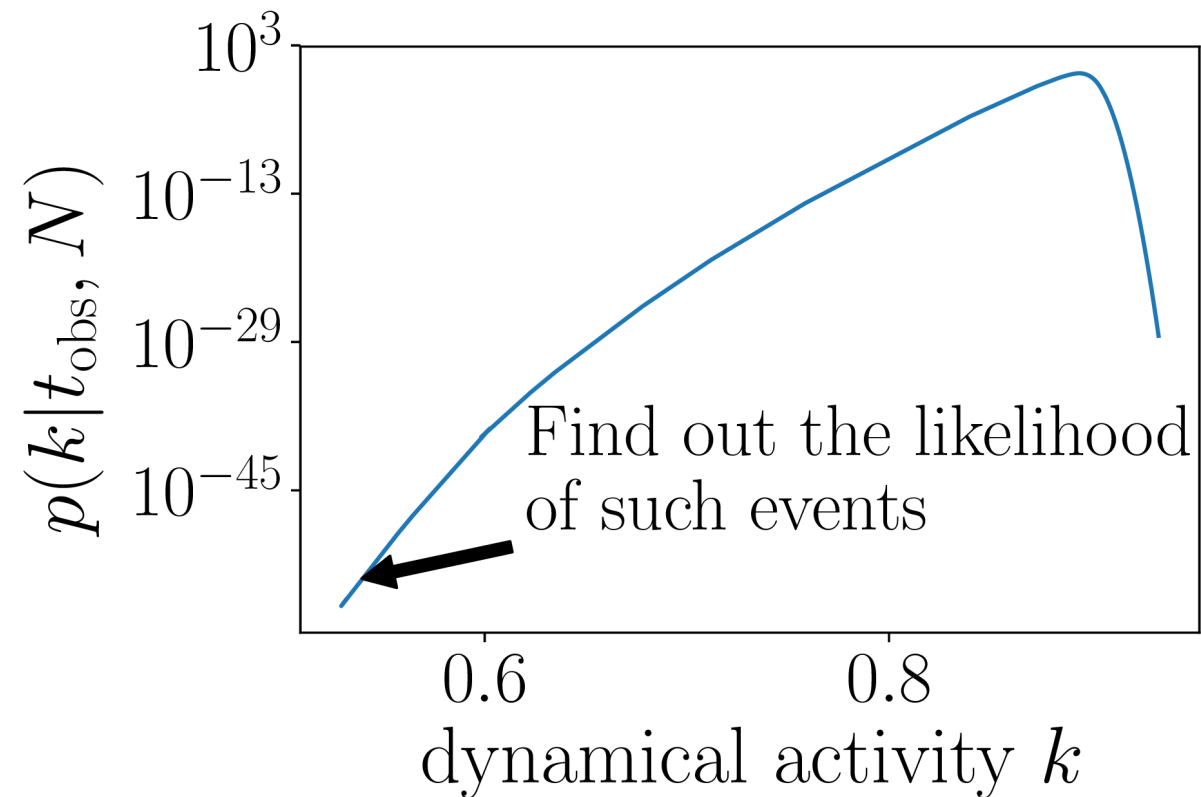
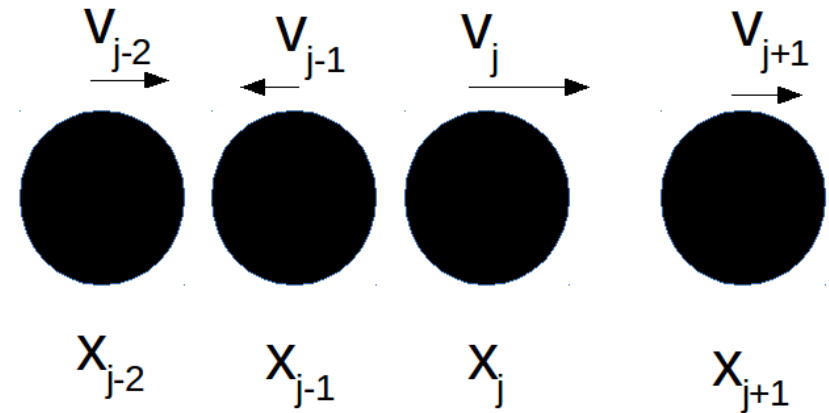


Large Deviations and Optimal Control Forces

Jakub Dolezal, Robert L. Jack

Model-
Diffusing hard particles
in periodic 1D system



Rare events useful
in many contexts
-Protein folding
-Glass formation
-Climate science

Brute Force



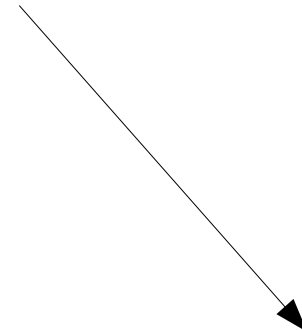
- Direct simulation of system
- Almost impossible to do



Using transition path sampling (TPS) to generate biased ensemble



- Simulate biased ensemble with Monte Carlo methods to sample rare events
- Makes sampling very rare events possible



Using controlled systems with TPS

- Analytically derive approximate control forces
- Simulate controlled system and then bias it
- At least 100 times improvement in sampling efficiency for larger systems over base TPS