Neural Estimation of Entropy Production in Coarse-Grained Systems via Trajectory Snippets: Application to Molecular Catenane Motors

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Estimating entropy production is essential for uncovering the non-equilibrium energetics of biophysical systems, yet traditional inference is often challenged by high levels of coarse-graining and sparse experimental data. We present a recurrent neural network (RNN)-based estimator that leverages the framework of trajectory snippets (trajectories between recurring Markovian events) to provide a fundamental lower bound on entropy production, even when underlying dynamics are partially hidden. By training a compact and computationally efficient RNN architecture to learn irreversibility from snippets, our method demonstrates superior data efficiency, capturing complex history dependencies in time-series data with significantly fewer dataset than conventional estimators. We apply it to a synthetic molecular Catenane motors, a prominent real-world model for autonomous chemically fueled small-molecule motor. Notably, under conditions of current reversal induced by varying track geometries, our neural estimator successfully extracts underlying entropy production and uncovers the explicit the physical origins of entropy production by identifying which localized shuttling ring currents drive the system’s irreversibility. This extensible framework provides a robust and scalable diagnostic tool for characterising energy dissipation, thermodynamic efficiency, and free energy landscapes directly from limited experimental time series data, such as single-molecule force spectroscopy or fluorescence trajectories.