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A Master equation approach to deciphering non-detailed balance systems

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Abstract. The world is filled with complex systems whether it is the traffic patterns in cities, weather patterns, information flow in the internet, or turbulence in fusion reactors. These complex systems are not often amenable to simple analytic solutions, understanding these systems requires a new statistical method beyond traditional equilibrium theory, i.e. Boltzmann Gibbs statistics. We present a novel method for understanding complex dynamics of such systems by using the Observable Representation which has been successfully applied to complex systems in detailed balance. Specifically we generalise it to non-equilibrium systems where detailed balance does not hold, i.e. the system has non zero currents. 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 correlation among variables. This is a very general method of understanding correlation in various systems, in particular, long-range correlation, or chaotic properties. As an example we show that these distances can be utilized to control chaos in a simple dynamical system given by the logistic map.

Keywords: detailed balance, non-equilibrium, chaos, complex systems.

1 Introduction

When studying a system in nature, we often devise experiments whose goal is to understand the interactions of a set of proposed variables. The ultimate goal of these investigations is to try and discover how the variables interact to form the underlying dynamical equations which govern the system. Often though the system is so complicated that finding these unknown equations is impossible. Instead of attempting to derive the underlying functions of a system, we take a different approach. Just as the field of dynamical systems uses graphical representations of systems that are difficult or impossible to solve analytically. We use a graphical representation of the system which comes from a master

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equation. The distances in this representation can be used to understand the original system without having any knowledge of its underlying functions which govern the system.

This representation of a system is called the Observable Representation (OR), it was originally developed by Schulman and Gaveau to try and understand non-equilibrium phase transitions, [4], [5]. Since its inception the OR has been applied to Ising models [6], course graining [1] and the reconstruction of coordinate spaces [2] among others. Coifmann et.al. have also used an extremely similar spectral approach which has been applied to the Fokker-Planck equation [3]. This paper will outline the notation of both the detailed balance OR and our non-detailed balance extension of the OR, the NOR. We will then show how to use this approach to control chaos in a simple dynamical system given by the Logistic map. Finally we will summarize with a brief conclusion.

2 Observable Representation with detailed balance

The system which is being studied is represented by the NxN stochastic matrix of transition probabilities R_{xy}. States of the system are given by $x, y \in \mathbf{X}$, $\mathbf{X}$ is a state space of cardinality $N < \infty$. The system moves according to R_{xy}, R_{xy} is defined as,

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

$p_o(x)$ is a unique strictly positive stationary distribution such that $\sum_x p_o = 1$, and $R_{xy} p_o(y) = p_o(x)$. There are several requirements of R_{xy}, the two main ones are that $\sum_x R_{xy} = 1$. We also require that R_{xy} is irreducible and assume R_{xy} is diagonalizable though the ideas should carry over if R_{xy} requires a Jordan form. These lead to an eigenvalue $\lambda_o = 1$ which corresponds to the stationary probabilities $p_o(x)$. We rearrange the eigenvalues in decreasing magnitude, $1 = \lambda_o \geq |\lambda_1| \geq |\lambda_2| \geq \ldots \geq |\lambda_N|$. The eigenvectors corresponding to each eigenvalue are reordered accordingly. The left and right eigenvectors of R_{xy} are defined as,

$$A_\alpha(x)^T R_{xy} = \lambda_\alpha A_\alpha^T(y), \quad R_{xy} P_\alpha(y) = \lambda_\alpha P_\alpha(x). \tag{2}$$

The subscript α denotes column number while the argument of the eigenvector x or y denotes the row, T is the transpose. The slowest decaying eigenfunctions of R_{xy}, will be the macroscopic "observables" which will give the averaged quantities of the system. While the faster decaying eigenvectors are the quickly fluctuating quantities of the system, which average themselves out. It follows from the form of R_{xy} that $\exists$ a left eigenvector, $A_o = 1$, s.t. $A_o^T R = A_o^T$. We normalize the eigenfunctions, A_j and P_k to form an orthonormal basis, $\langle A_j | P_k \rangle = \delta_{jk}$.

To see how the OR can be used to represent the coordinate space underlying system, we will build the basic structure of the Sierpinski fractal. This self similar fractal at its heart consists of three points or states as we will refer to them connected to form a triangle, with a smaller rotated triangle inside.

To find the coordinate space we first built an adjacency matrix $W^{N\times N}$ of the connections between the states of the system,

$$W = \begin{pmatrix} 0\,1\,0\,0\,0\,1 \\ 1\,0\,1\,1\,0\,1 \\ 0\,1\,0\,1\,0\,0 \\ 0\,1\,1\,0\,1\,1 \\ 0\,0\,0\,1\,0\,1 \\ 1\,1\,0\,1\,1\,0 \end{pmatrix} \tag{3}$$

Where each non zero value in W_{xy} says that the system can move from state y to state x in one time step. This is normalized so that $R_{xy} = \frac{W_{xy}}{\sum_x W_{xy}}$. Diagonalizing R_{xy} and plotting A_1, A_2 in figure (1) we recover the basic structure of the Sierpinski fractal. This process can be increased for as many layers of the fractal as one wishes. A 3-D version can also be created using the same process. This time plotting A_1, A_2 and A_3 in figure (2).

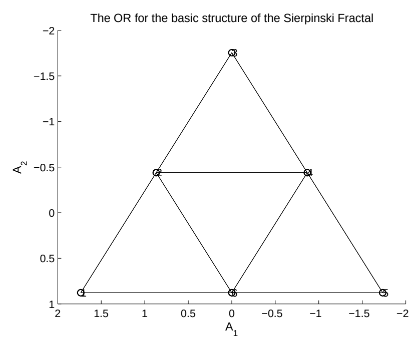

Fig. 1. Plotting the OR for the basic structure of the Sierpinski fractal. The lines have been added in to show connections.

It was shown in [2] that using the left eigenvectors, one can create a distance metric. The metric inequality is defined as,

$$\sum_x \left| \frac{R_{xi} - R_{xj}}{\sqrt{p_o(x)}} \right| \geq \sqrt{\sum_\alpha^m |\lambda_\alpha (A_\alpha(i) - A_\alpha(j))|^2}. \tag{4}$$

The right hand side is the distance in the OR called, D_{OR}. While the left hand side is a distance using R_{xy}. m is the dimension of the OR, where $m \leq N$. The inequality says that states of the system, which are related dynamically are also related in the OR. For the inequality to hold, R_{xy} must satisfy detailed balance, which is defined as,

$$J_{xy} = R_{xy}p_o(y) - R_{yx}p_o(x) = 0. \tag{5}$$

Though, even when $J_{xy} \neq 0$ the OR can often still recover the topology of the underlying coordinate space for simple systems. The derivation of the right

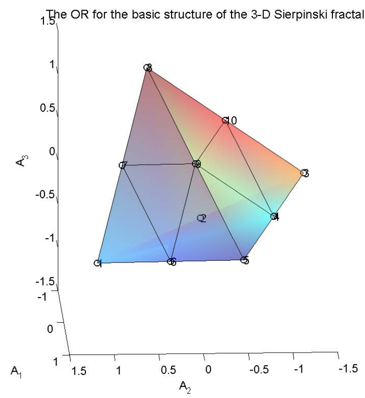

Fig. 2. Plotting the OR for the basic structure of the 3-D Sierpinski fractal. The lines have been added in to show connections.

hand side of equation (4) which represents the distance in the OR, abbreviated D_{OR}, relies on the eigenfunctions of R_{xy} having a one to one relation with a similarly symmetric matrix, S_{xy}. When $J_{xy} \neq 0$ this is not guaranteed. To recover the ability to relate distances in an OR, we define a new matrix B_{xy},

$$B_{xy} = R_{xy} - \frac{J_{xy}}{2p_o(y)}. \tag{6}$$

B_{xy} is an NxN matrix which is column wise stochastic. This is due to the fact that J_{xy} follows Kirchoff's loop rule, that the amount of current into a node is equal to the amount out. We also require B_{xy} to be irreducible. It can easily be shown that R_{xy} and B_{xy} share the same unique stationary distribution, $p_o(x)$. There is at least one eigenvalue of order unity, $\nu_o = 1$. The rest we again reorder into decreasing magnitude, $\nu_o \geq |\nu_1| \geq \ldots \geq |\nu_N|$. The right and left eigenvectors of B_{xy} are similarly defined as,

$$B_{xy}\varphi_\alpha(y) = \nu_\alpha \varphi_\alpha(x) \quad \Gamma_\alpha(x)^T B_{xy} = \nu_\alpha \Gamma_\alpha(y)^T. \tag{7}$$

There is a relationship between the matrix B_{xy} and the corresponding matrix S_{xy}, which can be shown to be symmetric even when $J_{xy} \neq 0$. The symmetry in S_{xy} is what guarantees the completeness of the eigenvectors of B_{xy}. The eigenvectors of B_{xy} and S_{xy} also share a relationship,

$$\frac{\varphi_\alpha(i)}{\sqrt{p_o(i)}} = \psi_\alpha(i), \quad \Gamma_\alpha(i)\sqrt{p_o(i)} = \psi_\alpha(i). \tag{8}$$

Using S_{xy} and the left eigenvectors of B_{ij} we can construct the non-detailed balance version of the OR, which we denote the (NOR). As was done in [2] we can also construct a distance metric where in equation (4) $\lambda_\alpha \rightarrow \nu_\alpha$ and $A_\alpha(i) \rightarrow \Gamma_\alpha(i)$. The metric which we will call D_{NOR} quantifies the relationship between the dynamical relations of a system to its macroscopic behavior when the system does not satisfy detail balance. The derivation of our metric conveniently follows just as was done in [2]. This simple extension opens up an entirely new class of systems to be studied using the NOR. As an example we will control the chaotic properties of the logistic map when its control parameter, $a = 4$.

3 Controlling chaos in the Logistic map

The Logistic map is defined as,

$$x_{n+1} = M(x_n) = ax_n(1 - x_n), \tag{9}$$

x_n is the position of a test particle in the system on iteration n, a is the control parameter which will be equal to 4 in the following. To control chaos in this system we initially track how the position of particles changes over many iterations and use this information to make, R_{xy} and B_{xy}. B_{xy} is then used to find the distances D_{NOR} between course grained points in the domain of the Logistic map. The minimum of the first off-diagonal of D_{NOR} will be the point that we perturb the system to when the Lyapunov exponents L, is greater than 0. L is defined as,

$$L = \frac{1}{n} \sum_i \log |M^{'}(x_n)|. \tag{10}$$

We see in figure (3) that from $1 \leq n \leq 50$, $L > 0$ for all the particles. From $n > 50$ we start to perturb the system on each iteration which is $50 < n \leq 75$ until $L \leq 0$ for all particles. From approximately $n > 75$ the system is allowed to freely evolve unless $L > 0$ for a particle, then it is perturbed back to the chosen position.

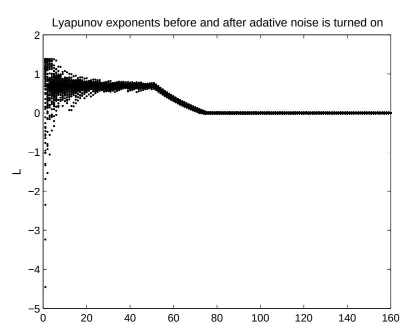

Fig. 3. The evolution of Lyapunov exponents for 100 particles in the Logistic map. we see the Lyapunov exponents become greater than zero until we begin to perturb the system at $n = 50$. Then the Lyapunov exponents approach and stay around zero.

4 Conclusion

In this paper we have shown a general method for deciphering the interactions of complex system when they no longer satisfy detailed balance. We have then applied this to the toy problem of stopping chaos in the Logistic map. Future work will consist of applying this method to real world system and system with more variables. We will also address questions with regards to the correct dimension of the OR and the NOR for a general system in future publications.
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