toolkit, which are intended to guide the user through how to use JIDT in their code. We begin with simple Java examples in Section 4.1 that includes a description of the general pattern of usage in instantiating a measure and making calculations, and walks the user through differences in calculators for discrete and continuous data, and multivariate calculations. We also describe how to take advantage of the polymorphism in JIDT's object-oriented design to facilitate run-time swapping of the estimator type for a given measure. Other demonstration sets from the distribution are presented also, including basic examples using the toolkit in MATLAB, GNU Octave, and Python (Sections 4.2 and 4.3); reproduction of the original transfer entropy examples from Schreiber (2000) (Section 4.4); and local information profiles for cellular automata (Section 4.5).

2. INFORMATION-THEORETIC MEASURES AND ESTIMATORS

We begin by providing brief overviews of information-theoretic measures (Section 2.1) and estimator types (Section 2.2) implemented in JIDT. These sections serve as summaries of Sections S.1 and S.2 in Supplementary Material. We also discuss related toolkits implementing some of these measures in Section 2.3.

2.1. INFORMATION-THEORETIC MEASURES

This section provides a brief overview of the information-theoretic measures (Cover and Thomas, 1991; MacKay, 2003), which are implemented in JIDT. All features discussed are available in JIDT unless otherwise noted. *A more complete description for each measure is provided in* Section S.1 in Supplementary Material.

We consider measurements x of a random variable X, with a probability distribution function (PDF) $p(x)$ defined over the

[1]Further commentary on links between information-theoretic analysis and traditional dynamical systems approaches are discussed by Beer and Williams (2014).

alphabet α_x of possible outcomes for x (where $\alpha_x = \{0, \ldots, M_X - 1\}$ without loss of generality for some M_X discrete symbols).

The fundamental quantity of information theory, for example, is the *Shannon entropy*, which represents the expected or average uncertainty associated with any measurement x of X:

$$H(X) = -\sum_{x \in \alpha_x} p(x) \log_2 p(x). \tag{1}$$

Unless otherwise stated, logarithms are taken by convention in base 2, giving units in bits. $H(X)$ for a measurement x of X can also be interpreted as the minimal expected or average number of bits required to encode or describe its value without losing information (Cover and Thomas, 1991; MacKay, 2003). X may be a joint or vector variable, e.g., $\mathbf{X} = \{Y, Z\}$, generalizing equation (1) to the *joint entropy* $H(\mathbf{X})$ or $H(Y, Z)$ for an arbitrary number of joint variables (see **Table 1**; equation (S.2) in Section S.1.1 in Supplementary Material). While the above definition of Shannon entropy applies to discrete variables, it may be extended to variables in the *continuous* domain as the *differential entropy* – see Section S.1.4 in Supplementary Material for details.

All of the subsequent Shannon information-theoretic quantities we consider may be written as sums and differences of the aforementioned marginal and joint entropies, and all may be extended to multivariate ($\mathbf{X}$, $\mathbf{Y}$, etc.) and/or continuous variables. The basic information-theoretic quantities: *entropy*, *joint entropy*, *conditional entropy*, *mutual information* (MI), *conditional mutual information* (Cover and Thomas, 1991; MacKay, 2003), and *multi-information* (Tononi et al., 1994); are discussed in detail in Section S.1.1 in Supplementary Material, and summarized here in **Table 1**. All of these measures are non-negative.

Also, we may write down *pointwise* or *local information-theoretic measures*, which characterize the information attributed with *specific* measurements x, y, and z of variables X, Y, and Z (Lizier, 2014), rather than the traditional expected or average information measures associated with these variables introduced above. Full details are provided in Section S.1.3 in Supplementary Material, and the local form for all of our basic measures is shown here in **Table 1**. For example, the *Shannon information content* or *local entropy* of an outcome x of measurement of the variable X is (Ash, 1965; MacKay, 2003):

$$h(x) = -\log_2 p(x). \tag{2}$$

By convention, we use lower-case symbols to denote local information-theoretic measures. The Shannon information content of a given symbol x is the *code-length* for that symbol in an optimal encoding scheme for the measurements X, i.e., one that produces the minimal expected code length. We can form all local information-theoretic measures as sums and differences of local entropies (see **Table 1**; Section S.1.3 in Supplementary Material), and each ordinary measure is the *average* or *expectation value* of their corresponding local measure, e.g., $H(X) = \langle h(x) \rangle$. Crucially, the *local MI* and *local conditional MI* (Fano, 1961) may be negative, unlike their averaged forms. This occurs for MI where the measurement of one variable is *misinformative* about the other variable (see further discussion in Section S.1.3 in Supplementary Material).

Applied to *time-series data*, these local variants return a time-series for the given information-theoretic measure, which with mutual information, for example, characterizes how the shared information between the variables fluctuates *as a function of time*. As such, they directly reveal the *dynamics* of information, and are gaining popularity in complex systems analysis (Shalizi, 2001;

Table 1 | Basic information-theoretic quantities (first six measures) and measures of information dynamics (last five measures) implemented in JIDT.

Measure	Average/expected form		Local form	
Entropy	$H(X) = -\sum_{x \in \alpha_x} p(x) \log_2 p(x)$	Eq. (S.1)	$h(x) = -\log_2 p(x)$	Eq. (S.32)
Joint entropy	$H(X, Y) = -\sum_{x \in \alpha_x, y \in \alpha_y} p(x, y) \log_2 p(x, y)$	Eq. (S.2)	$h(x, y) = -\log_2 p(x, y)$	Eq. (S.38)
Conditional entropy	$H(Y \mid X) = H(X, Y) - H(X)$	Eq. (S.3)	$h(x \mid y) = h(x, y) - h(x)$	Eq. (S.37)
Mutual information	$I(X; Y) = H(X) + H(Y) - H(X, Y)$	Eq. (S.6)	$i(x; y) = h(x) + h(y) - h(x, y)$	Eq. (S.41)
Multi-information	$I(X_1; X_2; \ldots; X_G) = \left(\sum_{g=1}^{G} H(X_g)\right) - H(X_1, X_2, \ldots, X_G)$	Eq. (S.7)	$i(x_1; x_2; \ldots; x_G) = \left(\sum_{g=1}^{G} h(x_g)\right) - h(x_1, x_2, \ldots, x_G)$	Eq. (S.47)
Conditional MI	$I(X; Y \mid Z) = H(X \mid Z) + H(Y \mid Z) - H(X, Y \mid Z)$	Eq. (S.11)	$i(x; y \mid z) = h(x \mid z) + h(y \mid z) - h(x, y \mid z)$	Eq. (S.44)
Entropy rate	$H_{\mu X}(k) = H(X_{n+1} \mid \mathbf{X}_n^{(k)})$	Eq. (S.18)	$h_{\mu X}(n+1, k) = h(x_{n+1} \mid \mathbf{x}_n^{(k)})$	Eq. (S.48)
Active information storage	$A_X(k) = I(\mathbf{X}_n^{(k)}; X_{n+1})$	Eq. (S.23)	$a_X(n+1, k) = i(\mathbf{x}_n^{(k)}; x_{n+1})$	Eq. (S.52)
Predictive information	$E_X(k) = I(\mathbf{X}_n^{(k)}; \mathbf{X}_{n+1}^{(k^+)})$	Eq. (S.21)	$e_X(n+1, k) = i(\mathbf{x}_n^{(k)}; \mathbf{x}_{n+1}^{(k^+)})$	Eq. (S.50)
Transfer entropy	$T_{Y \to X}(k, l, u) = I(\mathbf{Y}_{n+1-u}^{(l)}; X_{n+1} \mid \mathbf{X}_n^{(k)})$	Eq. (S.27)	$t_{Y \to X}(n+1, k, l, u) = i(\mathbf{y}_{n+1-u}^{(l)}; x_{n+1} \mid \mathbf{x}_n^{(k)})$	Eq. (S.54)
Conditional TE	$T_{Y \to X \mid Z}(k, l) = I(\mathbf{Y}_n^{(l)}; X_{n+1} \mid \mathbf{X}_n^{(k)}, Z_n)$	Eq. (S.29)	$t_{Y \to X \mid Z}(n+1, k, l) = i(\mathbf{y}_n^{(l)}; x_{n+1} \mid \mathbf{x}_n^{(k)}, z_n)$	Eq. (S.56)

Equations are supplied for both their average or expected form, and their local form. References are given to the presentation of these equations in Sections S.1.1 and S.1.2 in Supplementary Material.

Helvik et al., 2004; Shalizi et al., 2006; Lizier et al., 2007, 2008c, 2010, 2012b; Lizier, 2014; Wibral et al., 2014a).

Continuing with time-series, we then turn our attention to measures specifically used to quantify the dynamics of information processing in multivariate time-series, under a framework for *information dynamics*, which was recently introduced by Lizier et al. (2007, 2008c, 2010, 2012b, 2014) and Lizier (2013, 2014). The measures of information dynamics implemented in JIDT – which are the real focus of the toolkit – are discussed in detail in Section S.1.2 in Supplementary Material, and summarized here in **Table 1**.

These measures consider *time-series processes* X of the random variables $\{\ldots X_{n-1}, X_n, X_{n+1}\ldots\}$ with process realizations $\{\ldots x_{n-1}, x_n, x_{n+1}\ldots\}$ for countable time indices n. We use $\mathbf{X}_n^{(k)} = \{X_{n-k+1}, \ldots, X_{n-1}, X_n\}$ to denote the k consecutive variables of X up to and including time step n, which has realizations $\mathbf{x}_n^{(k)} = \{x_{n-k+1}, \ldots, x_{n-1}, x_n\}$[2]. The $\mathbf{x}_n^{(k)}$ are Takens' *embedding vectors* (Takens, 1981) with *embedding dimension* k, which capture the underlying *state* of the process X for Markov processes of order k[3].

Specifically, our framework examines how the information in variable X_{n+1} is related to previous variables or states (e.g., X_n or $\mathbf{X}_n^{(k)}$) of the process or other related processes, addressing the fundamental question: "*where does the information in a random variable X_{n+1} in a time series come from?*" As indicated in **Figure 1** and shown for the respective measures in **Table 1**, this question is addressed in terms of

1. information from the past of process X – i.e., the information *storage*, measured by the *active information storage* (Lizier et al., 2012b), and *predictive information* or *excess entropy* (Grassberger, 1986; Bialek et al., 2001; Crutchfield and Feldman, 2003);
2. information contributed from other source processes Y – i.e., the information *transfer*, measured by the *transfer entropy* (TE) (Schreiber, 2000), and *conditional transfer entropy* (Lizier et al., 2008c, 2010);
3. and how these sources combine – i.e., information *modification* (see *separable information* (Lizier et al., 2010) in Section S.1.2 in Supplementary Material).

The goal of the framework is to decompose the information in the next observation X_{n+1} of process X in terms of these information sources.

The transfer entropy, arguably the most important measure in the toolkit, has become a very popular tool in complex systems in general, e.g., (Lungarella and Sporns, 2006; Lizier et al., 2008c, 2011c; Obst et al., 2010; Williams and Beer, 2011; Barnett and Bossomaier, 2012; Boedecker et al., 2012), and in computational neuroscience, in particular, e.g., (Ito et al., 2011; Lindner et al., 2011; Lizier et al., 2011a; Vicente et al., 2011; Stramaglia et al., 2012). For multivariate Gaussians, the TE is equivalent (up to a factor of 2) to the *Granger causality* (Barnett et al., 2009). Extension of the TE to arbitrary source-destination lags is described by Wibral et al. (2013) and incorporated in **Table 1** (this is not shown for conditional TE here for simplicity, but is handled in JIDT). Further, one can consider multivariate sources $\mathbf{Y}$, in which case we refer to the measure $T_{\mathbf{Y}\rightarrow X}(k, l)$ as a *collective transfer entropy* (Lizier et al., 2010). See further description of this measure at Section S.1.2 in Supplementary Material, including regarding how to set the history length k.

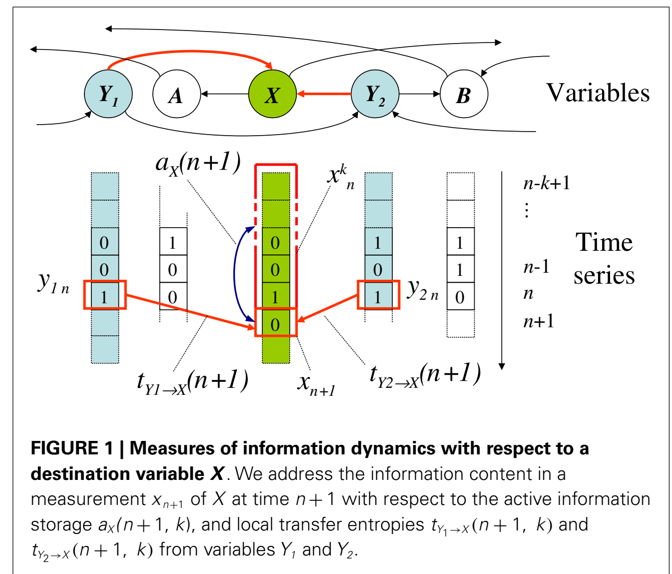

FIGURE 1 | Measures of information dynamics with respect to a destination variable X. We address the information content in a measurement x_{n+1} of X at time $n+1$ with respect to the active information storage $a_X(n+1, k)$, and local transfer entropies $t_{Y_1\rightarrow X}(n+1, k)$ and $t_{Y_2\rightarrow X}(n+1, k)$ from variables Y_1 and Y_2.

Table 1 also shows the local variants of each of the above measures of information dynamics (presented in full in Section S.1.3 in Supplementary Material). The use of these local variants is particularly important here because they provide a direct, model-free mechanism to analyze the *dynamics* of how information processing unfolds in time in complex systems. **Figure 1** indicates, for example, a local active information storage measurement for time-series process X, and a local transfer entropy measurement from process Y to X.

Finally, in Section S.1.5 in Supplementary Material, we describe how one can evaluate whether an MI, conditional MI, or TE is statistically different from 0, and therefore, represents sufficient evidence for a (directed) relationship between the variables. This is done (following (Chávez et al., 2003; Verdes, 2005; Lindner et al., 2011; Lizier et al., 2011a; Vicente et al., 2011; Barnett and Bossomaier, 2012; Wibral et al., 2014b)) via permutation testing to construct appropriate surrogate populations of time-series and measurements under the null hypothesis of no directed relationship between the given variables.

2.2. ESTIMATION TECHNIQUES

While the mathematical formulation of the quantities in Section 2.1 are relatively straightforward, empirically estimating them in practice from a finite number N of samples of time-series data can be a complex process, and is dependent on the type of data you have and its properties. Estimators are typically subject to bias and

[2]We use the corresponding notation $\mathbf{X}_{n+1}^{(k^+)}$ for the next k values *from* $n+1$ onwards, $\{X_{n+1}, X_{n+2}, \ldots, X_{n+k}\}$, with realizations $\mathbf{x}_{n+1}^{(k^+)} = \{x_{n+1}, x_{n+2}, \ldots, x_{n+k}\}$

[3]We can use an embedding delay τ to give $\mathbf{x}_n^{(k)} = \{x_{n-(k-1)\tau}, \ldots, x_{n-\tau}, x_n\}$, where this helps to better empirically capture the state from a finite sample size. Non-uniform embeddings (i.e., with irregular delays) may also be useful (Faes et al., 2011) (not implemented in JIDT at this stage).

variance due to finite sample size. Here, we briefly introduce the various types of estimators that are included in JIDT, referring the reader to Section S.2 in Supplementary Material (and also (Vicente and Wibral, 2014) for the transfer entropy, in particular) for more detailed discussion.

For *discrete* variables *X*, *Y*, *Z*, etc., the definitions in Section 2.1 may be used directly by counting the matching configurations in the available data to obtain the relevant plug-in probability estimates (e.g., $\hat{p}(x|y)$ and $\hat{p}(x)$ for MI). These estimators are simple and fast, being implemented in O (N) time. Several bias correction techniques are available, e.g., Paninski (2003), Bonachela et al. (2008), though not yet implemented in JIDT.

For *continuous* variables *X*, *Y*, *Z*, one could simply discretize or bin the data and apply the discrete estimators above. While this is simple and fast (O (N) as above), it is likely to sacrifice accuracy. Alternatively, we can use an estimator that harnesses the continuous nature of the variables, dealing with the differential entropy and probability density functions. The latter is more complicated but yields a more accurate result. We discuss several such estimators in Section S.2.2 in Supplementary Material, and summarize them in the following[4]:

- A *multivariate Gaussian model* may be used (Section S.2.2.1 in Supplementary Material) for the relevant variables, assuming linear interactions between them. This approach uses the known form of entropy for Gaussian multivariates (equation (S.61) in Supplementary Material, in nats) (Cover and Thomas, 1991) and sums and differences of these entropies to compute other measures (e.g., transfer entropy as per (Kaiser and Schreiber, 2002)). These estimators are fast (O (Nd^2), for dimensionality d of the given joint variable) and parameter-free, but subject to the linear-model assumption.
- *Kernel estimation* of the relevant PDFs via a *kernel function* are discussed in Section S.2.2.2 in Supplementary Material (and see, e.g., Schreiber (2000), Kaiser and Schreiber (2002), and Kantz and Schreiber (1997)). Such kernel functions measure similarity between pairs of samples using a specific resolution or *kernel width* r; e.g., the box-kernel (implemented in JIDT) results in counting the proportion of the N sample values, which fall within r of the given sample. They are then used as plug-in estimates for the entropy, and again sums and differences of these for the other measures. Kernel estimation can measure non-linear relationships and is model-free (unlike Gaussian estimators), though is sensitive to the parameter choice for r (Schreiber, 2000; Kaiser and Schreiber, 2002) and is biased. It is less time-efficient than the simple methods, although box-assisted methods can achieve O (N) time-complexity (Kantz and Schreiber, 1997). See Section S.2.2.2 in Supplementary Material for further comments, e.g., regarding selection of r.
- The Kraskov et al. (2004) (KSG) technique (see details in Section S.2.2.3 in Supplementary Material) improved on (box-) kernel estimation for MI (and multi-information) via the use of Kozachenko–Leonenko estimators (Kozachenko and Leonenko, 1987) of log-probabilities via nearest-neighbor counting; bias correction; and a fixed number K of nearest neighbors in the full X-Y joint space. The latter effectively means using a dynamically altered (box-) kernel width r to adjust to the density of samples in the vicinity of any given observation; this smooths out errors in the PDF estimation, especially when handling a small number of observations. These authors proposed two slightly different algorithms for their estimator – both are implemented in JIDT. The KSG technique has been directly extended to conditional MI by Frenzel and Pompe (2007) and transfer entropy (originally by Gomez-Herrero et al. (2010)) and later for algorithm 2 by Wibral et al. (2014b)). KSG estimation builds on the non-linear and model-free capabilities of kernel estimation with bias correction, better data efficiency and accuracy, and being effectively parameter-free (being relatively stable to choice of K). As such, it is widely used as best of breed solution for MI, conditional MI and TE for continuous data; see, e.g., Wibral et al. (2014b) and Vicente and Wibral (2014). It can be computationally expensive with naive algorithms requiring O (KN^2) time though fast nearest neighbor search techniques can reduce this to O ($KN\log N$). For release v1.0 JIDT only implements a naive algorithm, though fast nearest neighbor search is implemented and available via the project SVN repository (see Section 3.1) and as such will be included in future releases.
- *Permutation entropy* approaches (Bandt and Pompe, 2002) estimate the relevant PDFs based on the relative ordinal structure of the joint vectors (see Section S.2.2.4 in Supplementary Material). Permutation entropy has, for example, been adapted to estimate TE as the *symbolic transfer entropy* (Staniek and Lehnertz, 2008). Permutation approaches are computationally fast, but are model-based, however, (assuming all relevant information is in the ordinal relationships). This is not necessarily the case, and can lead to misleading results, as demonstrated by Wibral et al. (2013).

2.3. RELATED OPEN-SOURCE INFORMATION-THEORETIC TOOLKITS

We next consider other existing open-source information-theoretic toolkits for computing the aforementioned measures empirically from time-series data. In particular, we consider those that provide implementations of the transfer entropy. For each toolkit, we describe its purpose, the type of data it handles, and which measures and estimators are implemented.

TRENTOOL[5] (GPL v3 license) by Lindner et al. (2011) is a MATLAB toolbox, which is arguably the most mature open-source toolkit for computing TE. It is not intended for general-purpose use, but designed from the ground up for transfer entropy analysis of (continuous) neural data, using the data format of the FieldTrip toolbox (Oostenveld et al., 2011) for EEG, MEG, and LFP recordings. In particular, it is designed for performing effective connectivity analysis between the input variables (see Vicente et al. (2011) and Wibral et al. (2011)), including statistical significance testing of TE results (as outlined in Section S.1.5 in Supplementary Material) and processing steps to deal with volume conduction and identify cascade or common-driver effects in the inferred network. Conditional/multivariate TE is not yet available, but planned. TRENTOOL automates selection of parameters for embedding input time-series data and for source-target

[4]Except where otherwise noted, JIDT implements the most efficient described algorithm for each estimator.

[5]http://www.trentool.de

delays, and implements KSG estimation (see Section S.2.2.3 in Supplementary Material), harnessing fast nearest neighbor search, parallel computation, and GPU-based algorithms (Wollstadt et al., 2014).

The MuTE toolbox by Montalto et al. (2014a,b) (CC-BY license)[6] provides MATLAB code for TE estimation. In particular, MuTE is capable of computing conditional TE, includes a number of estimator types (discrete or binned, Gaussian, and KSG including fast nearest neighbor search), and adds non-uniform embedding (see Faes et al. (2011)). It also adds code to assist with embedding parameter selection, and incorporates statistical significance testing.

The Transfer entropy toolbox (TET, BSD license)[7] by Ito et al. (2011) provides C-code callable from MATLAB for TE analysis of spiking data. TET is limited to binary (discrete) data only. Users can specify embedding dimension and source-target delay parameters.

MILCA (Mutual Information Least-dependent Component Analysis, GPL v3 license)[8] provides C-code (callable from MATLAB) for mutual information calculations on continuous data (Kraskov et al., 2004; Stögbauer et al., 2004; Astakhov et al., 2013). MILCA's purpose is to use the MI calculations as part of Independent Component Analysis (ICA), but they can be accessed in a general-purpose fashion. MILCA implements KSG estimators with fast nearest neighbor search; indeed, MILCA was co-written by the authors of this technique. It also handles multidimensional variables.

TIM (GNU Lesser GPL license)[9] by Rutanen (2011) provides C++ code (callable from MATLAB) for general-purpose calculation of a wide range of information-theoretic measures on continuous-valued time-series, including for multidimensional variables. The measures implemented include entropy (Shannon, Renyi, and Tsallis variants), Kullback–Leibler divergence, MI, conditional MI, TE, and conditional TE. TIM includes various estimators for these, including Kozachenko–Leonenko (see Section S.2.2.3 in Supplementary Material), Nilsson and Kleijn (2007), and Stowell and Plumbley (2009) estimators for (differential) entropy, and KSG estimation for MI and conditional MI (using fast nearest neighbor search).

The MVGC (multivariate Granger causality toolbox, GPL v3 license)[10] by Barnett and Seth (2014) provides a MATLAB implementation for general-purpose calculation of the Granger causality (i.e., TE with a linear-Gaussian model, see Section S.1.2 in Supplementary Material) on continuous data. MVGC also requires the MATLAB Statistics, Signal Processing, and Control System Toolboxes.

There is a clear gap for a general-purpose information-theoretic toolkit, which can run in multiple code environments, implementing all of the measures in Sections S.1.1 and S.1.2 in Supplementary Material, with various types of estimators, and with implementation of local values, measures of statistical significance, etc. In the next section, we introduce JIDT, and outline how it addresses this gap. Users should make a judicious choice of which toolkit suits their requirements, taking into account data types, estimators and application domain. For example, TRENTOOL is built from the ground up for effective network inference in neural imaging data, and is certainly the best tool for that application in comparison to a general-purpose toolkit.

3. JIDT INSTALLATION, CONTENTS, AND DESIGN

JIDT (Java Information Dynamics Toolkit, GPL v3 license)[11] is unique as a general-purpose information-theoretic toolkit, which provides all of the following features in one package:

- Implementation of a large array of measures, including all conditional/multivariate forms of the transfer entropy, complementary measures such as active information storage, and allows full specification of relevant embedding parameters;
- Implementation a wide variety of estimator types and applicability to both discrete and continuous data;
- Implementation of local measurement for all estimators;
- Inclusion of statistical significance calculations for MI, TE, etc., and their conditional variants;
- No dependencies on other installations (except Java).

Furthermore, JIDT is written in Java[12], taking advantage of the following features:

- The code becomes platform agnostic, requiring only an installation of the Java Virtual Machine (JVM) to run;
- The code is object-oriented, with common code shared and an intuitive hierarchical design using interfaces; this provides flexibility and allows different estimators of same measure can be swapped dynamically using polymorphism;
- The code can be called directly from MATLAB, GNU Octave, Python, etc., but runs faster than native code in those languages (still slower but comparable to C/C++, see Computer Language Benchmarks Game, 2014); and
- Automatic generation of Javadoc documents for each class.

In the following, we describe the (minimal) installation process in Section 3.1, and contents of the version 1.0 JIDT distribution in Section 3.2. We then describe which estimators are implemented for each measure in Section 3.3, and architecture of the source code in Section 3.4. We also outline how the code has been tested in Section 3.5, how to build it (if required) in Section 3.6 and point to other sources of documentation in Section 3.7.

3.1. INSTALLATION AND DEPENDENCIES

There is *little to no installation* of JIDT required beyond downloading the software. The software can be run on any platform, which supports a standard edition Java Runtime Environment (i.e., Windows, Mac, Linux, and Solaris).

[6] http://figshare.com/articles/MuTE_toolbox_to_evaluate_Multivariate_Transfer_Entropy/1005245/1
[7] http://code.google.com/p/transfer-entropy-toolbox/
[8] http://www.ucl.ac.uk/ion/departments/sobell/Research/RLemon/MILCA/MILCA
[9] http://www.cs.tut.fi/%7etimhome/tim/tim.htm
[10] http://www.sussex.ac.uk/sackler/mvgc/

[11] http://code.google.com/p/information-dynamics-toolkit/
[12] The JIDT v1.0 distribution is compiled by Java Standard Edition 6; it is also verified as compatible with Edition 7.

Table 2 | Relevant web/wiki pages on JIDT website.

Name	URL
Project home	http://code.google.com/p/information-dynamics-toolkit/
Installation	http://code.google.com/p/information-dynamics-toolkit/wiki/Installation
Downloads	http://code.google.com/p/information-dynamics-toolkit/wiki/Downloads
MATLAB/Octave use	http://code.google.com/p/information-dynamics-toolkit/wiki/UseInOctaveMatlab
Octave-Java array conversion	http://code.google.com/p/information-dynamics-toolkit/wiki/OctaveJavaArrayConversion
Python use	http://code.google.com/p/information-dynamics-toolkit/wiki/UseInPython
JUnit test cases	http://code.google.com/p/information-dynamics-toolkit/wiki/JUnitTestCases
Documentation	http://code.google.com/p/information-dynamics-toolkit/wiki/Documentation
Demos	http://code.google.com/p/information-dynamics-toolkit/wiki/Demos
Simple Java examples	http://code.google.com/p/information-dynamics-toolkit/wiki/SimpleJavaExamples
Octave/MATLAB examples	http://code.google.com/p/information-dynamics-toolkit/wiki/OctaveMatlabExamples
Python examples	http://code.google.com/p/information-dynamics-toolkit/wiki/PythonExamples
Cellular Automata demos	http://code.google.com/p/information-dynamics-toolkit/wiki/CellularAutomataDemos
Schreiber TE demos	http://code.google.com/p/information-dynamics-toolkit/wiki/SchreiberTeDemos
jidt-discuss group	http://groups.google.com/group/jidt-discuss
SVN URL	http://information-dynamics-toolkit.googlecode.com/svn/trunk/

Material pertaining to installation is described in full at the "Installation" wiki page for the project (see **Table 2** *for all relevant project URLs*); summarized as follows:

1. Download a code release package from the "Downloads" wiki page. Full distribution is recommended (described in Section 3.2) so as to obtain, e.g., access to the examples described in Section 4, though a "Jar only" distribution provides just the JIDT library `infodynamics.jar` in Java archive file format.
2. Unzip the full `.zip` distribution to the location of your choice, and/or move the `infodynamics.jar` file to a relevant location. Ensure that `infodynamics.jar` is on the Java classpath when your code attempts to access it (see Section 4).
3. To update to a new version, simply copy the new distribution over the top of the previous one.

As an alternative, advanced users can take an SVN checkout of the source tree from the SVN URL (see **Table 2**) and build the `infodynamics.jar` file using `ant` scripts (see Section 3.6).

In general, there are no dependencies that a user would need to download in order to run the code. Some exceptions are as follows:

1. Java must be installed on your system in order to run JIDT; most systems will have Java already installed. To simply run JIDT, you will only need a Java Runtime Environment (JRE, also known as Java Virtual Machine or JVM), whereas to modify and/or build to software, or write your own Java code to access it, you will need the full Java Development Kit (JDK), standard edition (SE). Download it from http://java.com/. For using JIDT via MATLAB, a JVM is included in MATLAB already.
2. If you wish to build the project using the `build.xml` script – this requires `ant` (see Section 3.6).
3. If you wish to run the unit test cases (see Section 3.5) – this requires the `JUnit` framework: http://www.junit.org/ – for how to run `JUnit` with our ant script see "JUnit test cases" wiki page.
4. Additional preparation may be required to use JIDT in GNU Octave or Python. Octave users must install the `octave-java` package from the `Octave-forge` project – see description of these steps at "MATLAB/Octave use" wiki page. Python users must install a relevant Python-Java extension – see description at "Python use" wiki page. Both cases will depend on a JVM on the system (as per point 1 above), though the aforementioned extensions may install this for you.

Note that JIDT does *adapt* code from a number of sources in accordance with their open-source license terms, including Apache Commons Math v3.3[13], the JAMA project[14], and the octave-java package from the Octave-Forge project[15]. Relevant notices are supplied in the `notices` folder of the distribution. Such code is included in JIDT, however, and does not need to be installed separately.

3.2. CONTENTS OF DISTRIBUTION

The contents of the current (version 1.0) JIDT (full) distribution are as follows:

- The top-level folder contains the `infodynamics.jar` library file, a GNU GPL v3 license, a `readme.txt` file and an ant `build.xml` script for (re-)building the code (see Section 3.6);
- The `java` folder contains source code for the library in the `source` subfolder (described in Section 3.3), and unit tests in the `unittests` subfolder (see Section 3.5).

[13]http://commons.apache.org/proper/commons-math/
[14]http://math.nist.gov/javanumerics/jama/
[15]http://octave.sourceforge.net/java/

- The `javadocs` folder contains automatically generated Javadocs from the source code, as discussed in Section 3.7.
- The `demos` folder contains several example applications of the software, described in Section 4, sorted into folders to indicate that environment they are intended to run in, i.e., `java`, `octave` (which is compatible with `MATLAB`), and `python`. There is also a `data` folder here containing sample data sets for these demos and unit tests.
- The `notices` folder contains notices and licenses pertaining to derivations of other open-source code used in this project.

3.3. SOURCE CODE AND ESTIMATORS IMPLEMENTED

The Java source code for the JIDT library contained in the `java/source` folder is organized into the following Java *packages* (which map directly to subdirectories):

- `infodynamics.measures` contains all of the classes implementing the information-theoretic measures, split into:
  - `infodynamics.measures.discrete` containing all of the measures for discrete data;
  - `infodynamics.measures.continuous` which at the top-level contains Java *interfaces* for each of the measures as applied to continuous data, then a set of sub-packages (`gaussian`, `kernel`, `kozachenko`, `kraskov`, and `symbolic`), which map to each estimator type in Section 2.2 and contain *implementations* of such estimators for the interfaces defined for each measure (Section 3.4 describes the object-oriented design used here). **Table 3** identifies which estimators are measured for each estimator type;
  - `infodynamics.measures.mixed` includes *experimental* discrete-to-continuous MI calculators, though these are not discussed in detail here.
- `infodynamics.utils` contains classes providing a large number of utility functions for the measures (e.g., matrix manipulation, file reading/writing including in Octave text format);
- `infodynamics.networkinference` contains implementations of higher-level algorithms, which use the information-theoretic calculators to infer an effective network structure from time-series data (see Section 4.6).

As outlined above, **Table 3** describes which estimators are implemented for each measure. This effectively maps the definitions of the measures in Section 2.1 to the estimators in Section 2.2 (note that the efficiency of these estimators is also discussed in Section 2.1). All estimators provide the corresponding *local* information-theoretic measures (as introduced in Section S.1.3 in Supplementary Material). Also, for the most part, the estimators include a generalization to multivariate **X**, **Y**, etc., as identified in the table.

3.4. JIDT ARCHITECTURE

The measures for continuous data have been organized in a strongly *object-oriented* fashion[16]. **Figure 2** provides a sample (partial) Unified Modeling Language (UML) class diagram of the implementations of the conditional mutual information (equation (S.11) in Supplementary Material) and transfer entropy (equation (S.25) in Supplementary Material) measures using KSG estimators (Section S.2.2.3 in Supplementary Material). This diagram shows the typical object-oriented hierarchical structure of the implementations of various estimators for each measure. The class hierarchy is organized as follows.

3.4.1. Interfaces

Interfaces at the top layer define the available *methods* for each measure. At the top of this figure we see the `ConditionalMutualInfoCalculatorMultiVariate` and `TransferEntropyCalculator` interfaces, which define the methods each estimator *class* for a given measure must implement. Such interfaces are defined for each information-theoretic measure in the `infodynamics.measures.continuous` package.

3.4.2. Abstract classes

Abstract classes[17] at the intermediate layer provide basic functionality for each measure. Here, we have abstract classes `ConditionalMutualInfoMultiVariateCommon` and `TransferEntropyCalculatorViaCondMutualInfo` which *implement* the above interfaces, providing common code bases for the given measures that various child classes can build on to specialize themselves to a particular estimator type. For instance, the `TransferEntropyCalculatorViaCondMutualInfo` class provides code which abstractly *uses* a `ConditionalMutualInfoCalculatorMultiVariate` interface in order to make transfer entropy calculations, but neither concretely specify which type of conditional MI estimator to use nor fully set its parameters.

3.4.3. Child classes

Child classes at the lower layers add specialized functionality for each estimator type for each measure. These child classes *inherit* from the above parent classes, building on the common code base to add specialization code for the given estimator type. Here, that is the KSG estimator type. The child classes at the bottom of the hierarchy have no remaining abstract functionality, and can thus be used to make the appropriate information-theoretic calculation. We see that `ConditionalMutualInfoCalculatorMultiVariateKraskov` begins to *specialize* `ConditionalMutualInfoMultiVariateCommon` for KSG estimation, with further specialization by its child class `ConditionalMutualInfoCalculatorMultiVariateKraskov1` which implements the KSG algorithm 1 (equation (S.64) in Supplementary Material). Not shown here is `ConditionalMutualInfoCalculatorMultiVariateKraskov2` which implements the KSG algorithm 2 (equation (S.65) in Supplementary Material) and has similar class relationships. We also see that `TransferEntropyCalculatorKraskov` specializes `TransferEntropyCalculatorViaCond`

[16]This is also the case for the measures for discrete data, though to a lesser degree and without multiple estimator types, so this is not focused on here.

[17]Abstract classes provide implementations of some but not all methods required for a class, so they cannot be directly instantiated themselves but child classes, which provide implementations for the missing methods and may be instantiated.

Table 3 | An outline of which estimation techniques are implemented for each relevant information-theoretic measure.

Measure			Discrete estimator (Section S.2.1)	Continuous estimators			
Name	**Notation**	**Defined at**		**Gaussian (Section S.2.2.1)**	**Box-kernel (Section S.2.2.2)**	**Kraskov et al. (KSG) (Section S.2.2.3)**	**Permutation (Section S.2.2.4)**
Entropy	$H(X)$	Eqs. (S.1) and (S.32)	✓	✓	✓	*	
Entropy rate	$H_{\mu X}$	Eqs. (S.18) and (S.48)	✓	*Use two multivariate entropy calculators*			
Mutual information (MI)	$I(X;Y)$	Eqs. (S.6) and (S.41)	✓	✓	✓	✓	
Conditional MI	$I(X;Y\|Z)$	Eqs. (S.11) and (S.44)	✓	✓		✓	
Multi-information	$I(\mathbf{X})$	Eqs. (S.7) and (S.47)	✓		✓^{u}	✓^{u}	
Transfer entropy (TE)	$T_{Y\rightarrow X}$	Eqs. (S.25) and (S.54)	✓	✓	✓	✓	✓^{u}
Conditional TE	$T_{Y\rightarrow X\|Z}$	Eqs. (S.29) and (S.56)	✓	✓^{u}		✓^{u}	
Active information storage	A_X	Eqs. (S.23) and (S.52)	✓	✓^{u}	✓^{u}	✓^{u}	
Predictive information	E_X	Eqs. (S.21) and (S.50)	✓	†u	†u	†u	
Separable information	S_X	Eq. (S.31)	✓				

*The ✓ symbol indicates that the measure is implemented for the given estimator and is applicable to both univariate and multivariate time-series (e.g., collective transfer entropy, where the source is multivariate), while the addition of superscript "u" (i.e., ✓^{u}) indicates the measure is implemented for univariate time-series only. The section numbers and equation numbers refer to the definitions in the Supplementary Material for the expected and local values (where provided) for each measure. Also, while the KSG estimator is not applicable for entropy, the * symbol there indicates the implementation of the estimator by Kozachenko and Leonenko (1987) for entropy (which the KSG technique is based on for MI; see Section S.2.2.3 in Supplementary Material). Finally, †indicates that the (continuous) predictive information calculators are not available in the v1.0 release but are available via the project SVN and future releases.*

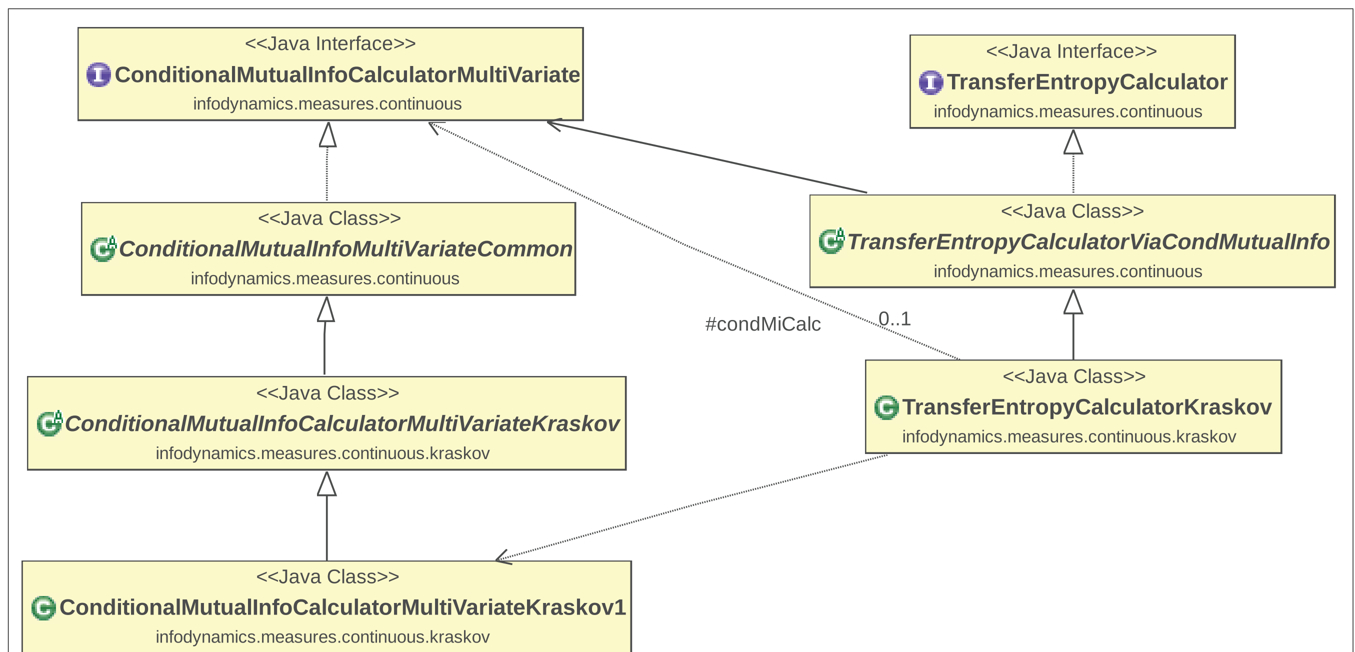

FIGURE 2 | Partial UML class diagram of the implementations of the conditional mutual information (equation (S.11) in Supplementary Material) and transfer entropy (equation (S.25) in Supplementary Material) measures using KSG estimators. As explained in the main text, this diagram shows the typical *object-oriented* structure of the implementations of various estimators for each measure. The relationships indicated on the class diagram are as follows: dotted lines with hollow triangular arrow heads indicate the realization or *implementation* of an interface by a class; solid lines with hollow triangular arrow heads indicate the generalization or *inheritance* of a child or subtype from a parent or superclass; lines with plain arrow heads indicate that one class *uses* another (with the solid line indicating direct usage and dotted line indicating indirect usage via the superclass).

MutualInfo for KSG estimation, by using ConditionalMutualInfoCalculatorMultiVariateKraskov1 (or ConditionalMutuaInfoCalculatorMultiVariateKraskov2, not shown) as the specific implementation of ConditionalMutualInfoCalculatorMultiVariate. The implementations of these interfaces for other estimator types (e.g., TransferEntropyCalculatorGaussian) sit at the same level here inheriting from the common abstract classes above.

This type of object-oriented hierarchical structure delivers two important benefits: (i) the *decoupling* of common code away from specific estimator types and into common parent classes allows code re-use and simpler maintenance, and (ii) the use of interfaces delivers *subtype polymorphism* allowing *dynamic dispatch*, meaning that one can write code to compute a given measure using the methods on its interface and only specify the estimator type at runtime (see a demonstration in Section 4.1.8).

3.5. VALIDATION

The calculators in JIDT are validated using a set of *unit tests* (distributed in the java/unittests folder). Unit testing is a method of testing software by the use of a set of small test cases which call parts of the code and check the output against expected values, flagging errors if they arise. The unit tests in JIDT are implemented via the JUnit framework version 3[18]. They can be run via the ant script (see Section 3.6).

At a high level, the unit tests include validation of the results of information-theoretic calculations applied to the sample data in demos/data against measurements from various other existing toolkits, e.g.,

- The KSG estimator (Section S.2.2.3 in Supplementary Material) for MI is validated against values produced from the *MILCA* toolkit (Kraskov et al., 2004; Stögbauer et al., 2004; Astakhov et al., 2013);
- The KSG estimator for conditional MI and TE is validated against values produced from scripts within *TRENTOOL* (Lindner et al., 2011);
- The discrete and box-kernel estimators for TE are validated against the plots in the original paper on TE by Schreiber (2000) (see Section 4.4);
- The Gaussian estimator for TE (Section S.2.2.1 in Supplementary Material) is verified against values produced from (a modified version of) the computeGranger.m script of the *ChaLearn Connectomics Challenge Sample Code* (Orlandi et al., 2014).

Further code coverage by the unit tests is planned in future work.

3.6. (RE-)BUILDING THE CODE

Users may wish to build the code, perhaps if they are directly accessing the source files via SVN or modifying the files. The source code may be compiled manually of course, or in your favorite IDE (Integrated Development Environment). JIDT also provides an ant build script, build.xml, to guide and streamline this process. Apache ant – see http://ant.apache.org/– is a command-line tool to build various interdependent targets in software projects, much like the older style Makefile for C/C++.

To build any of the following targets using build.xml, either integrate build.xml into your IDE and run the selected <targetName >, or run ant <targetName> from the command line in the top-level directory of the distribution, where <targetName> may be any of the following:

- build or jar (this is the default if no <targetName> is supplied) – creates a jar file for the JIDT library;
- compile – compiles the JIDT library and unit tests;
- junit – runs the unit tests;
- javadocs – generates automated Javadocs from the formatted comments in the source code;
- jardist – packages the JIDT jar file in a distributable form, as per the jar-only distributions of the project;
- dist – runs unit tests, and packages the JIDT jar file, Javadocs, demos, etc., in a distributable form, as per the full distributions of the project;
- clean – delete all compiled code, etc., built by the above commands.

3.7. DOCUMENTATION AND SUPPORT

Documentation to guide users of JIDT is composed of

1. This manuscript!
2. The Javadocs contained in the javadocs folder of the distribution (main page is index.html), and available online via the Documentation page of the project wiki (see **Table 2**). Javadocs are html formatted documentation for each package, class, and interface in the library, which are automatically created from formatted comments in the source code. The Javadocs are very useful tools for users, since they provide specific details about each class and their methods, in more depth than we are able to do here; for example, which properties may be set for each class. The Javadocs can be (re-)generated using ant as described in Section 3.6.
3. The demos; as described further in Section 4, on the Demos wiki page (see **Table 2**), and the individual wiki page for each demo;
4. The project wiki pages (accessed from the project home page, see **Table 2**) provide additional information on various features, e.g., how to use JIDT in MATLAB or Octave and Python;
5. The unit tests (as described in Section 3.5) provide additional examples on how to run the code.

You can also join our email discussion group jidt-discuss on Google Groups (see URL in **Table 2**) or browse past messages, for announcements, asking questions, etc.

[18]http://www.junit.org/

4. JIDT CODE DEMONSTRATIONS

In this section, we describe some simple demonstrations on how to use the JIDT library. Several sets of demonstrations are included in the JIDT distribution, some of which are described here. More detail is provided for each demo on its wiki page, accessible from the main Demos wiki page (see **Table 2**). We begin with the main set of *Simple Java Demos*, focusing, in particular, on a detailed walk-through of using a KSG estimator to compute transfer entropy since the calling pattern here is typical of all estimators for continuous data. Subsequently, we provide more brief overviews of other examples available in the distribution, including how to run the code in MATLAB, GNU Octave, and Python, implementing the transfer entropy examples from Schreiber (2000), and computing spatiotemporal profiles of information dynamics in Cellular Automata.

4.1. SIMPLE JAVA DEMOS

The primary set of demos is the "Simple Java Demos" set at `demos/java` in the distribution. This set contains eight standalone Java programs to demonstrate simple use of various aspects of the toolkit. This set is described further at the `SimpleJavaExamples` wiki page (see **Table 2**).

The Java source code for each program is located at `demos/java/infodynamics/demos` in the JIDT distribution, and shell scripts (with mirroring batch files for Windows)[19] to run each program are found at `demos/java/`. The shell scripts demonstrate how to compile and run the programs from command line, e.g., `example1TeBinaryData.sh` contains the following commands in **Listing 1**:

Listing 1 | Shell script `example1TeBinaryData.sh`.

```
# Make sure the latest source file is
  compiled.
javac -classpath "../../infodynamics.jar"
  "infodynamics/demos/Example1TeBinaryData
  .java"
# Run the example:
java -classpath ".:../../infodynamics.jar"
  infodynamics.demos.Example1TeBinaryData
```

The examples focus on various transfer entropy estimators (though similar calling paradigms can be applied to all estimators), including

1. computing transfer entropy on *binary (discrete) data*;
2. computing transfer entropy for specific channels within *multi-dimensional* binary data;
3. computing transfer entropy on *continuous* data using *kernel estimation*;
4. computing transfer entropy on *continuous* data using *KSG estimation*;
5. computing *multivariate* transfer entropy on *multidimensional* binary data;
6. computing *mutual information* on continuous data, using *dynamic dispatch* or *late-binding* to a particular estimator;
7. computing transfer entropy from an *ensemble* of time-series samples;
8. computing transfer entropy on *continuous* data using *binning* then *discrete* calculation.

[19]The batch files are not included in release v1.0, but are currently available via the SVN repository and will be distributed in future releases.

In the following, we explore selected salient examples in this set. We begin with `Example1TeBinaryData.java` and `Example4TeContinuousDataKraskov.java` as typical calling patterns to use estimators for discrete and continuous data, respectively, then add extensions for how to compute local measures and statistical significance, use ensembles of samples, handle multivariate data and measures, and dynamic dispatch.

4.1.1. *Typical calling pattern for an information-theoretic measure on discrete data*

`Example1TeBinaryData.java` (see **Listing 2**) provides a typical calling pattern for calculators for *discrete data*, using the `infodynamics.measures.discrete.TransferEntropyCalculatorDiscrete` class. *While the specifics of some methods may be slightly different, the general calling paradigm is the same for all discrete calculators.*

Listing 2 | Estimation of TE from discrete data; source code adapted from `Example1TeBinaryData.java`.

```
int arrayLengths = 100;
RandomGenerator rg = new RandomGenerator();
// Generate some random binary data:
int[] sourceArray = rg.generateRandomInts
   (arrayLengths, 2);
int[] destArray = new int[arrayLengths];
destArray[0] = 0;
System.arraycopy(sourceArray, 0, destArray,
   1, arrayLengths - 1);
// Create a TE calculator and run it:
TransferEntropyCalculatorDiscrete teCalc =
   new TransferEntropyCalculatorDiscrete
   (2, 1);
teCalc.initialise();
teCalc.addObservations(sourceArray,
   destArray);
double result = teCalc.
   computeAverageLocalOfObservations();
```

The data type used for all discrete data are `int[]` time-series arrays (indexed by time). Here, we are computing TE for *univariate time series* data, so `sourceArray` and `destArray` at line 4 and line 5 are single dimensional `int[]` arrays. Multidimensional time series are discussed in Section 4.1.6.

The first step in using any of the estimators is to construct an instance of them, as per line 9 above. Parameters/properties

for calculators for discrete data are *only* supplied in the constructor at line 9 (this is not the case for continuous estimators, see Section 4.1.2). See the Javadocs for each calculator for descriptions of which parameters can be supplied in their constructor. The arguments for the TE constructor here include the number of discrete values ($M = 2$), which means the data can take values {0, 1} (the allowable values are always enumerated $0, \ldots, M-1$); and the embedded history length $k = 1$. Note that for measures such as TE and AIS, which require embeddings of time-series variables, the user must provide the embedding parameters here.

All calculators must be initialized before use or re-use on new data, as per the call to `initialise()` at line 10. This call clears any PDFs held inside the class, The `initialise()` method provides a mechanism by which the same object instance may be used to make separate calculations on multiple data sets, by calling it in between each application (i.e., looping from line 12 back to line 10 for a different data set – see the full code for `Example1TeBinaryData.java` for an example).

The user then supplies the data to construct the PDFs with which the information-theoretic calculation is to be made. Here, this occurs at line 11 by calling the `addObservations()` method to supply the source and destination time series values. This method can be called multiple times to add multiple sample time-series before the calculation is made (see further commentary for handling ensembles of samples in Section 4.1.5).

Finally, with all observations supplied to the estimator, the resulting transfer entropy may be computed via `computeAverageLocalOfObservations()` at line 12. The information-theoretic *measurement is returned in bits* for all discrete calculators. In this example, since the destination copies the previous value of the (randomized) source, then `result` should approach 1 bit.

4.1.2. Typical calling pattern for an information-theoretic measure on continuous data

Before outlining how to use the continuous estimators, we note that the discrete estimators above may be applied to continuous `double[]` data sets by first *binning* them to convert them to `int[]` arrays, using either `MatrixUtils.discretise(double data[], int numBins)` for even bin sizes or `MatrixUtils.discretiseMaxEntropy(double data[], int numBins)` for maximum entropy binning (see `Example8TeContinuousDataByBinning`). This is very efficient, however, as per section 2.2 it is more accurate to use an estimator, which utilizes the continuous nature of the data.

As such, we now review the use of a KSG estimator (Section S.2.2.3 in Supplementary Material) to compute transfer entropy (equation (S.25) in Supplementary Material), as a *standard calling pattern* for all estimators applied to *continuous data*. The sample code in **Listing 3** is adapted from `Example4TeContinuousDataKraskov.java`. (That this is a standard calling pattern can easily be seen by comparing to `Example3TeContinuousDataKernel.java`, which uses a box-kernel estimator but has very similar method calls, except for which parameters are passed in).

Listing 3 | Use of KSG estimator to compute transfer entropy; adapted from `Example4TeContinuousDataKraskov.java`.

```
double[] sourceArray, destArray;
// ...
// Import values into sourceArray and
   destArray
// ...
TransferEntropyCalculatorKraskov teCalc = new
   TransferEntropyCalculatorKraskov();
teCalc.setProperty("k", "4");
teCalc.initialise(1);
teCalc.setObservations(sourceArray,
   destArray);
double result = teCalc.
   computeAverageLocalOfObservations();
```

Notice that the calling pattern here is almost the same as that for discrete calculators, as seen in **Listing 2**, with some minor differences outlined below.

Of course, for continuous data we now use `double[]` arrays (indexed by time) for the univariate time-series data here at line 1. Multidimensional time series are discussed in Section 4.1.7.

As per discrete calculators, we begin by constructing an instance of the calculator, as per line 5 above. Here, however, parameters for the operation of the estimator are not only supplied via the constructor (see below). As such, all classes offer a constructor with no arguments, while only some implement constructors which accept certain parameters for the operation of the estimator.

Next, almost all relevant properties or parameters of the estimators can be supplied by passing key-value pairs of `String` objects to the `setProperty(String, String)` method at line 6. The key values for properties, which may be set for any given calculator are described in the Javadocs for the `setProperty` method for each calculator. Properties for the estimator may be set by calling `setProperty` at any time; in most cases, the new property value will take effect immediately, though it is only guaranteed to hold after the next initialization (see below). At line 6, we see that property "`k`" (shorthand for `ConditionalMutualInfoCalculatorMultiVariateKraskov.PROP_K`) is set to the value "4." As described in the Javadocs for `TransferEntropyCalculatorKraskov.setProperty`, this sets the number of nearest neighbors K to use in the KSG estimation in the full joint space. Properties can also easily be extracted and set from a file, see `Example6LateBindingMutualInfo.java`.

As per the discrete calculators, all continuous calculators must be initialized before use or re-use on new data (see line 7). This clears any PDFs held inside the class, but additionally finalizes any property settings here. Also, the `initialise()` method for continuous estimators may accept some parameters for the calculator – here, it accepts a setting for the k embedded history length parameter for the transfer entropy (see equation (S.25) in Supplementary Material). Indeed, there may be several *overloaded* forms of `initialise()` for a given class, each accepting different sets of parameters. For example, the

`TransferEntropyCalculatorKraskov` used above offers an `initialise(k, tau_k, l, tau_l, u)` method taking arguments for both source and target embedding lengths k and l, embedding delays τ_k and τ_l (see Section S.1.2 in Supplementary Material), and source-target delay u (see equation (S.27) in Supplementary Material). Note that currently such embedding parameters must be supplied by the user, although we intend to implement automated embedding parameter selection in the future. Where a parameter is not supplied, the value given for it in a previous call to `initialise()` or `setProperty()` (or otherwise its default value) is used.

The supply of samples is also subtly different for continuous estimators. Primarily, all estimators offer the `setObservations()` method (line 8) for supplying a single time-series of samples (which can only be done once). See Section 4.1.5 for how to use multiple time-series realizations to construct the PDFs via an `addObservations()` method.

Finally, the information-theoretic measurement (line 9) is returned in *either bits or nats* as per the standard definition for this type of estimator in Section 2.2 (i.e., bits for discrete, kernel, and permutation estimators; nats for Gaussian and KSG estimators).

At this point (before or after line 9) once all observations have been supplied, there are other quantities that the user may compute. These are described in the next two subsections.

4.1.3. Local information-theoretic measures

Listing 4 computes the *local* transfer entropy (equation (S.54) in Supplementary Material) for the observations supplied earlier in **Listing 3**:

Listing 4 | Computing local measures after Listing 3; adapted from `Example4TeContinuousDataKraskov.java`.

```
double[] localTE = teCalc.
  computeLocalOfPreviousObservations();
```

Each calculator (discrete or continuous) provides a `computeLocalOfPreviousObservations()` method to compute the relevant local quantities for the given measure (see Section S.1.3 in Supplementary Material). This method returns a `double[]` array of the local values (local TE here) at every time step n for the supplied time-series observations. For TE estimators, note that the first k values (history embedding length) will have value 0, since local TE is not defined without the requisite history being available[20].

4.1.4. Null distribution and statistical significance

For the observations supplied earlier in **Listing 3**, **Listing 5** computes a distribution of surrogate TE values obtained via resampling under the null hypothesis that `sourceArray` and `destArray` have no temporal relationship (as described in Section S.1.5 in Supplementary Material).

[20]The return format is more complicated if the user has supplied observations via several `addObservations()` calls rather than `setObservations()`; see the Javadocs for `computeLocalOfPreviousObservations()` for details.

Listing 5 | Computing null distribution after Listing 3; adapted from `Example3TeContinuousDataKernel.java`.

```
EmpiricalMeasurementDistribution dist =
  teCalc.computeSignificance(1000);
```

The method `computeSignificance()` is implemented for all MI and conditional MI based measures (including TE), for both discrete and continuous estimators. It returns an `EmpiricalMeasurementDistribution` object, which contains a `double[]` array `distribution` of an empirical distribution of values obtained under the null hypothesis (the sample size for this distribution is specified by the argument to `computeSignificance()`). The user can access the mean and standard deviation of the distribution, a p-value of whether these surrogate measurements were greater than the actual TE value for the supplied source, and a corresponding t-score (which assumes a Gaussian distribution of surrogate scores) via method calls on this object (see Javadocs for details).

Some calculators (discrete and Gaussian) overload the method `computeSignificance()` (without an input argument) to return an object encapsulating an *analytically* determined p-value of surrogate distribution where this is possible for the given estimation type (see Section S.1.5 in Supplementary Material). The availability of this method is indicated when the calculator implements the `AnalyticNullDistributionComputer` interface.

4.1.5. Ensemble approach: using multiple trials or realizations to construct PDFs

Now, the use of `setObservations()` for continuous estimators implies that the PDFs are computed from a single *stationary* time-series realization. One may supply multiple time-series realizations (e.g., as multiple stationary trials from a brain-imaging experiment) via the following alternative calling pattern to line 8 in **Listing 3**:

Listing 6 | Supply of multiple time-series realizations as observations for the PDFs; an alternative to line 8 in Listing 3. Code is adapted from `Example7EnsembleMethodTeContinuousDataKraskov.java`.

```
teCalc.startAddObservations();
teCalc.addObservations(sourceArray1,
  destArray1);
teCalc.addObservations(sourceArray2,
  destArray2);
teCalc.addObservations(sourceArray3,
  destArray3);
// ...
teCalc.finaliseAddObservations();
```

Computations on the PDFs constructed from this data can then follow as before. Note that other variants of `addObservations()` exist, e.g., which pull out sub-sequences from the time series arguments; see the Javadocs for each calculator to see the options available. Also, for the discrete estimators, `addObservations()` may be called multiple times

directly without the use of a `startAddObservations()` or `finaliseAddObservations()` method. This type of calling pattern may be used to realize an *ensemble approach* to constructing the PDFs (see Gomez-Herrero et al. (2010), Wibral et al. (2014b), Lindner et al. (2011), and Wollstadt et al. (2014)), in particular, by supplying only short corresponding (*stationary*) parts of each trial to generate the PDFs for that section of an experiment.

4.1.6. Joint-variable measures on multivariate discrete data

For calculations involving *joint variables* from *multivariate discrete data* time-series (e.g., collective transfer entropy, see Section S.1.2 in Supplementary Material), we use the *same* discrete calculators (unlike the case for continuous-valued data in Section 4.1.7). This is achieved with one simple pre-processing step, as demonstrated by `Example5TeBinaryMultivarTransfer.java`:

Listing 7 | Java source code adapted from `Example5TeBinaryMultivarTransfer.java`.

```
int[][] source, dest;
// ...
// Import binary values into the arrays,
// with two columns each.
// ...
TransferEntropyCalculatorDiscrete teCalc =
   new TransferEntropyCalculatorDiscrete
   (4, 1);
teCalc.initialise();
teCalc.addObservations(
   MatrixUtils.
   computeCombinedValues(source, 2),
   MatrixUtils.
   computeCombinedValues(dest, 2));
double result = teCalc.
   computeAverageLocalOfObservations();
```

We see that the multivariate discrete data is represented using two-dimensional `int [][]` arrays at line 1, where the first array index (row) is time and the second (column) is variable number.

The important pre-processing at line 9 and line 10 involves combining the joint vector of discrete values for each variable at each time step into a single discrete number, i.e., if our joint vector `source[t]` at time t has v variables, each with M possible discrete values, then we can consider the joint vector as a v-digit base-M number, and directly convert this into its decimal equivalent. The `computeCombinedValues()` utility in `infodynamics.utils.MatrixUtils` performs this task for us at each time step, taking the `int [][]` array and the number of possible discrete values for each variable $M = 2$ as arguments. Note also that when the calculator was constructed at line 6, we need to account for the total number of possible combined discrete values, being $M^v = 4$ here.

4.1.7. Joint-variable measures on multivariate continuous data

For calculations involving *joint variables* from *multivariate continuous data* time-series, JIDT provides *separate* calculators to be used. `Example6LateBindingMutualInfo.java` demonstrates this for calculators implementing the `MutualInfoCalculatorMultiVariate` interface[21]:

Listing 8 | Java source code adapted from `Example6LateBindingMutualInfo.java`.

```
double[][] variable1, variable2;
MutualInfoCalculatorMultiVariate miCalc;
// ...
// Import continuous values into the arrays
// and instantiate miCalc
// ...
miCalc.initialise(2, 2);
miCalc.setObservations(variable1, variable2);
double miValue = miCalc.
   computeAverageLocalOfObservations();
```

First, we see that the multivariate continuous data is represented using two-dimensional `double [][]` arrays at line 1, where (as per section 4.1.6) the first array index (row) is time and the second (column) is variable number. The instantiating of a class implementing the `MutualInfoCalculatorMultiVariate` interface to make the calculations is not shown here (but is discussed separately in Section 4.1.8).

Now, a crucial step in using the multivariate calculators is specifying in the arguments to `initialise()` the number of dimensions (i.e., the number of variables or columns) for each variable involved in the calculation. At line 7, we see that each variable in the MI calculation has two dimensions (i.e., there will be two columns in each of `variable1` and `variable2`).

Other interactions with these multivariate calculators follow the same form as for the univariate calculators.

4.1.8. Coding to interfaces; or dynamic dispatch

Listing 8 (`Example6LateBindingMutualInfo.java`) also demonstrates the manner in which a user can write code to use the *interfaces* defined in `infodynamics.measures.continuous` – rather than any particular *class* implementing that measure – and dynamically alter the instantiated class implementing this interface at runtime. This is known as *dynamic dispatch*, enabled by the *polymorphism* provided by the interface (described at Section 3.4). This is a useful feature in object-oriented programing where, here, a user wishes to write code which requires a particular measure, and dynamically switch-in different estimators for that measure at runtime. For example, in **Listing 8**, we may normally use a KSG estimator, but switch-in a linear-Gaussian estimator if we happen to know our data is Gaussian.

To use dynamic dispatch with JIDT:

1. Write code to use an interface for a calculator (e.g., `MutualInfoCalculatorMultiVariate` in **Listing 8**), rather than to directly use a particular implementing class (e.g., `MutualInfoCalculatorMultiVariateKraskov`);

[21] In fact, for MI, JIDT does not actually define a separate calculator for univariates – the multivariate calculator `MutualInfoCalculatorMultiVariate` provides interfaces to supply univariate `double[]` data where each variable is univariate.

2. Instantiate the calculator object by *dynamically* specifying the implementing class (compare to the static instantiation at line 5 of **Listing 3**), e.g., using a variable name for the class as shown in **Listing 9**:

Listing 9 | Dynamic instantiation of a mutual information calculator, belonging at line 5 in Listing 8. Adapted from `Example6LateBindingMutualInfo.java`.

```
String implementingClass;
// Load the name of the class to be used into
// the variable implementingClass
miCalc = (MutualInfoCalculatorMultiVariate)
  Class.forName(implementingClass).
  newInstance();
```

Of course, to be truly dynamic, the value of `implementingClass` should not be hard-coded but must be somehow set by the user. For example, in the full `Example6LateBindingMutualInfo.java` it is set from a properties file.

4.2. MATLAB/OCTAVE DEMOS

The "Octave/MATLAB code examples" set at `demos/octave` in the distribution provide a basic set of demonstration scripts for using the toolkit in GNU Octave or MATLAB. The set is described in some detail at the `OctaveMatlabExamples` wiki page (**Table 2**). See Section 3.1 regarding installation requirements for running the toolkit in Octave, with more details at the `UseInOctaveMatlab` wiki page (see **Table 2**).

The scripts in this set mirror the Java code in the "Simple Java Demos" set (Section 4.1), to demonstrate that *anything which JIDT can do in a Java environment can also be done in MATLAB/Octave*. The user is referred to the distribution or the `OctaveMatlabExamples` wiki page for more details on the examples. An illustrative example is provided in **Listing 10**, which converts **Listing 2** into MATLAB/Octave:

Listing 10 | Estimation of TE from discrete data in MATLAB/Octave; adapted from `example1TeBinaryData.m`.

```
javaaddpath('../../infodynamics.jar');
sourceArray=(rand(100,1)>0.5)*1;
destArray = [0; sourceArray(1:99)];
teCalc=javaObject('infodynamics.measures.
  discrete.TransferEntropyCalculatorDiscrete',
  2, 1);
teCalc.initialise();
teCalc.addObservations(
  octaveToJavaIntArray(sourceArray),
  octaveToJavaIntArray(destArray));
result = teCalc.
  computeAverageLocalOfObservations()
```

This example illustrates several important steps for using JIDT from a MATLAB/Octave environment:

1. Specify the classpath (i.e., the location of the `infodynamics.jar` library) before using JIDT with the function `javaaddpath(samplePath)` (at line 1);
2. Construct classes using the `javaObject()` function (see line 4);
3. Use of objects is otherwise almost the same as in Java itself, however,
   a. In Octave, conversion between native *array* data types and Java arrays is not straightforward; we recommend using the supplied functions for such conversion in `demos/octave`, e.g., `octaveToJavaIntArray.m`. These are described on the `OctaveJavaArrayConversion` wiki page (**Table 2**), and see example use in line 7 here, and in `example2TeMultidimBinaryData.m` and `example5TeBinaryMultivarTransfer.m`.
   b. In Java arrays are indexed from 0, whereas in Octave or MATLAB these are indexed from 1. So when you call a method on a Java object such as `MatrixUtils.select(double data, int fromIndex, int length)` – even from within MATLAB/Octave – you must be aware that `fromIndex` will be indexed from 0 inside the toolkit, not 1!

4.3. PYTHON DEMOS

Similarly, the "Python code examples" set at `demos/python` in the distribution provide a basic set of demonstration scripts for using the toolkit in Python. The set is described in some detail at the `PythonExamples` wiki page (**Table 2**). See Section 3.1 regarding installation requirements for running the toolkit in Python, with more details at the `UseInPython` wiki page (**Table 2**).

Again, the scripts in this set mirror the Java code in the "Simple Java Demos" set (Section 4.1), to demonstrate that *anything which JIDT can do in a Java environment can also be done in Python*.

Note that this set uses the `JPype` library[22] to create the Python-Java interface, and the examples would need to be altered if you wish to use a different interface. The user is referred to the distribution or the `PythonExamples` wiki page for more details on the examples.

An illustrative example is provided in **Listing 11**, which converts **Listing 2** into Python:

Listing 11 | Estimation of TE from discrete data in Python; adapted from `example1TeBinaryData.py`.

```
from jpype import *
import random
startJVM(getDefaultJVMPath(), "-ea",
  "-Djava.class.path=../../infodynamics.jar")
sourceArray = [random.randint(0,1) for
  r in xrange(100)]
destArray = [0] + sourceArray[0:99];
teCalcClass = JPackage("infodynamics.measures.
 discrete").TransferEntropyCalculatorDiscrete
teCalc = teCalcClass(2,1)
teCalc.initialise()
teCalc.addObservations(sourceArray,
destArray)
result = teCalc.
  computeAverageLocalOfObservations()
shutdownJVM()
```

[22] http://jpype.sourceforge.net/

This example illustrates several important steps for using JIDT from Python via JPype:

1. Import the relevant packages from JPype (line 1);
2. Start the JVM and specify the classpath (i.e., the location of the `infodynamics.jar` library) before using JIDT with the function `startJVM()` (at line 3);
3. Construct classes using a reference to their package (see line 6 and 7);
4. Use of objects is otherwise almost the same as in Java itself, however, conversion between native *array* data types and Java arrays can be tricky – see comments on the `UseInPython` wiki page (see **Table 2**).
5. Shutdown the JVM when finished (line 11).

4.4. SCHREIBER'S TRANSFER ENTROPY DEMOS

The "Schreiber Transfer Entropy Demos" set at `demos/octave/SchreiberTransferEntropyExamples` in the distribution recreates the original examples introducing transfer entropy by Schreiber (2000). The set is described in some detail at the `SchreiberTeDemos` wiki page (see **Table 2**). The demo can be run in MATLAB or Octave.

The set includes computing TE with a discrete estimator for data from a Tent Map simulation, with a box-kernel estimator for data from a Ulam Map simulation, and again with a box-kernel estimator for heart and breath rate data from a sleep apnea patient[23] (see Schreiber (2000)) for further details on all of these examples and map types). Importantly, the demo shows correct values for important parameter settings (e.g., use of bias correction), which were not made clear in the original paper.

We also revisit the heart-breath rate analysis using a KSG estimator, demonstrating how to select embedding dimensions k and l for this data set. As an example, we show in **Figure 3**, a calculation of AIS (equation (S.23) in Supplementary Material) for the heart and breath rate data, using a KSG estimator with $K=4$ nearest neighbors, as a function of embedding length k. This plot is produced by calling the MATLAB function: `activeInfoStorageHeartBreathRatesKraskov(1:15, 4)`. Ordinarily, as an MI the AIS will be non-decreasing with k, while an observed increase may be simply because bias in the underlying estimator increases with k (as the statistical power of the estimator is exhausted). This is not the case, however, when we use an underlying KSG estimator, since the bias is automatically subtracted away from the result. As such, we can use the peak of this plot to suggest that an embedded history of $k=2$ for both heart and breath time-series is appropriate to capture all relevant information from the past without adding more spurious than relevant information as k increases. (The result is stable with the number of nearest neighbors K.) We then continue on to use those embedding lengths for further investigation with the TE in the demonstration code.

[23]This data set was made available via the Santa Fe Institute time series contest held in 1991 (Rigney et al., 1993) and redistributed with JIDT with kind permission from Andreas Weigend.

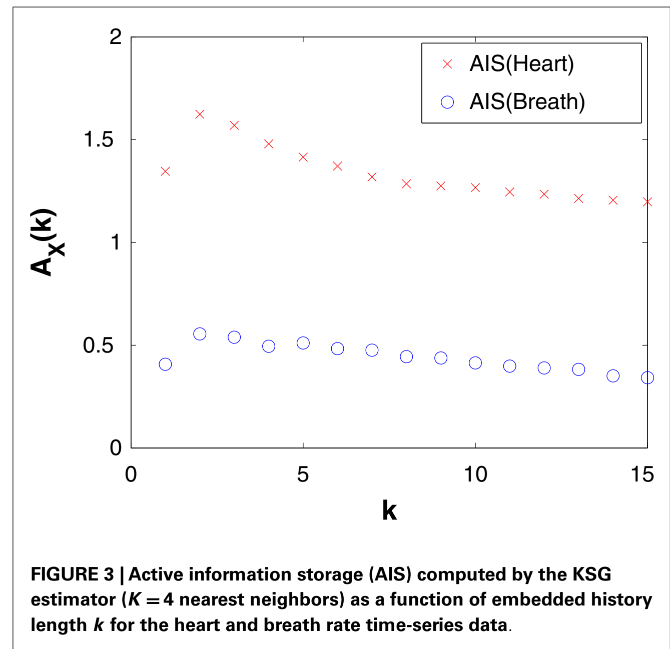

FIGURE 3 | Active information storage (AIS) computed by the KSG estimator ($K=4$ nearest neighbors) as a function of embedded history length k for the heart and breath rate time-series data.

4.5. CELLULAR AUTOMATA DEMOS

The "Cellular Automata Demos" set at `demos/octave/CellularAutomata` in the distribution provide a standalone demonstration of the utility of *local* information dynamics profiles. The scripts allow the user to reproduce the key results from Lizier et al. (2008c, 2010, 2012b, 2014); (Lizier, 2013); (Lizier and Mahoney, 2013), etc., i.e., plotting local information dynamics measures at every point in space-time in the cellular automata (CA). These results confirmed the long-held conjectures that gliders are the dominant information transfer entities in CAs, while blinkers and background domains are the dominant information storage components, and glider/particle collisions are the dominant information modification events.

The set is described in some detail at the `CellularAutomataDemos` wiki page (see **Table 2**). The demo can be run in MATLAB or Octave. The main file for the demo is `plotLocalInfoMeasureForCA.m`, which can be used to specify a CA type to run and which measure to plot an information profile for. Several higher-level scripts are available to demonstrate how to call this, including `DirectedMeasuresChapterDemo2013.m` which was used to generate the figures by Lizier (2014) (reproduced in **Figure 4**).

4.6. OTHER DEMOS

The toolkit contains a number of other demonstrations, which we briefly mention here:

- The "Interregional Transfer demo" set at `demos/java/interregionalTransfer/` is a higher-level example of computing information transfer between two regions of variables (e.g., brain regions in fMRI data), using multivariate extensions to the transfer entropy, to infer effective connections between the regions. This demonstration implements the method originally

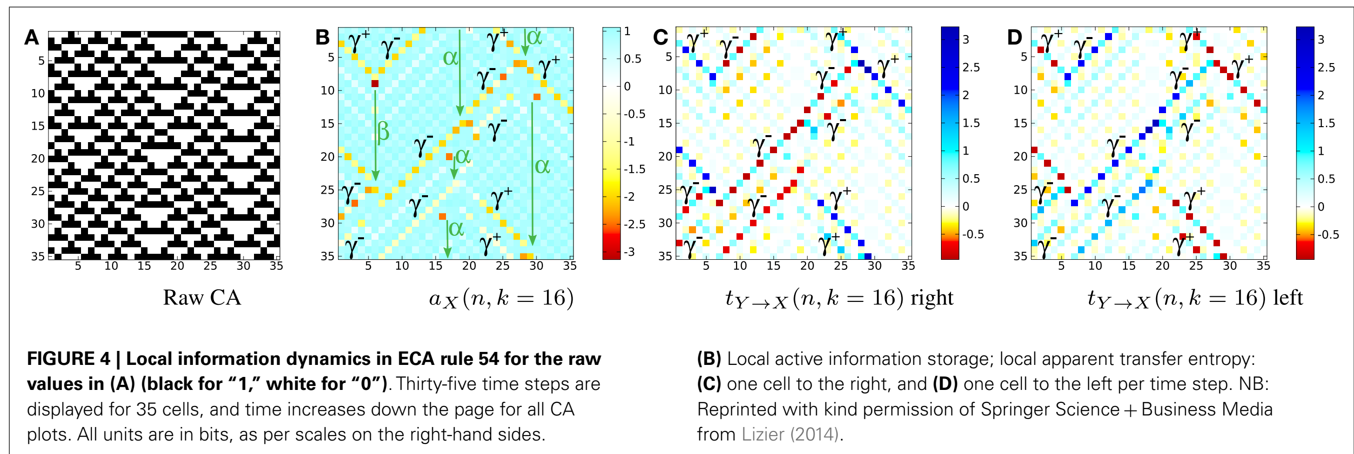

FIGURE 4 | Local information dynamics in ECA rule 54 for the raw values in (A) (black for "1," white for "0"). Thirty-five time steps are displayed for 35 cells, and time increases down the page for all CA plots. All units are in bits, as per scales on the right-hand sides. **(B)** Local active information storage; local apparent transfer entropy: **(C)** one cell to the right, and **(D)** one cell to the left per time step. NB: Reprinted with kind permission of Springer Science + Business Media from Lizier (2014).

described by Lizier et al. (2011a). Further documentation is provided via the `Demos` wiki page (see **Table 2**).

- The "Detecting interaction lags" demo set at `demos/octave/DetectingInteractionLags` shows how to use the transfer entropy calculators to investigate a source-destination lag that is different to 1 (the default). In particular, this demo was used to make the comparisons of using transfer entropy (TE) and momentary information transfer (MIT) (Pompe and Runge, 2011) to investigate source-destination lags by Wibral et al. (2013) (see Test cases Ia and Ib therein). In particular, the results show that TE is most suitable for investigating source-destination lags as MIT can be deceived by source memory, and also that symbolic TE (Section S.2.2.4 in Supplementary Material) can miss important components of information in an interaction. Further documentation is provided via the `Demos` wiki page (see **Table 2**).
- The "Null distribution" demo set at `demos/octave/NullDistributions` explores the match between analytic and resampled distributions of MI, conditional MI and TE under null hypotheses of no relationship between the data sets (see Section S.1.5 in Supplementary Material). Further documentation is provided via the `Demos` wiki page (see **Table 2**).

Finally, we note that demonstrations on using JIDT within several additional languages (Julia, Clojure, and R) are currently available within the SVN repository only, and will be distributed in future releases.

5. CONCLUSION

We have described the Java Information Dynamics Toolkit (JIDT), an open-source toolkit available on Google code, which implements information-theoretic measures of dynamics via several different estimators. We have described the architecture behind the toolkit and how to use it, providing several detailed code demonstrations.

In comparison to related toolkits, JIDT provides implementations for a wider array of information-theoretic measures, with a wider variety of estimators implemented, adds implementations of local measures and statistical significance, and is standalone software. Furthermore, being implemented in Java, JIDT is platform agnostic and requires little to no installation, is fast, exhibits an intuitive object-oriented design, and can be used in MATLAB, Octave, Python, and other environments.

JIDT has been used to produce results in publications by both this author and others (Wang et al., 2012, 2014; Dasgupta et al., 2013; Lizier and Mahoney, 2013; Wibral et al., 2013, 2014a,c; Gómez et al., 2014; Lizier, 2014; Lizier et al., 2014).

It may be complemented by the Java Partial Information Decomposition (JPID) toolkit (Lizier and Flecker, 2012; Lizier et al., 2013), which implements early attempts (Williams and Beer, 2010b) to separately measure redundant and synergistic components of the conditional mutual information (see Section S.1.1 in Supplementary Material).

We are planning the extension or addition of several important components in the future. Of highest priority, we are exploring the use of multi-threading and GPU computing, and automated parameter selection for time-series embedding. We will add additional implementations to complete **Table 3**, and aim for larger code coverage by our unit tests. Most importantly, however, we seek collaboration on the project from other developers in order to expand the capabilities of JIDT, and we will welcome volunteers who wish to contribute to the project.

ACKNOWLEDGMENTS

I am grateful to many collaborators and contacts who have tested JIDT in their applications, provided test data, found bugs, provided feedback, and reviewed this manuscript, etc. These include primarily X. Rosalind Wang, Michael Wibral, Oliver Cliff, Siddharth Pritam, Rommel Ceguerra, Ipek Özdemir, and Oliver Obst; as well as Sakyasingha Dasgupta, Heni Ben Amor, Mizuki Oka, Christoph Hartmann, Michael Harré, and Patricia Wollstadt.

SUPPLEMENTARY MATERIAL

The Supplementary Material for this article can be found online at http://www.frontiersin.org/Journal/10.3389/frobt.2014.00011/abstract

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Conflict of Interest Statement: The Review Editor Keyan Ghazi-Zahedi declares that, despite being affiliated to the same institution as author Joseph T. Lizier, the review process was handled objectively and no conflict of interest exists. The author declares that the research was conducted in the absence of any commercial or financial relationships that could be construed as a potential conflict of interest.

Received: 15 August 2014; paper pending published: 23 September 2014; accepted: 24 October 2014; published online: 02 December 2014.

*Citation: Lizier JT (2014) JIDT: an information-theoretic toolkit for studying the dynamics of complex systems. Front. Robot. AI **1**:11. doi: 10.3389/frobt.2014.00011*

This article was submitted to Computational Intelligence, a section of the journal Frontiers in Robotics and AI.

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