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Deciphering interactions of complex systems that do not satisfy detailed balance

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ABSTRACT

We present an extension of a novel method for understanding complex systems, which has been applied to non-equilibrium systems both in and out of detailed balance. For the non-detailed balance case, in which non-zero currents are a principal indicator of complexity, there has been an incomplete understanding of the distance function in the observable representation embedding. To deal with this we construct a new transition matrix by accounting for this current and compute the eigenvalues and eigenvectors. From these, we define a metric whose distance provides a useful measure of the relation among variables. Use of this method provides insights into long-range correlation, and chaotic properties. As an example we show that these distances can be used to control chaos in a simple dynamical system.

1. Introduction

Natural systems that come under the (often vague) heading of *complex*, are typically far from equilibrium, involve many degrees of freedom, exhibit irreversibility, do not satisfy detailed balance, and are not described by traditional Boltzmann–Gibbs statistics (properties that are not independent of one another). Examples include neural networks [10], gene activity [2], and turbulent flows [1,12]. A special class of complex systems has already been extensively studied in the past. These systems can have their slow variables differentiated from those changing rapidly when there is scale separation in time and/or space. In these cases analytical progress can be made for example by using the projection method [3].

A recently developed technique that does not assume this scale separation and has been used in the study of dynamical systems is to use a graphical representation that implicitly reflects dynamical correlations in phase space [6]. This is done by using a subset of "macroscopic observables" obtained by calculating transition probabilities from the dynamics of the system. The metric distance in this representation is a direct measure of correlation, and is useful in understanding the dynamics of the system without detailed knowledge of the complex interactions among all of the underlying constituents. This is called the Observable Representation (OR) and is an example of a spectral method.

Spectral methods to aid visualization and highlight relationships are used both in spectral graph theory [13] and the OR [9] (see [9] for a comparison; see [4] for the continuous case). The OR was originally developed to understand non-equilibrium phase transitions, [5,6]. It has been applied to several examples, including spin glasses [17], coarse graining models [7], and the reconstruction of coordinate spaces [9]. In this Letter we present a new framework, called the Non-detailed balance Observable Representation (NOR), which allows the study of non-detailed balance systems. To explain the NOR we first briefly recall the framework of the OR (the NOR's detailed balance version).

States of the system are given by $x, y \in \mathbf{X}$, where $\mathbf{X}$ is a space of cardinality $N < \infty$. We represent the transition probabilities between two states x and y as R_{xy}, where

$$R_{xy} = \Pr(x \leftarrow y) = \Pr\big[\text{state at } (t+1) \text{ is } x \,\big|\, \text{state at } t \text{ is } y\big]. \tag{1}$$

Assuming R to be irreducible leads to a unique eigenvalue $\lambda_0 = 1$ with eigenvector $p_0(x)$. $p_0(x)$ is strictly positive and satisfies $\sum_y R_{xy} p_0(y) = p_0(x)$, with $\sum_x p_0(x) = 1$. There are several other requirements on R_{xy}; the first is the conservation of total probability $\sum_x R_{xy} = 1$. Second, we assume R_{xy} is diagonalizable. We arrange the eigenvalues in order of decreasing magnitude, $1 = \lambda_0 \geqslant |\lambda_1| \geqslant |\lambda_2| \geqslant \cdots \geqslant |\lambda_N|$. The eigenvectors corresponding to each

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eigenvalue are ordered accordingly. The left and right eigenvectors of R_{xy} are defined as

$$\sum_x A_\alpha(x)R_{xy} = \lambda_\alpha A_\alpha(y), \qquad \sum_y R_{xy}p_\alpha(y) = \lambda_\alpha p_\alpha(x). \tag{2}$$

Here the subscript denotes the column index, and the argument denotes the row index. The slowest decaying left eigenfunctions of R_{xy} will be the macroscopic "observables" which characterize the system on the macroscale of interest. (See [7] for elaboration on this terminology.) The faster decaying eigenvectors are the rapidly fluctuating quantities of the system, which average to zero over the macroscale. It follows from the form of R_{xy} that there is a left eigenvector, $A_0 = 1$, such that $A_0 R = A_0$. We normalize the eigenfunctions A_j and p_k to form an orthonormal basis, $\langle A_j | p_k \rangle = \delta_{jk}$.

It was shown in [9] that for the detailed balance case using the left eigenvectors, there is an inequality between a metric intuitively related to the state-to-state dynamics (the left-hand side of Eq. (3)) and a natural metric in the OR (on the right) as

$$\sum_x \left| \frac{R_{xi} - R_{xj}}{\sqrt{p_0(x)}} \right| \geqslant \sqrt{\sum_\alpha^m \left|\lambda_\alpha \big(A_\alpha(i) - A_\alpha(j)\big)\right|^2}. \tag{3}$$

Here m is the dimension of the OR, where $m \leqslant N$. $A_\alpha(i)$ is the α element in the m-tuple corresponding to the ith point in the OR. The appropriate value of m is typically given by a spectral gap in the eigenvalues, when $\lambda_{m+1} \ll \lambda_m$ [4,7]. If the system does not exhibit a spectral gap, it may be necessary to consider more dimensions than is feasible to faithfully represent the system. As remarked, for the inequality (3) to hold, R_{xy} must also satisfy detailed balance, which is equivalent to the currents' vanishing (no summation over x or y),

$$J_{xy} = R_{xy}p_0(y) - R_{yx}p_0(x) = 0. \tag{4}$$

The crux of the derivation of Eq. (3) is the existence of a complete set of eigenvalues and orthogonal eigenvectors of a symmetric matrix $S_{xy} = \frac{1}{\sqrt{p_0(x)}} R_{xy} \sqrt{p_0(y)}$.

The purpose of this Letter is to generalize Eq. (3) when $J_{xy} \neq 0$. When $J_{xy} \neq 0$, the symmetric property of S_{xy} based on R_{xy} no longer holds. It was shown in [7] that even when $J_{xy} \neq 0$ the first few eigenvectors and eigenvalues could be used to find the phases of simple systems. As J_{xy} grows or the complexity of the system increases, A_α no longer gives an accurate representation of the system. As a result Eq. (3) fails and we need an extension to the theory. To be able to use the idea of relating distances in a coordinate space to the original dynamical system, i.e. by Eq. (3), when $J_{xy} \neq 0$, we propose a new matrix B_{xy},

$$B_{xy} = R_{xy} - \frac{J_{xy}}{2p_0(y)}. \tag{5}$$

Here B_{xy} is an $N \times N$ matrix which is column-wise stochastic. This is due to the fact that J_{xy} follows Kirchoff's loop rule: net current into a node equals net current out. One can show that if R_{xy} is irreducible then B_{xy} is irreducible. Writing B_{xy} as $B_{xy} = \frac{R_{xy}}{2} + \frac{R_{yx}p_0(x)}{2p_0(y)}$. It is clear that by adding a non-negative term to R_{xy}, B_{xy} must also be irreducible. Interestingly, it can also be shown that R_{xy} and B_{xy} share the same unique stationary distribution, $p_0(x)$. It is also true that B_{xy} has one eigenvalue of unity, $\nu_0 = 1$. We list the remaining eigenvalues in decreasing order: $\nu_0 \geqslant |\nu_1| \geqslant \cdots \geqslant |\nu_N|$. The right and left eigenvectors of B_{xy} are similarly defined as

$$B_{xy}\varphi_\alpha(y) = \nu_\alpha \varphi_\alpha(x), \qquad \Gamma_\alpha(x)B_{xy} = \nu_\alpha \Gamma_\alpha(y). \tag{6}$$

The completeness of the eigenfunctions for B_{xy}, Eq. (5), is guaranteed by the fact that B_{xy} can be transformed into a symmetric matrix S_{xy}, by a similarity transform, even when the system does not satisfy detailed balance. To demonstrate this, we define

$$S_{xy} = \frac{1}{\sqrt{p_0(x)}} B_{xy} \sqrt{p_0(y)}. \tag{7}$$

It is straightforward to verify that S is symmetric. Note that the eigenvectors $\psi_\alpha(x)$ of S_{xy} are related to the eigenvectors of B_{xy} as follows:

$$\frac{\varphi_\alpha(x)}{\sqrt{p_0(x)}} = \psi_\alpha(x), \qquad \Gamma_\alpha(x)\sqrt{p_0(x)} = \psi_\alpha(x). \tag{8}$$

Given that $\sqrt{p_0(x)} \geqslant 0$ and that Eq. (8) is a one to one relationship between the real eigenvectors and eigenvalues of S_{xy} we have a guarantee that the eigenvectors and eigenvalues of B_{xy} will also be real. The matrix B_{xy} is reminiscent of the inverse construction in [8]. It turns out that the distance computed from the left eigenvectors of B_{xy} based on S_{xy} gives a physically meaningful distance, for example correlations, by removing the contribution from the anti-symmetric part which includes oscillating transition probabilities and rotation in the phase space. For a more in depth discussion of the symmetric anti-symmetric properties see [16]. Using S_{xy} and the left eigenvectors of B_{xy}, we construct the non-detailed balance version of the OR, which we denote the (NOR). Specifically we can also construct a distance metric by replacing λ_α by ν_α and $A_\alpha(i)$ by $\Gamma_\alpha(i)$ in Eq. (3), so that one now has the inequality,

$$\sum_x \left| \frac{B_{xi} - B_{xj}}{\sqrt{p_0(x)}} \right| \geqslant \sqrt{\sum_\alpha^m \left|\nu_\alpha \big(\Gamma_\alpha(i) - \Gamma_\alpha(j)\big)\right|^2}. \tag{9}$$

This metric whose right-hand side we designate D_{NOR}, quantifies the correlation between the macroscopic states of the system and its underlying dynamics when the system does not satisfy detailed balance. It provides an intuitive and quantitative basis for the embedding induced by the NOR for B_{xy}, just as Eq. (3) does for detailed balance situations. Eq. (9) provides a dynamical basis for the study of non-detailed balance systems.

To illustrate that the D_{NOR} gives a correct measure of the correlation among different elements of X, we consider the logistic map which is a simple irreversible system due to its strong currents (i.e., $J_{xy} \neq 0$, in Eq. (4)). Note, that although the logistic map has an infinite number of states, we will shortly show that a finite coarse grained approximation of these states is enough to control the system. D_{NOR} is computed by following an ensemble of different orbits, which are the corresponding constituents in this case. We show how using these orbits, D_{NOR} can be usefully exploited to eliminate chaos in the system.

2. Application of NOR on the logistic map

The logistic map is defined as

$$x_{n+1} = M(x_n) = ax_n(1 - x_n), \tag{10}$$

in $[0, 1]$. Here, a is the control parameter. We consider the irreversible chaotic case by choosing $a = 4$, which results in a positive Lyapunov exponent L. For this mapping (Eq. (10)), the Lyapunov exponent is given as

$$L = \frac{1}{n}\sum_{i=1}^{n} l_i,$$
$$l_i = \log\left|\Omega'(x_i)\right|, \tag{11}$$

where n is the nth iteration or time step of the map and $\Omega'(x_i)$ is the derivative of the map at point x_i, $1 \leqslant i \leqslant n$. l_i is the local contribution to L at each time step. We spread M initial positions