An information-theoretic approach to distributions of trajectories

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Abstract — **We explore the trajectory space of two-state dynamics in a single-particle system. A single particle makes Brownian-activated hops between two energy wells which are `sculpted' arbitrarily and dynamically. We model the trajectories of the particle using an information-theoretic approach – essentially, the principle of Maximum Entropy for time-dependent systems. We recover the probability distribution (all moments) of quantities such as the dwell times and switching rates. The measured moments are in good agreement with the theory, which is parameter-free. We also predict a hierarchy of fluctuation relations, resembling Onsager's relations of coupled transport coefficients and the Maxwell relations of equilibrium thermodynamics.**

Keywords — **Nonequilibrium statistical mechanics, maximum caliber, optical trapping.**

I. Purpose

TRADITIONALLY, the trajectories of random, discrete processes are characterized by master equations, differential equations that solve for the time-dependent probability distribution of the random variable [1]. Such type of random processes which appear in the cell are motor proteins movement along microtubules [2], protein oscillations such as ion channels [3], and the regulation of protein expression by DNA looping [4] among others. The resultant probability distributions are predicated on models.

For single-particle and few-particle systems, however, the most direct and convenient experimental observables are often the individual dynamical trajectories themselves, rather than the density functions. This suggests an approach for finding the probability distribution of trajectories.

By analyzing trajectories from the variational point of view of the time-dependent Maximum Entropy algorithm (which uses the Shannon missing information criterion), we derive a systematic approach for deriving the Boltzmann-like weights for each trajectory.

Trajectories are broken down into a series of different observables that are tuned by Lagrange multipliers. The first moments of the observables set the Lagrange multipliers, which in turn are used to predict higher moments of the observables of each trajectory. This trajectory-based approach is similar to what ET Jaynes called Maximum Caliber [5].

II. Results

By determining a Boltzmann-like weight for each trajectory, we can derive the partition function for all possible trajectories which serves as a moment generating function for the observables on the trajectories. We show that the theory predicts second and higher moments and covariances of the observables, as well as the complete probability distribution of trajectories of the random-telegraph type.

Moreover, we also uncover hierarchies of fluctuation-relations between trajectories and their perturbations which are reminiscent to the Maxwell relations of thermodynamics [6] or Onsager reciprocal relations under nonequilibrium regimes [7, 8].

III. Conclusion

We provide a framework for examining time series through an information theory approach and thereby uncover the probability distribution on trajectories. Such types of analysis may be useful in the analysis of cellular processes. Moreover, by understanding the covariances within time series, one deduces how trajectories are related to each other.

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