The network Liouville equation and the quest to understand complex networks on a general dynamical trajectory

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Extended Abstract

The incorporation of statistical-mechanics-inspired concepts, such as entropy, has provided a wide array of fields, from biology to information theory, with powerful mathematical tools. Following this fruitful pattern, in recent years various attempts have been made to build a similar formalism for complex networks. Among them, the introduction of the network density matrix ρ and its corresponding von Neumann entropy $S = -\mathrm{Tr}[\rho \log \rho]$ [1] has proven to be one of the most prolific. This formalism measures the response of a network to an ensemble of perturbations and is able to explain the emergence of sparsity in many real-world networks by expressing the subtle interplay between network structure and dynamics in terms of thermodynamic efficiency [2]. Moreover, the aforementioned network entropy S is interpreted as a measure of the dynamical functional diversity of a complex network. Thus, it has been exploited to assess the fragility and resilience of complex networks [3], as well as to investigate the presence of structural features such as communities.

However, despite its promising results, this theoretical framework is limited to describing the dynamics of a complex network only near its steady state, thereby overlooking the richness of the dynamics along a general trajectory. In fact, many real-world complex systems are known to exist and operate in regimes far from steady-state dynamics, and their study would greatly benefit from an extension of the density-matrix formalism to encompass these cases.

Here we present a first step towards such an extension, in the form of a Liouville-type matrix equation that describes the evolution of the density matrix ρ along a general trajectory of the complex system $\mathbf{x}(t)$:

$$\frac{\partial \rho(t)}{\partial t} = \mathbf{J}(\mathbf{x})\,\rho(t) + \rho(t)\,\mathbf{J}^T(\mathbf{x}) - 2\rho\ \mathrm{Tr}[\rho\,\mathbf{J}(\mathbf{x})] \tag{1}$$

where $\mathbf{J}(\mathbf{x})$ is the Jacobian of the generally non-linear dynamical system $\dot{\mathbf{x}} = \mathbf{F}(\mathbf{x})$, which describes the time evolution of the trajectory.

Equation (1) not only extends the previously existing framework to the case of a general trajectory but also deepens our understanding by introducing new theoretical tools. First, we consider the trace $\mathrm{Tr}[\rho\,\mathbf{J}(\mathbf{x})]$, which appears in the equation to preserve the trace normalization of ρ by counterbalancing the perturbation-averaged phase-space stretching along the trajectory. Thus, it corresponds to the local average rate of change of the network phase space and can be used to assess the persistence of a diverse dynamical response in a given portion of the trajectory (Fig. 1). Secondly, we derive from (1) an explicit expression for the network entropy production rate $\dot{S}$, which has been a fundamental quantity in non-equilibrium thermodynamics since its beginnings [4]. We then exploit this expression to prove that the functional diversity of a complex network linearized near its steady state is bounded to decrease or remain constant. This result is a complex-network version of the Boltzmann H-theorem and strongly supports the need for a trajectory-based formalism not limited to the neighborhood of the steady state, since real networks often preserve or even increase their functional diversity. In this regard, our work shows many points of contact with Maximum Caliber methods, which have recently received attention [5], and paves the way for further integration with such approaches in the broader quest to describe complex systems far from equilibrium.

Finally, since our work is focused on the foundational aspects of the statistical mechanics of complex networks and is still in a preliminary phase, we do not foresee any immediate ethical concerns. Nevertheless, constant vigilance is required to ensure that unethical applications do not arise from it.

References

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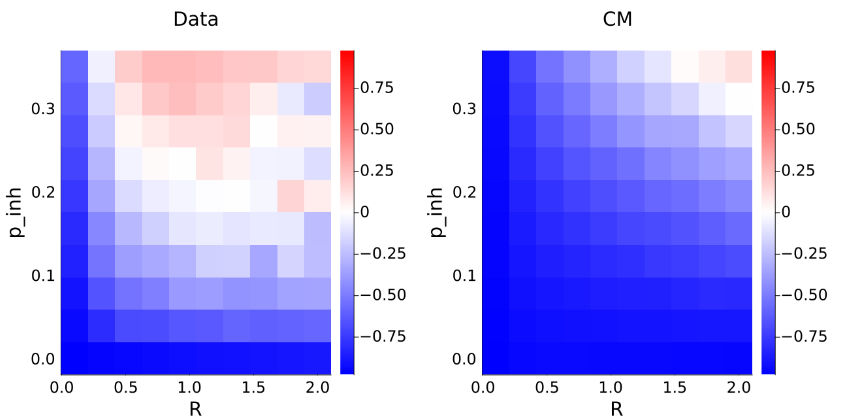

Figure 1: **Network dynamical response along a general trajectory.** The value of $\mathrm{Tr}[\rho\,\mathbf{J}(\mathbf{x})]$, time-integrated over a portion of a general trajectory, is a measure of the perturbation-averaged local stretching of the network phase space. Thus, it can be used to evaluate the local dynamical response: the more negative it is, the stronger the average tendency to contract the phase space, rapidly losing diversity in the dynamical response to perturbations. As an example, here we consider neuronal dynamics of the type $\dot{x}_i = -Bx_i + C\tanh(x_i) + R\sum_{j=1}^{N} A_{ij}\tanh(x_j)$ and compare the dynamical response $\int_0^t ds\,\mathrm{Tr}[\rho\,\mathbf{J}(\mathbf{x})]$ of the real *C. elegans* neural network (Data) with its configuration model (CM) for different values of the parameter R and different percentages of inhibitory links. This comparison unveils the more variegated response of the real network, underlining the dynamical importance of structural correlations.