Dynamical large deviations of kinetically constrained models using neural-network states

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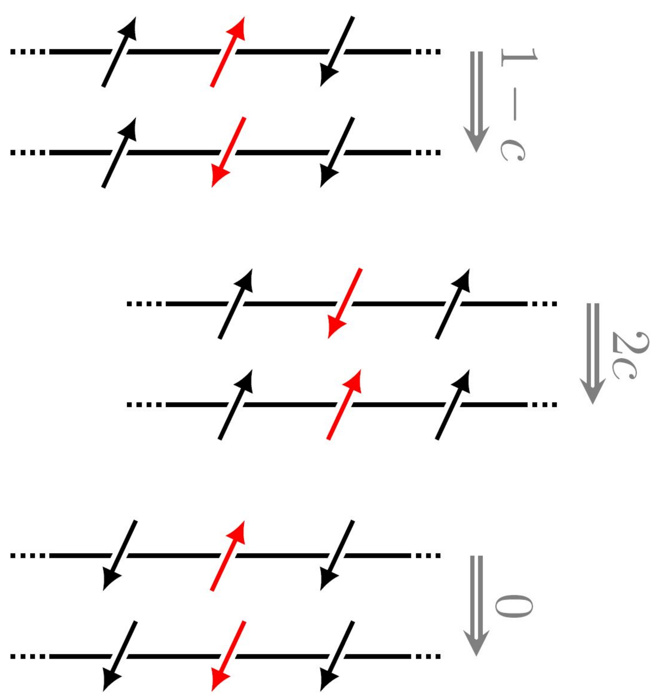
In brief

- Dynamical large-deviation functions describe the fluctuations of observables measured over stochastic trajectories, and play the role of thermodynamic potentials for trajectories
- They can be found as the largest eigenvalue of a modified version of the Markov generator
- We do so using recurrent neural-network states, and efficiently determine large-deviation functions in two dimensions

The Fredrickson-Andersen model



The FA model describes slow or glassy dynamics by placing kinetic constraints on the dynamics.

It consists of *N* spins on a lattice which are either up ($n_i = 1$) or down ($n_i = 0$), and evolves according to the generator

$$W = \sum_i f_i \left[c(\sigma_i^+ + n_i - 1) + (1-c)(\sigma_i^- - n_i) \right],$$

where $\sigma_i^+ (\sigma_i^-)$ flips a site up (down) and the kinetic constraint $f_i = \sum_{j \in \mathrm{nn}(i)} n_j$ is the number of neighboring up-spins.

The dynamical activity $K(t)$, which is the number of configuration changes during a trajectory of time t, can be found through large-deviation theory.

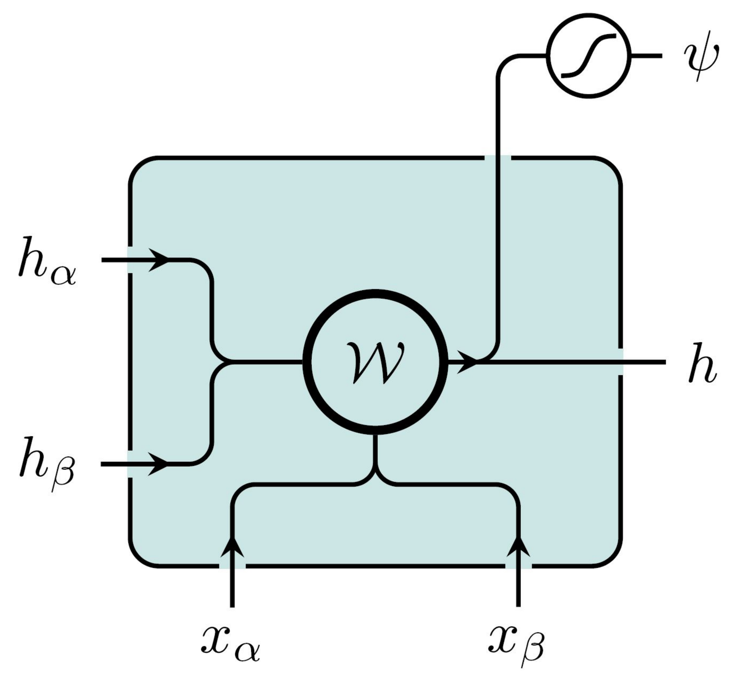
Dynamical activity of the FA model

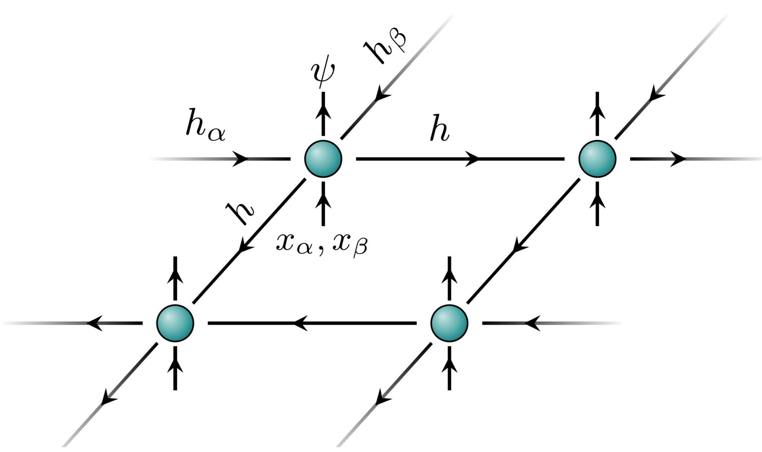
The distribution of $K(t)$ follows $P(K) \approx e^{-tJ(k)}$, where $J(k)$ is the rate function and $k \equiv K/t$. The cumulants of the dynamical activity can be found through the scaled cumulant-generating function $\theta(s) = \lim_{t\to\infty} \frac{1}{t} \ln \langle e^{-sK} \rangle$. These large-deviation functions are connected through a Legendre transform.

$\theta(s)$ can be found as the largest eigenvalue of a modified generator, $W^s|P^s\rangle = \theta(s)|P^s\rangle$, where the off-diagonal elements of W^s are multiplied by a factor e^{-s}.

Recurrent neural-network states

We use recurrent neural-network states to solve this eigenproblem variationally. At each site, a recurrent cell receives a previous visible and hidden state from each spatial direction, and calculates a new hidden state and the conditional probability amplitude $\psi(x_i|x_{j<i})$.

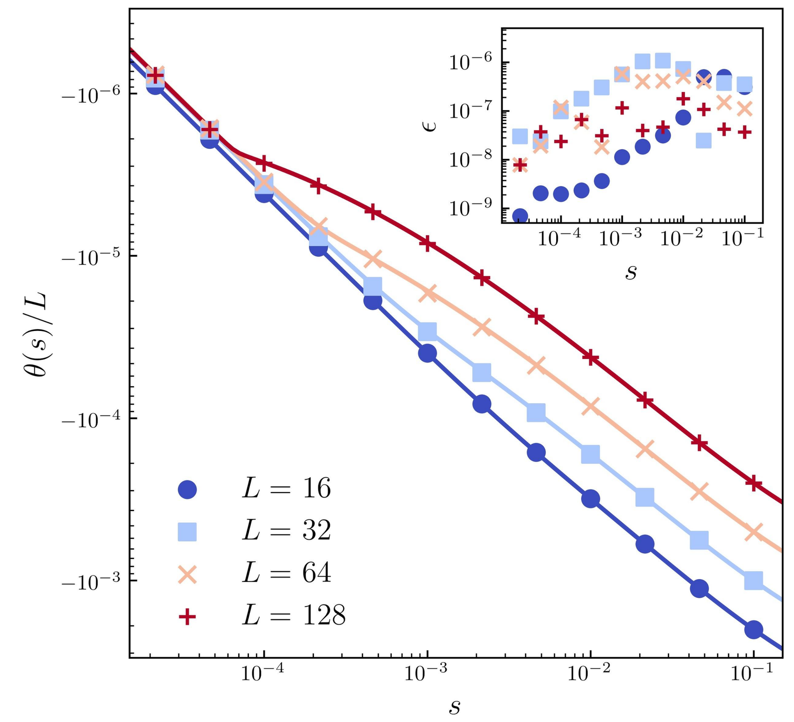




This is done for every site, and the total probability amplitude for the configuration is given by $\Psi(\mathbf{x}) = \prod_{i=1}^{N} \psi(x_i|x_{i-1},\ldots,x_1)$.

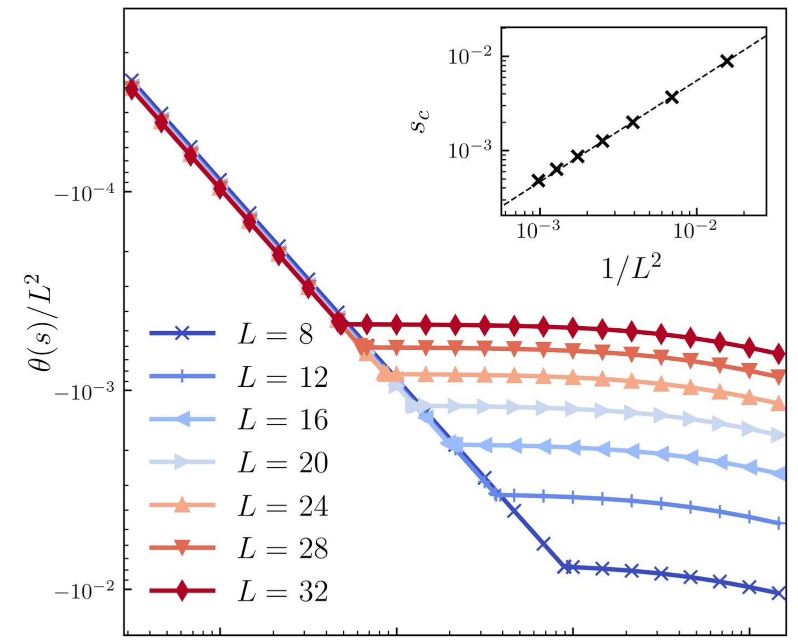
The weights of the recurrent cell are variationally optimized in order to find the state with the largest eigenvalue of the modified generator.

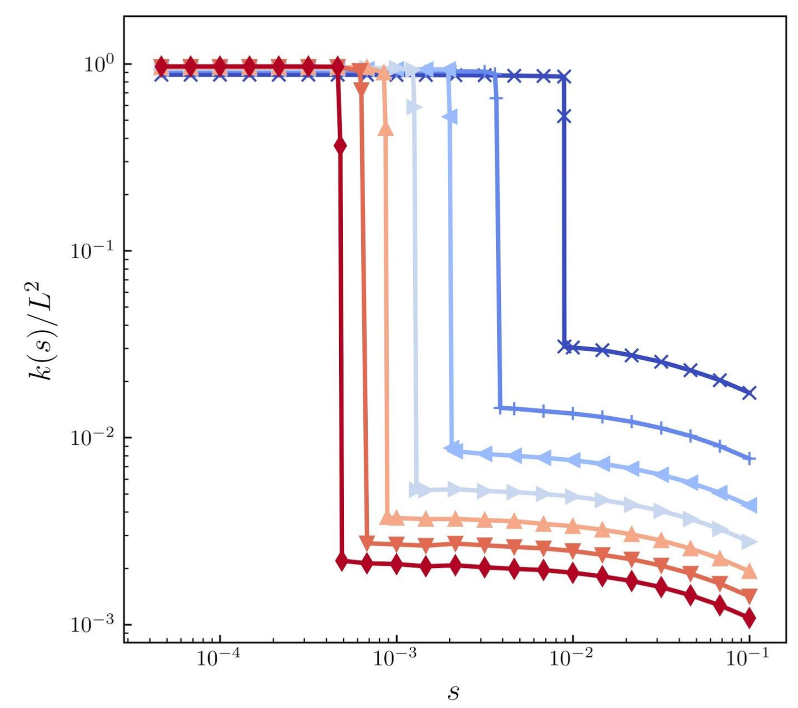
Results



We optimize RNN states for a 1D chain, and can describe the dynamical phase transition between an active and inactive phase, marked by a singularity in $\theta(s)$. Our results are competitive with DMRG.

We uncover a similar phase diagram for the previously unstudied two-dimensional FA model. Large lattices can be studied efficiently by using the RNN cell optimized for a small system as starting point for larger lattices. The derivative of $\theta(s)$ unveils a transition between dynamical phases with low and high activity at a size-dependent value, $s_c \sim N^{-1.07}$.





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