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Ranking nodes according to their path-complexity

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ABSTRACT

Thermalization is one of the most important phenomena in statistical physics. Often, the transition probabilities between different states in the phase space is or can be approximated by constants. In this case, the system can be described by Markovian transition kernels, and when the phase space is discrete, by Markov chains. In this paper, we introduce a macroscopic entropy on the states of paths of length k and, studying the recursion relation, obtain a fixed point entropy. This analysis leads to a centrality approach to Markov chains entropy.

1. Introduction

Physical systems require very often different descriptions at the micro and macro scale. It is the case for instance in systems which exhibit emergent phenomena, and for systems which undergo a phase transition. In this case, one could argue that the degrees of freedoms change with the scale effectively, and thus phase space counting should be different depending on the lens with which one look at the system. This line of thinking has been very fruitful in the last century, since the very initial work of Gell-Man and Low on the renormalization group. The concept of emergence, in particular, has enlighted many physical phenomena, giving them in the first place a renewed appeal from the new interpretation. With this same line of reasoning, dynamical systems can often exhibit correlations which are not only time dependent, but that at short time scales with respect to thermalization typical time scale, exhibit different behaviors.

The introduction of a macroscopic entropy functional for statistical systems has been introduced by Lloyd and Pagels in [1], and at the same time by Lindgren [2]. Lloyd and Pagels showed that the depth of a Hamiltonian system is proportional to the difference between the system and the coarse grained entropy. This paper introduced the concept of "thermodynamic depth". If p_i is the probability that a certain system arrived at a macroscopic state i, then the thermodynamic depth of that state is proportional to $\ln(p_i)$. This implies that the average depth of a system, the complexity, is proportional to the Shannon entropy, or the Boltzmann entropy. In addition, it has been shown in [1] that the only functional that is continuous, monotonically increasing with system size, and is extensive is the Boltzmann functional up to a constant [3]. One can show that such argument is true also for *macroscopic states*, described by trajectories $i_1 \to i_2 \to i_3 \cdots \to i_n$. In this case, the thermodynamic depth of this state is given by $-\alpha \log p(i_1, i_2, i_3, \cdots | i_n)$. In general, the average depth of a system with many macroscopic states can be very large. In fact, it has been shown in [2] that the macroscopic entropy defined by:

$$S_m = \sum_{i_1 i_2 \ldots i_m} - p_m(i_1 i_2 \ldots i_m) \log(p_m(i_1 i_2 \ldots i_m)) \tag{1}$$

is monotonically increasing, i.e. $\Delta S_m = S_m - S_{m-1} \geqslant 0$, and $\Delta S_m - \delta S_{m-1} \leqslant 0$. It has been also shown that, if the macrostate is described by a string of length L, one can obtain a finite specific thermodynamic depth,

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$$\mu(\chi) = \lim_{m\to\infty} \frac{S_m}{m},$$

with χ being the infinite string. The idea of thermodynamic depth has inspired Ekroot and Cover to introduce the entropy of Markov trajectories in [4]. If P_i denote the ith row of a Markov transition matrix, one can define the entropy of a state i as:

$$H(P_i) = -\sum_j M_{ij} \log(M_{ij}) \tag{2}$$

with M_{ij} being the Markov operator. If one introduces the probability of a trajectory going from i to j as p_{ij}, then, the macroscopic entropy of the Markov trajectory is given by:

$$H_{ij} = -\sum_j P(t_{ij}) \log(P(t_{ij})). \tag{3}$$

For Markov chains, one has that $p_{ij} = \sum_{k_1,k_2,\ldots,k_n} M_{ik_1} \ldots M_{k_nj}$, which thus leads to a recurrence relation:

$$H_{ij} = H(P_i) + \sum_{k\neq j} P_{ij} H_{kj}, \tag{4}$$

which follows from the chain rule of the entropy, and allows to calculate a closed formula for H_{ij} in terms of the entropy of the nodes, that we will call ${}^1S_i$, and the asymptotic, stationary distribution of the Markov chain, π.

Over the last decade, a huge effort has been devoted to understanding processes on networks [5], understanding their statistical properties, as interactions very often occur on nontrivial network topologies, as for instance scale free or small world networks, called complex networks. With this widespread interest in networks, the study of global properties of graphs and graph ensembles has given a renewed impetuous to the study of entropies on graphs. In general, in analogy with what happens for Markov chains, one is interested in quantifying their complexity by means of information theory approach. Since for strongly connected graphs, the transition kernel, given by $M = D^{-1}A$, with A being the adjacency matrix of the graph and D being the diagonal matrix of degree with $D_{ii} = \sum_j A_{ij}$. If M is an ergodic operator (which depends on the topological properties of the underlying graph), one can study operators based on the asymptotic properties of a random walk.

The dynamics and the structure of many physical networks, such as those involved in biological, physical, economical and technological systems, is often characterized by the topology of the network itself.

In order to quantify the complexity of a network, several measures of complexity of a network have been introduced, as for instance in [6], studying the entropy associate to a certain partitioning of a network. The standard Boltzmann entropy per node was defined as the transition kernel of a random walk in [7]. In general, in complex networks, one is interested in the average complexity of an ensemble of networks of the same type, as for instance Erdòs–Renyi or Watts–Strogats and Barabási–Albert random graphs. Along these lines in particular, we mention the entropy based on the transition kernel of Anand and Bianconi [8]. One can in fact write the partition function of a network ensemble subject to a micro-canonical constraint (the energy) and then, given the probability of certain microcanonical ensemble, calculate its entropy, similarly to what proposed in [9] for random graphs.

In general, an entropy of a complex network can be associated from a test particle performing a diffusion process on the network, as in [10]; for scale free networks, it is found that the entropy production rate depends on the tail of the distribution of nodes, and thus on the exponent of the tail.

Along these lines, in [11] a von Neumann entropy based on the graph Laplacian has been introduced, merging results inspired from pure states in Quantum Mechanics, and networks, and finding that the von Neumann entropy is related to the spectrum of the Laplacian [8]. In particular, it has been shown that many graph properties can be identified using this Laplacian approach.

In general, these approaches rely on a local operator (transition kernels, Laplacians) with support on the graph. Therefore, if one is interested in knowing macroscopic properties of the graph, is indeed forced to use non-local operators. In addition to the theoretical interest of describing the macroscopic properties of a graph in terms of information theory quantities, it is important to remark that very often these have important applications in classifying systems according to their topological properties. For instance, in [12] it has been shown that graph entropy can be used to differentiate and identify cancerogenic cells. In particular, [12] shows the importance of studying entropies based on the non-local (macroscopic) properties of a network, as for instance the *higher-order* network entropy given by

$$S^{(n)} = -\sum_j K_{ij}^{(n)} \log\left(K_{ij}^{(n)}\right), \tag{5}$$

with $K_{ij}^{(n)}$ satisfying an approximate diffusion equation at nth order,

$$K_{ij}^{(n)} \approx e^M + O(M^n).$$

In addition to the approaches just described, one could think of using, instead of the diffusion kernel above, a node-entropy based on diffusion as $S_i = \sum_j M_{ij}^k log(M_{ij}^k)$. It is easy to see, however that for $k \to \infty$, if the operator is ergodic, the asymptotic entropy is independent from the initial state: it easy a known fact that if M has a unique Perron root, $(M^k)_{ij} \approx \pi(j) + (N^k)_{ij}$, where N is a Nilpotent operator such that $\lim_{k\to\infty} N^k = 0$. The same happens for the diffusion kernel at long times: in this case the diffusion kernel approaches the asymptotic distribution, which indeed has forgotten from which node the diffusion started. With the aim of retaining the information on the node, we introduce the entropy on the paths originating at a node which, as we shall show, has very interesting asymptotic properties for long walks. In the next section we describe the construction of the non-local entropy, and an application to random graphs and fractals. Conclusions follow.