

# Hidden Markov state models

Simon Olsson

2020 PyEMMA Workshop  
FU Berlin  
Tuesday, Feb 18th

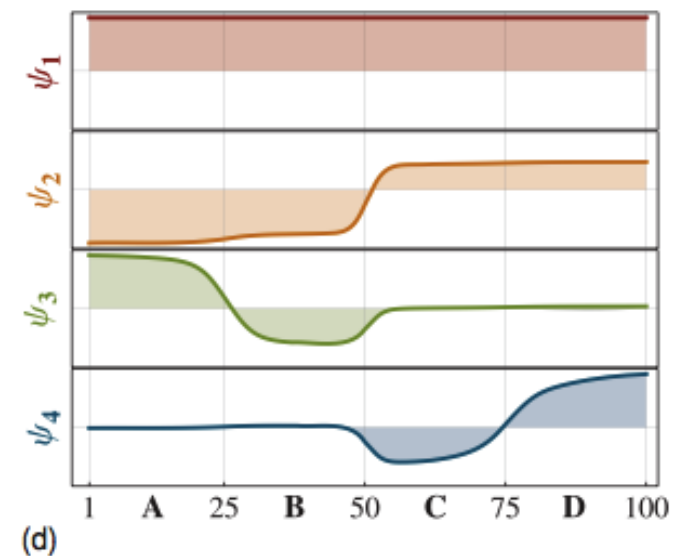
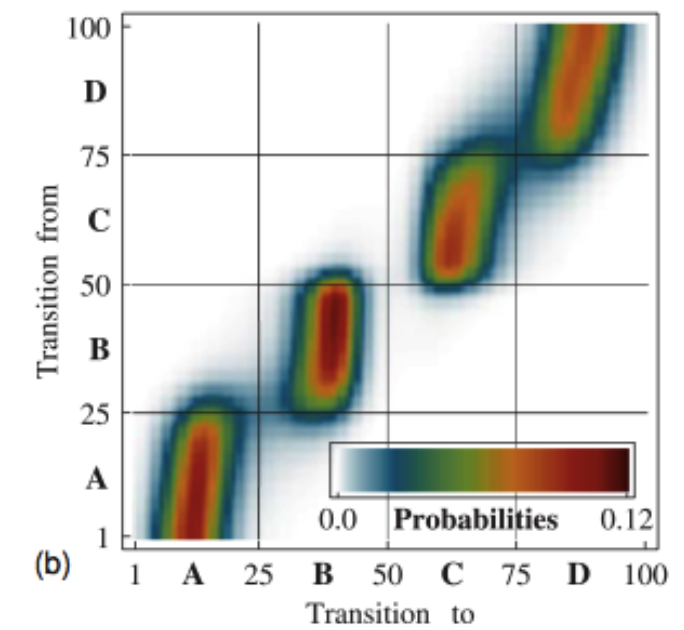
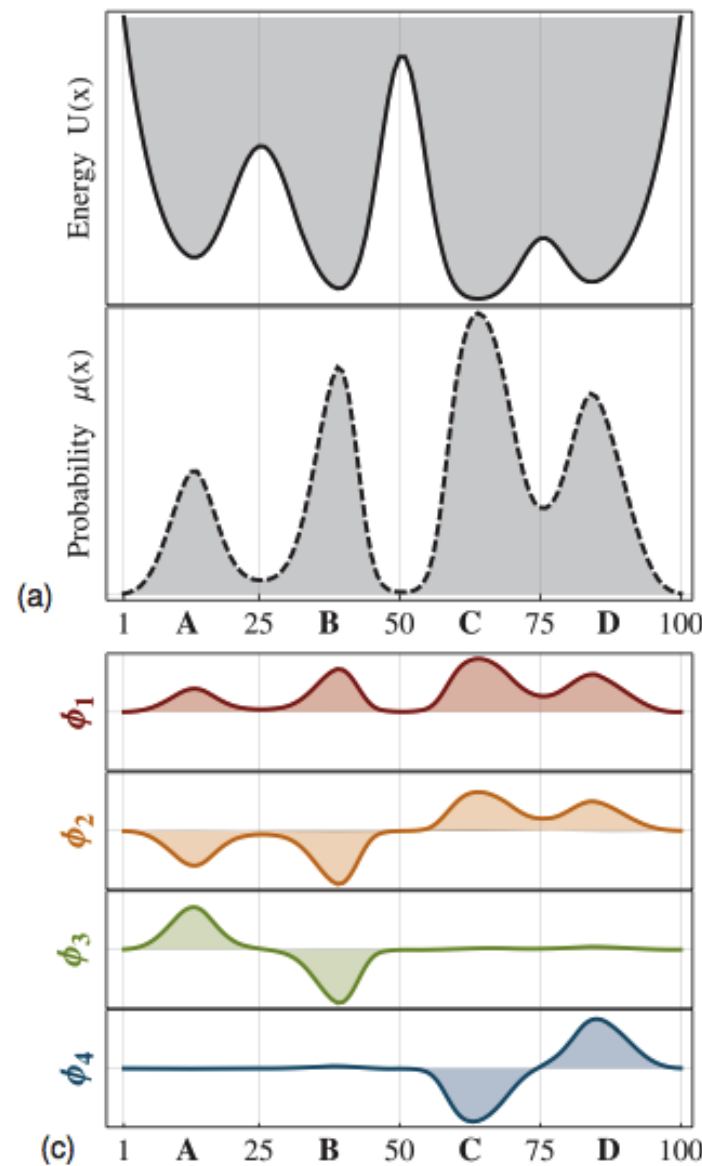
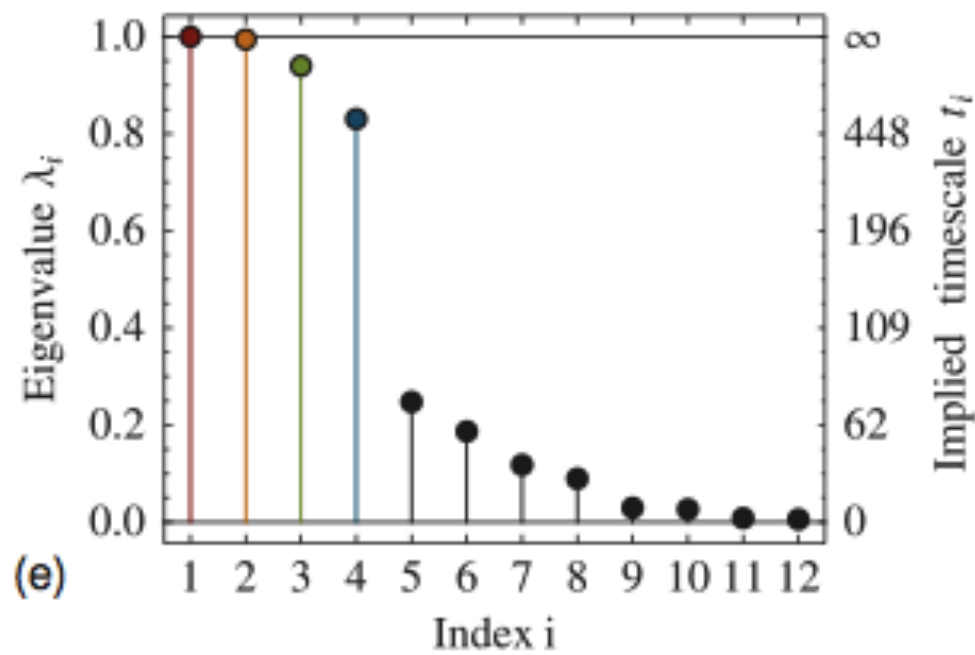
# Discretization

Backward propagator

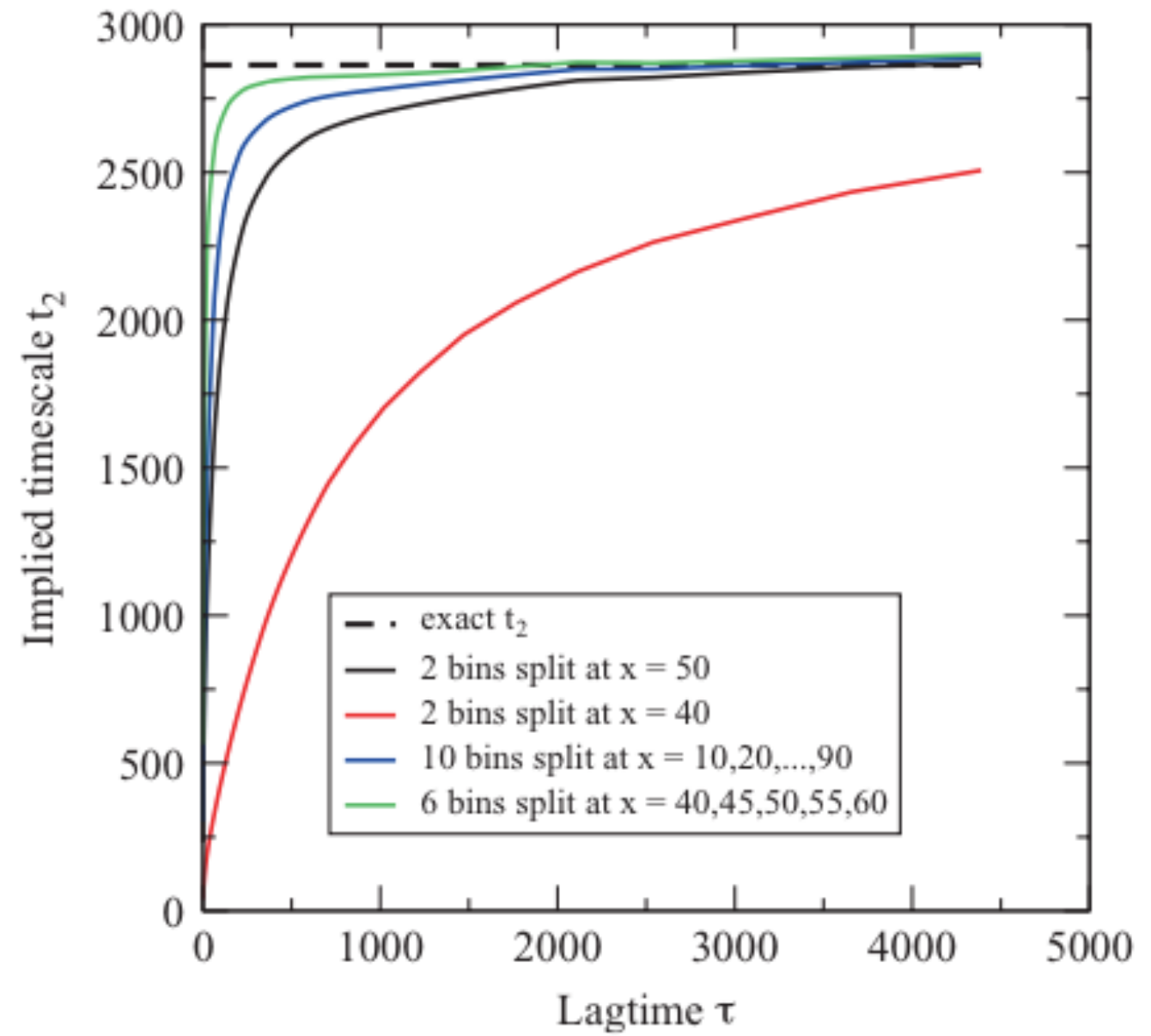
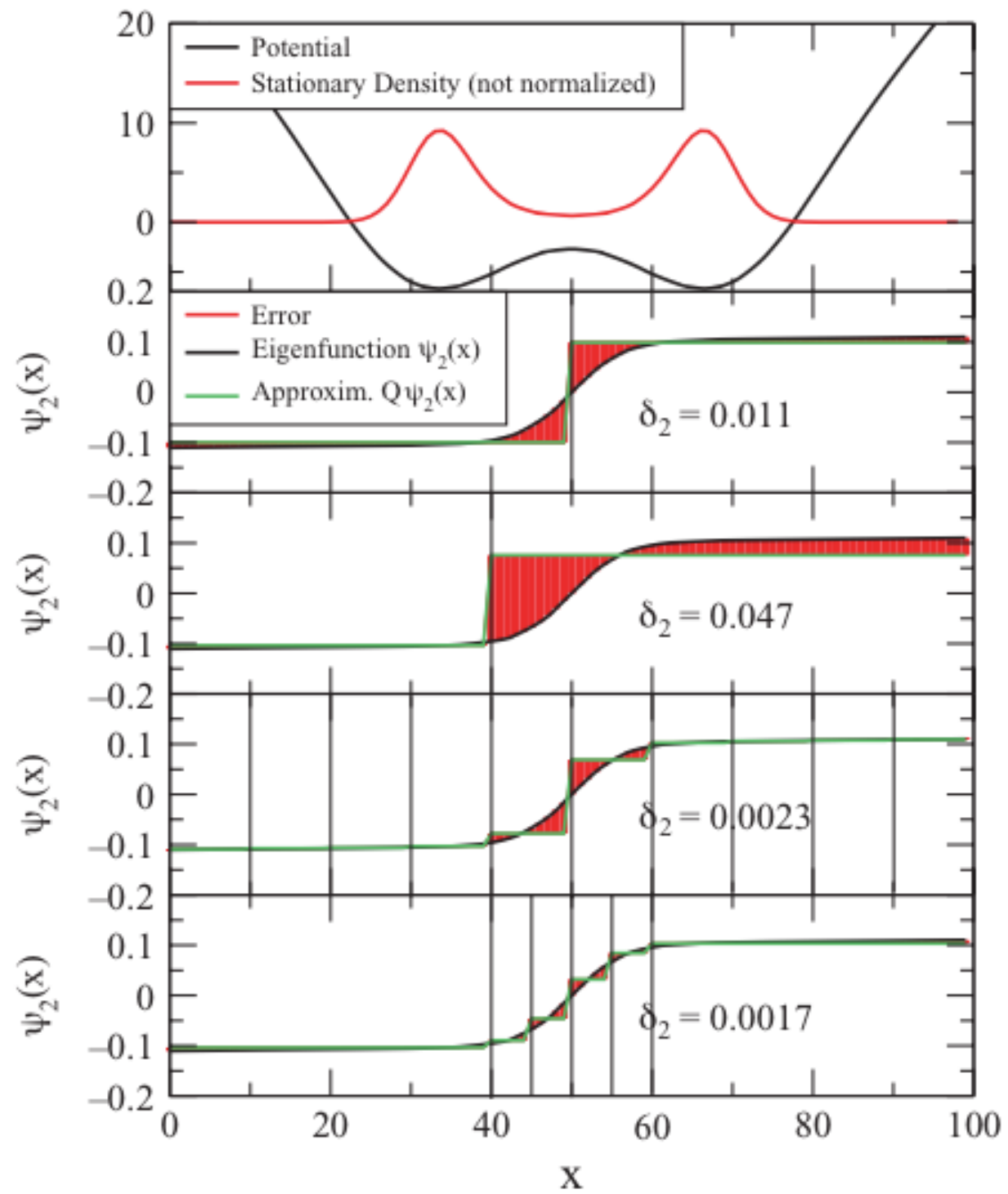
$$\rho_\tau = \mathcal{T}(\tau)\rho_0$$

Spectral decomposition

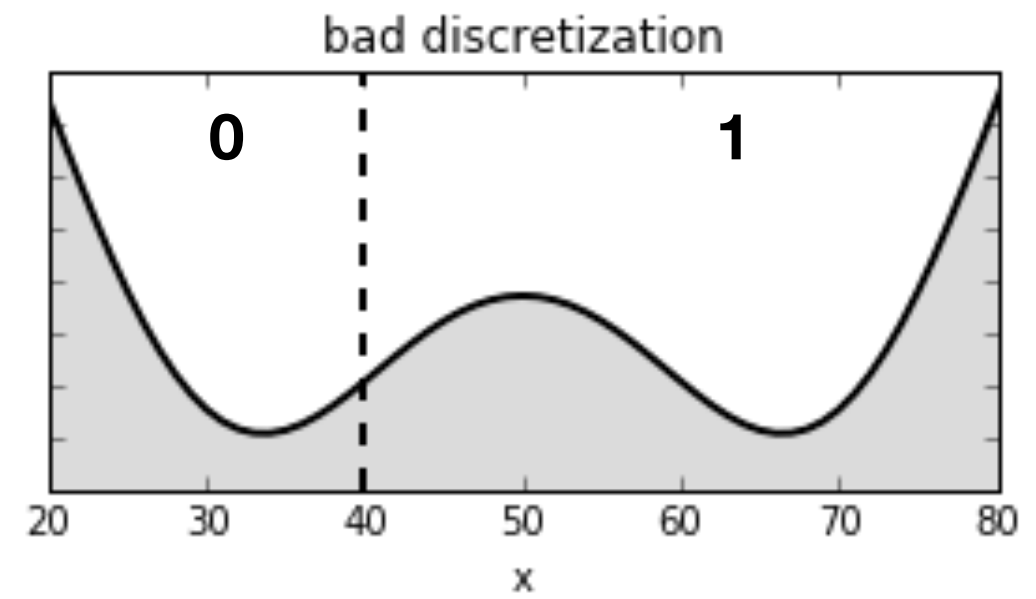
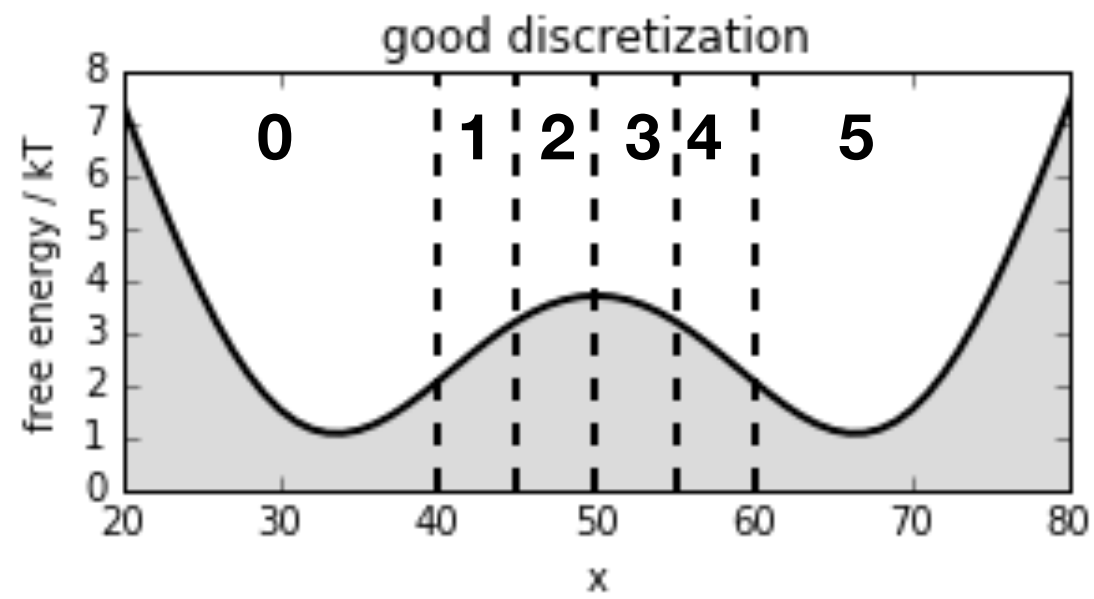
$$\rho_\tau = \sum_{i=1}^{\infty} e^{-\tau\kappa_i} \langle \psi_i | \rho_0 \rangle \psi_i$$



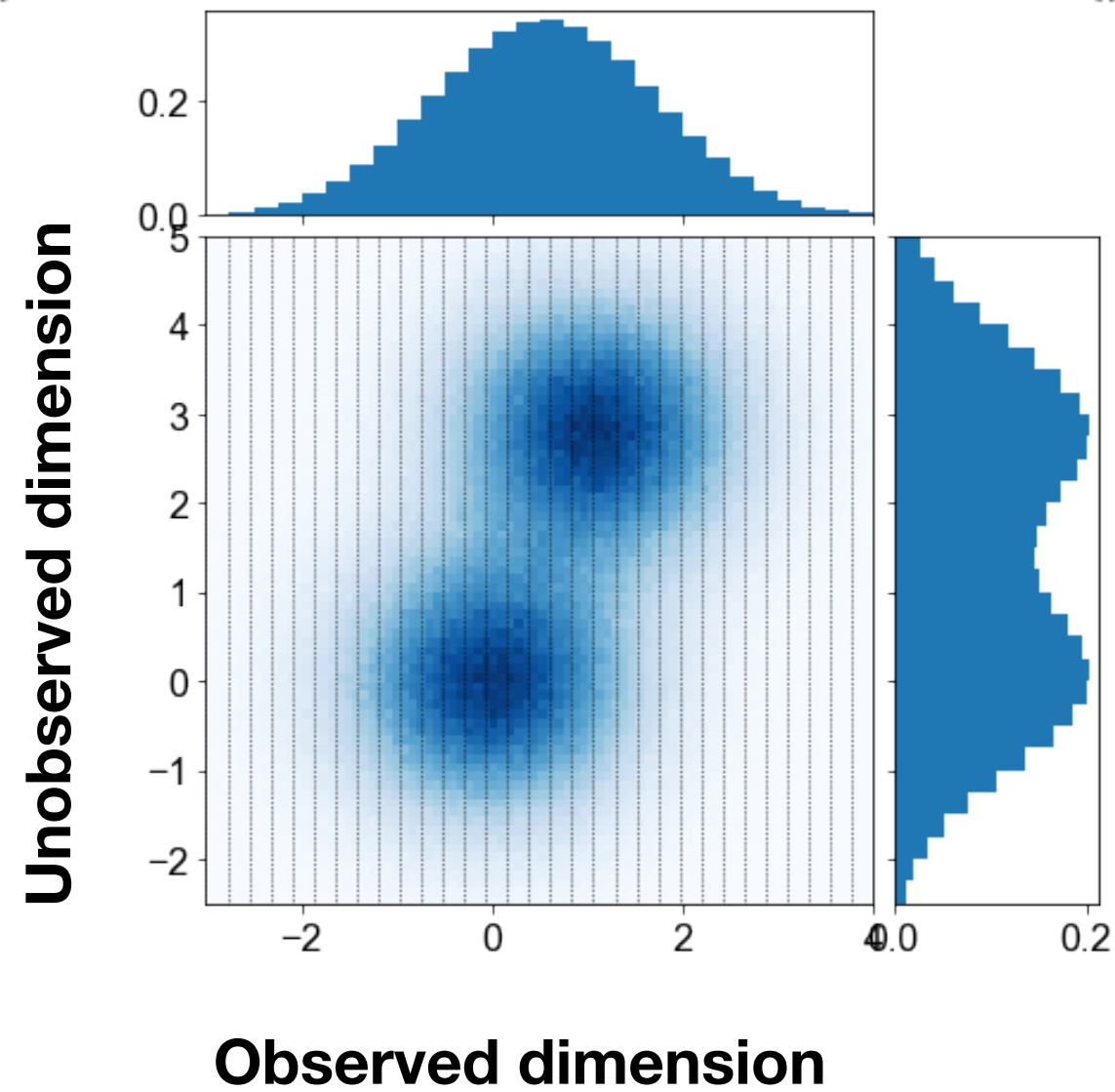
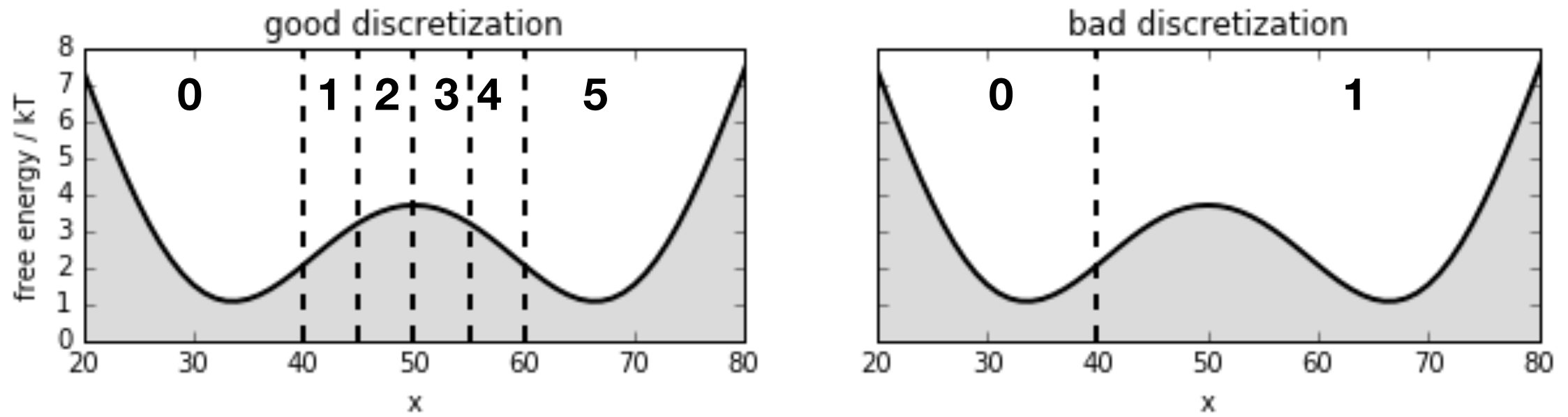
# Discretization



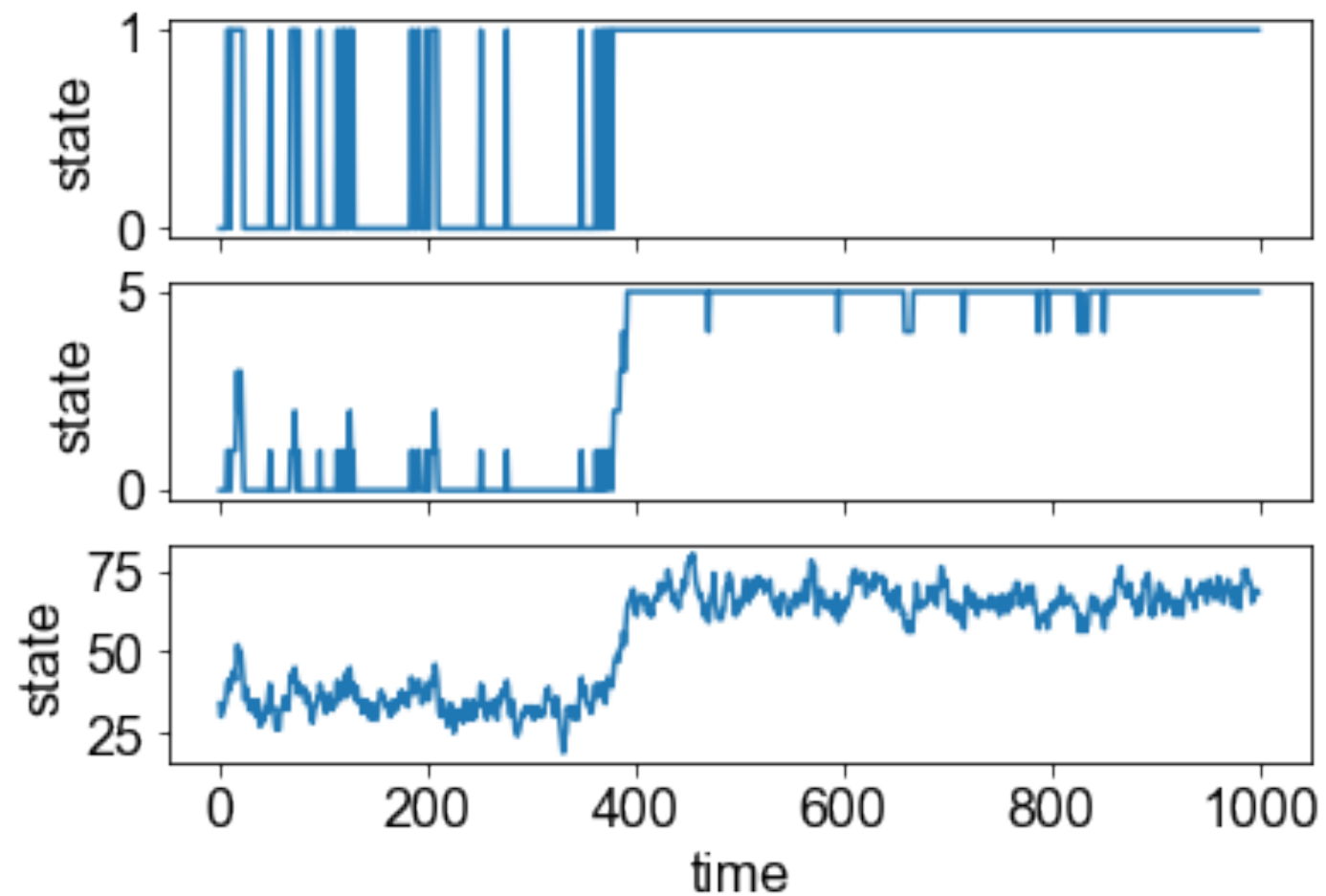
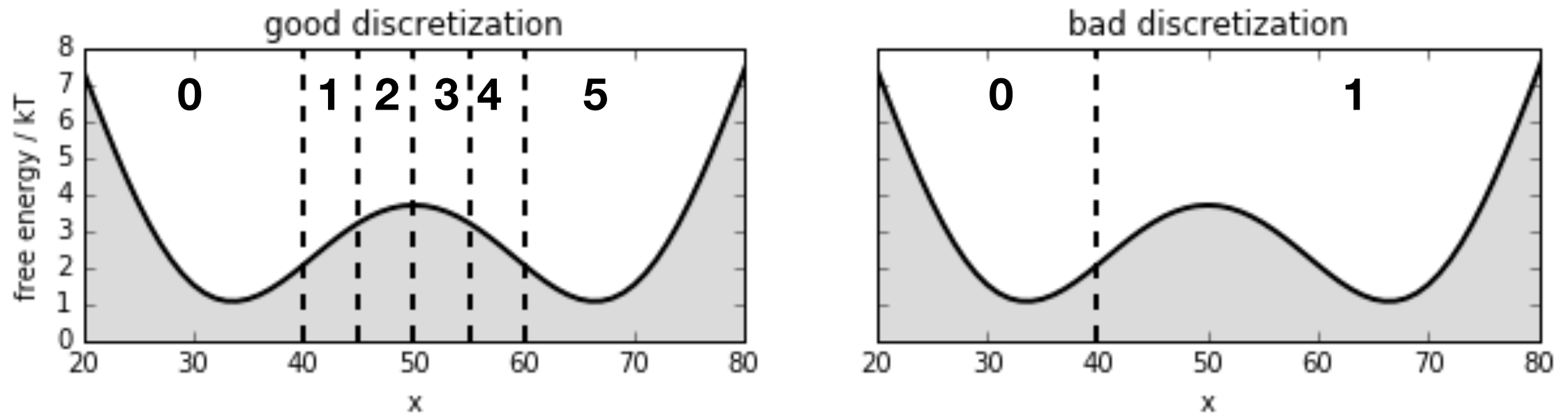
# There are two flavors of discretization/projection error



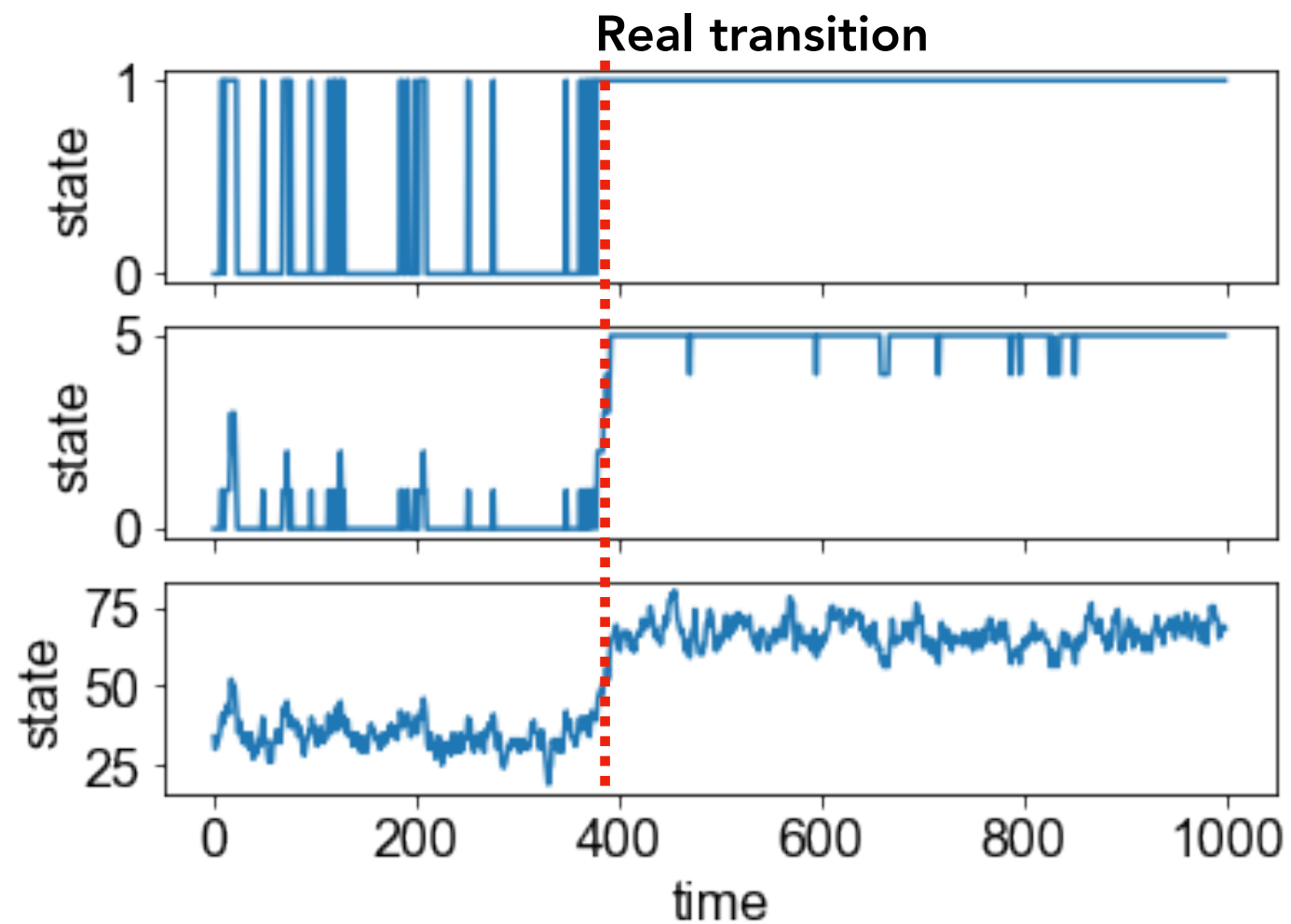
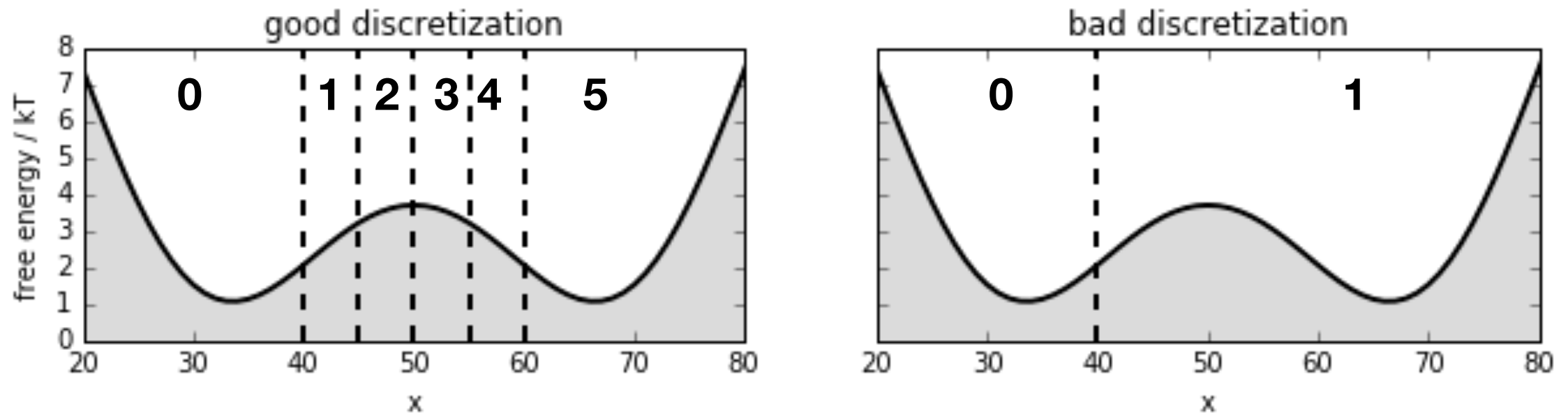
# There are two flavors of discretization/projection error



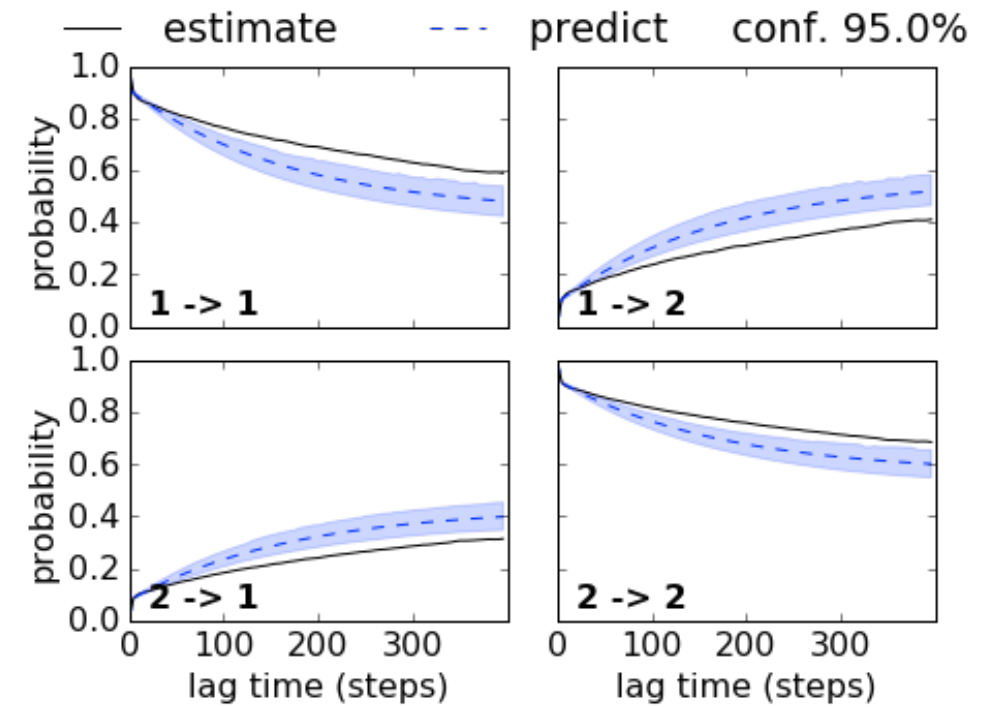
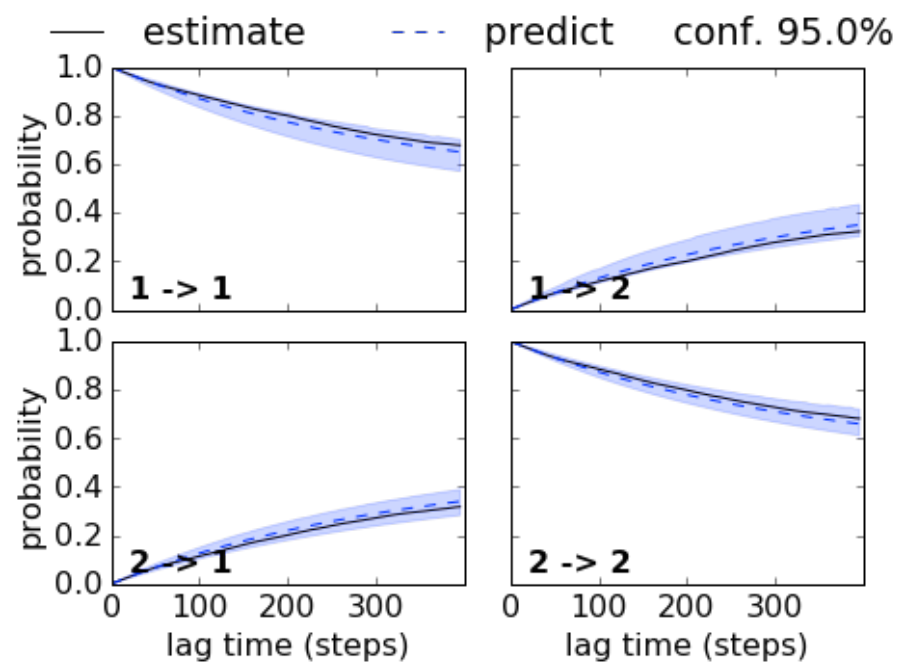
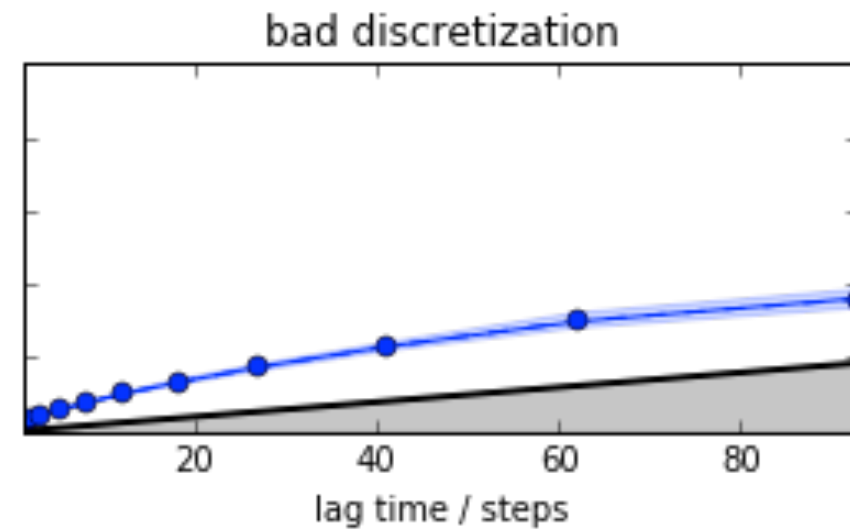
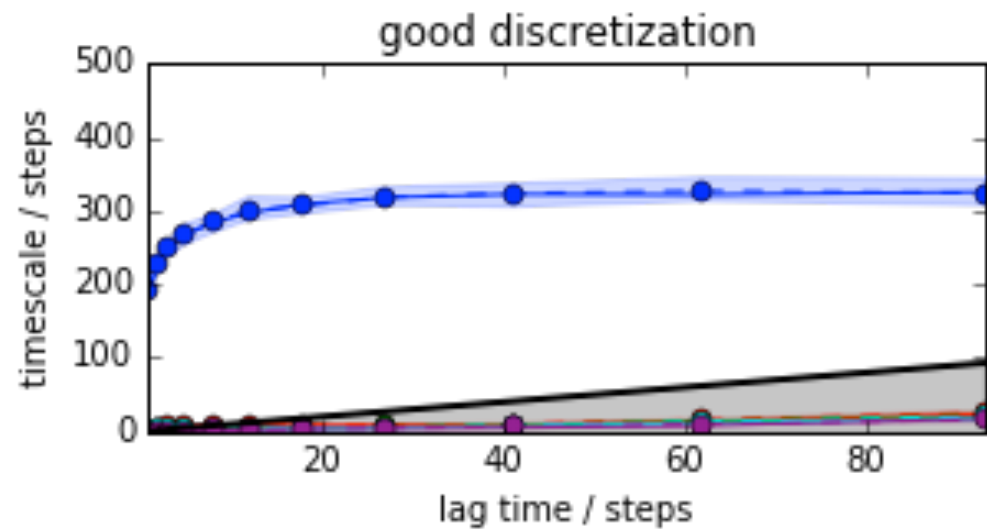
# There are two flavors of discretization/projection error



# There are two flavors of discretization/projection error



# There are two flavors of discretization/projection error





# Projection/discretization error leads to systematic errors

- Discretization and projection errors hampers our ability to distinguish between meta-stable states
- Apparent non-Markovian behavior of the dynamics.

# Projection/discretization error leads to systematic errors

- Discretization and projection errors hampers our ability to distinguish between meta-stable states
- Apparent non-Markovian behavior of the dynamics.

## Remedies:

- Increase lag-time when estimating MSM
- Improve featurization and clustering

# Projection/discretization error leads to systematic errors

- Discretization and projection errors hampers our ability to distinguish between meta-stable states
- Apparent non-Markovian behavior of the dynamics.

Remedies:

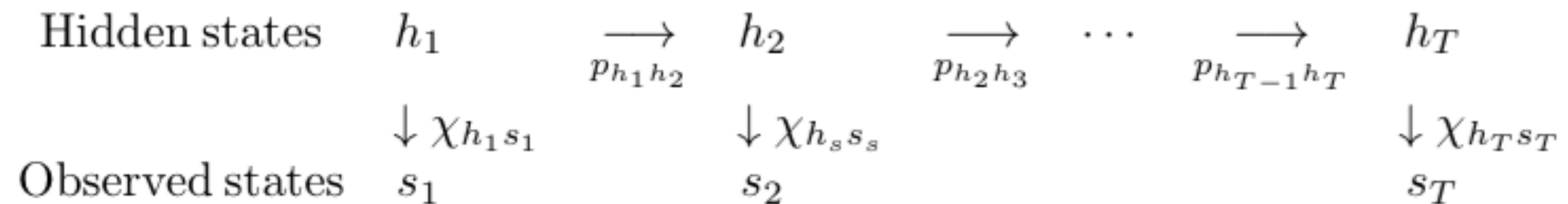
- Increase lag-time when estimating MSM
- Improve featurization and clustering

However we know that the underlying dynamics is Markovian,  
can we exploit fact in some way?

# Hidden Markov state models

We assume the existence of an underlying (hidden) Markovian dynamics described by the transition probabilities  $\mathbf{P} = \{p_{ij}\}$

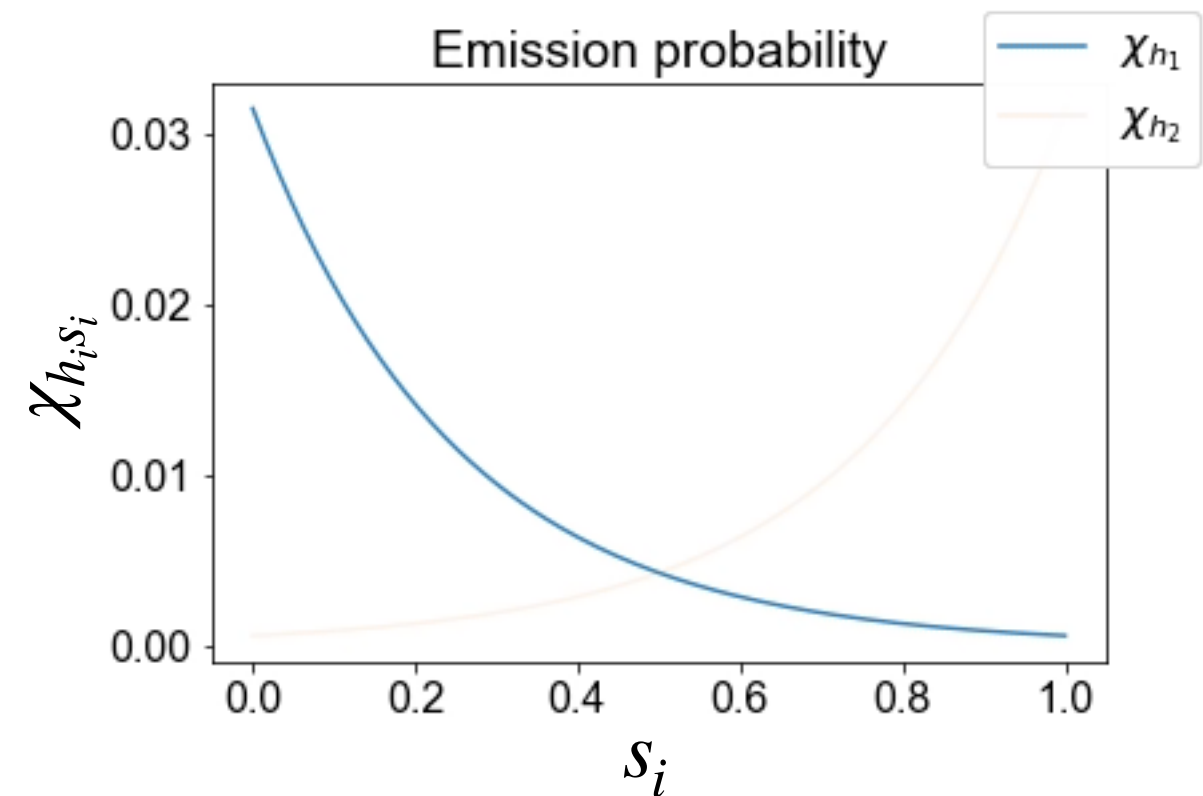
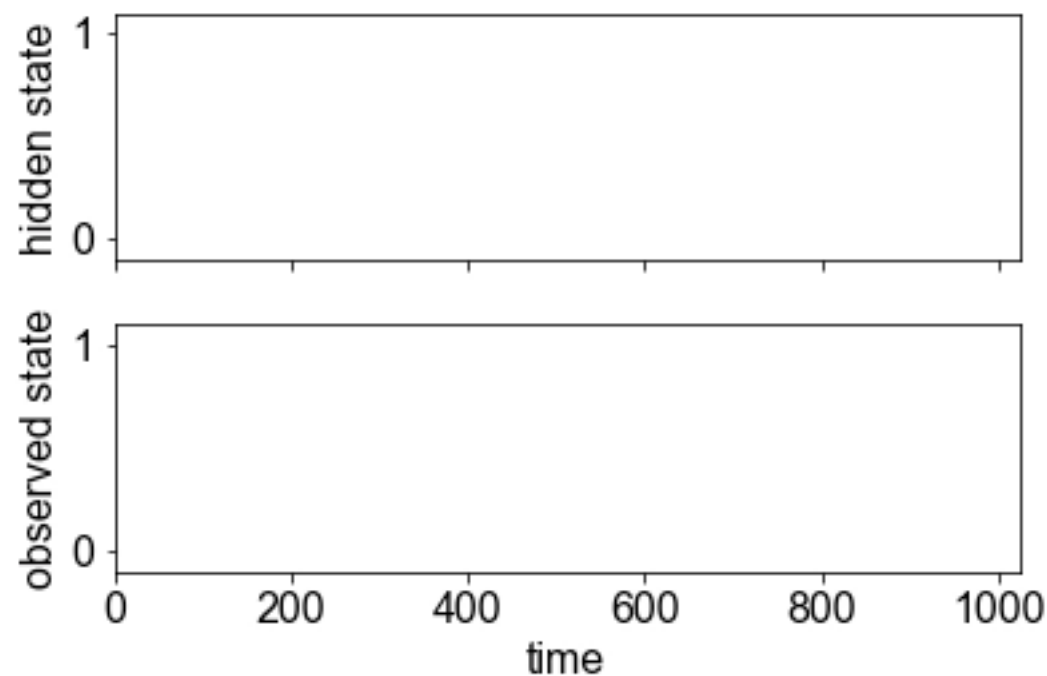
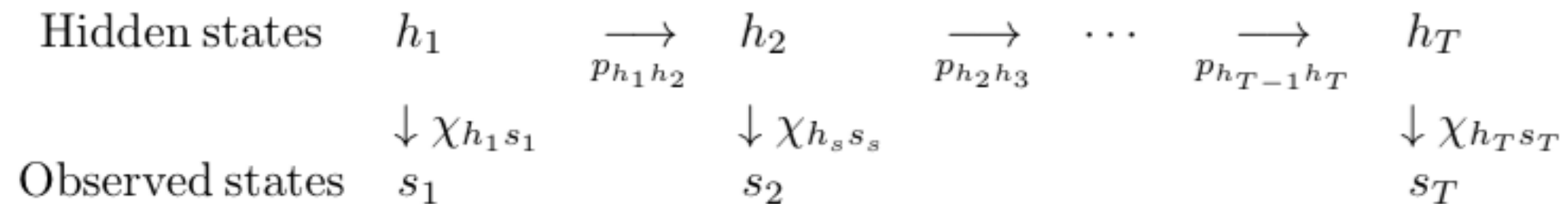
Instead of observing the state  $h_i$  directly we observe some distorted representation,  $s_i$  with a probability  $\chi_{h_i s_i}$  — the emission probabilities.



# Hidden Markov state models

We assume the existence of an underlying (hidden) Markovian dynamics described by the transition probabilities  $\mathbf{P} = \{p_{ij}\}$

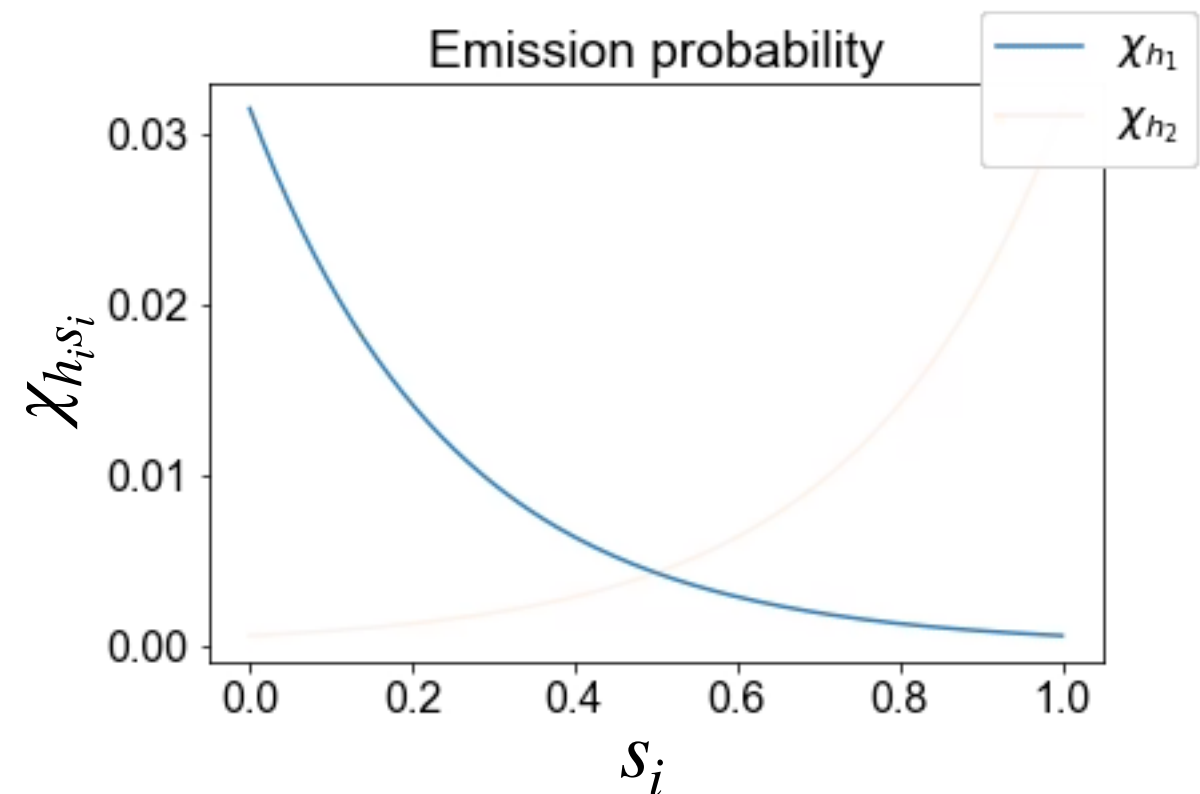
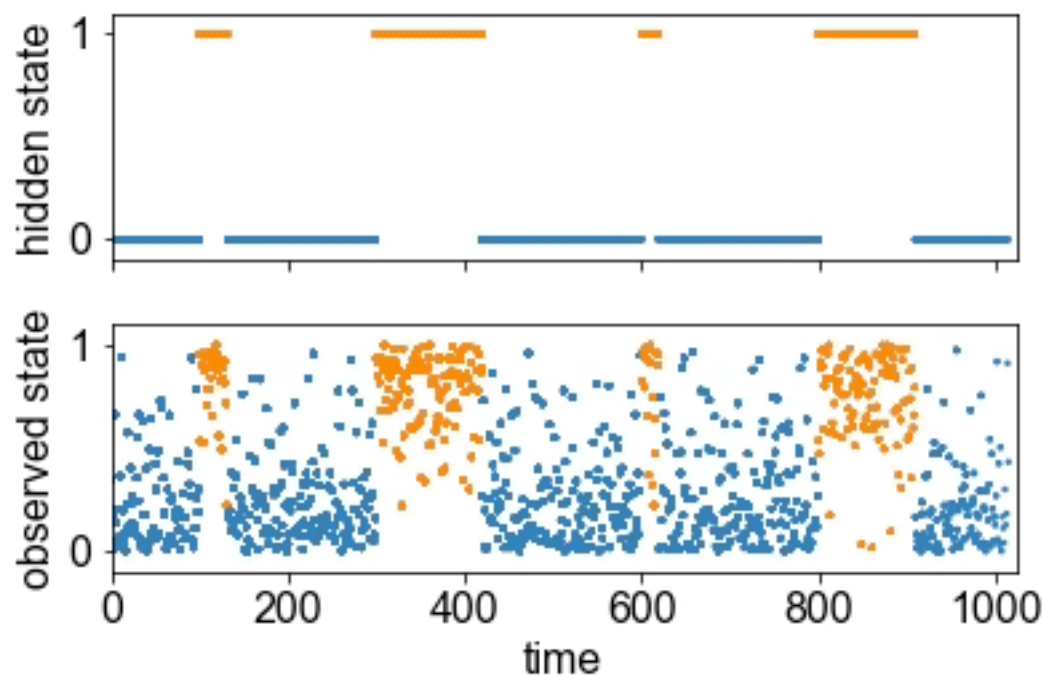
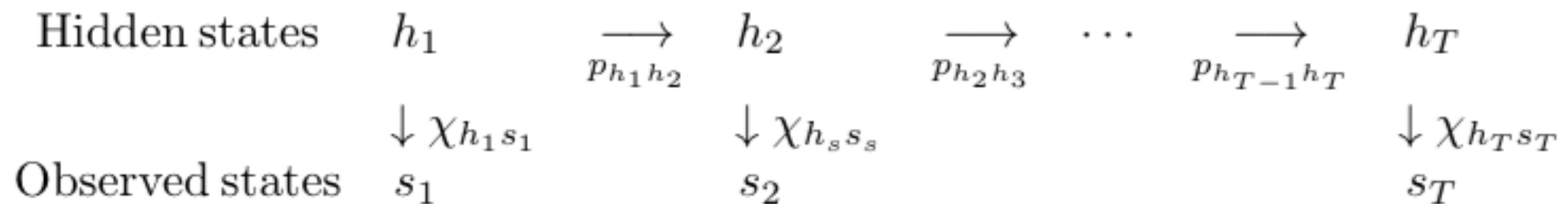
Instead of observing the state  $h_i$  directly we observe some distorted representation,  $s_i$  with a probability  $\chi_{h_i s_i}$  — the emission probabilities.



# Hidden Markov state models

We assume the existence of an underlying (hidden) Markovian dynamics described by the transition probabilities  $\mathbf{P} = \{p_{ij}\}$

Instead of observing the state  $h_i$  directly we observe some distorted representation,  $s_i$  with a probability  $\chi_{h_i s_i}$  — the emission probabilities.



Maximum-Likelihood and Bayesian estimators are available:

- Rabiner Proc IEEE (1989) 77,2, pp.257
- Noé et al. JCP (2013) 139, 184114
- Chodera et al. arxiv:1108:1430

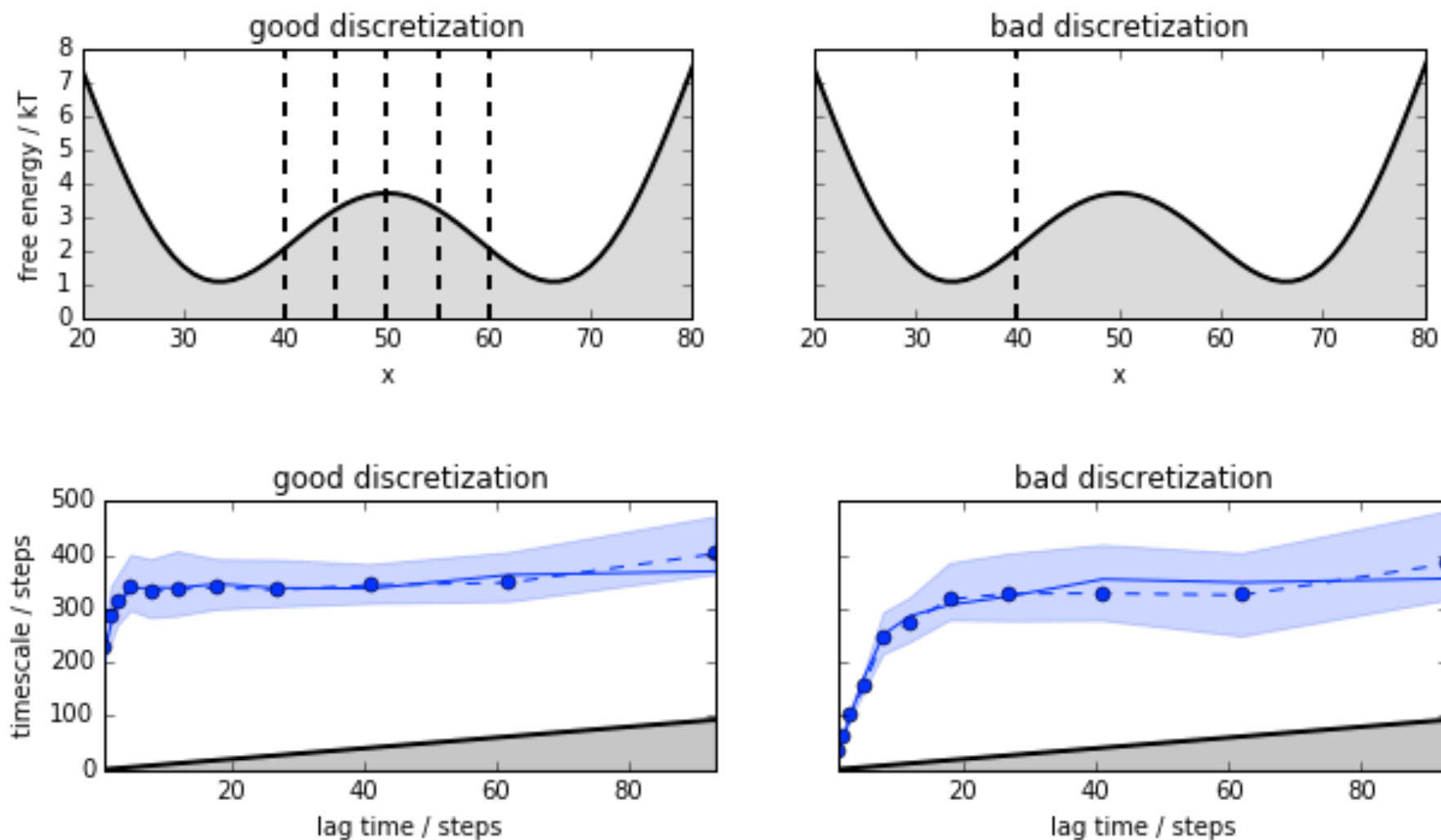
# Hidden Markov state models — an alternative to MSMs

- Models the system dynamics by estimation of transition probabilities of hidden Markov process, and emission probability distributions.
- We need to decide the number of states of the hidden Markov process a priori (the number of meta-stable states)

# Hidden Markov state models — an alternative to MSMs

- Models the system dynamics by estimation of transition probabilities of hidden Markov process, and emission probability distributions.
- We need to decide the number of states of the hidden Markov process a priori (the number of meta-stable states)

Let's revisit our two well potential from before:



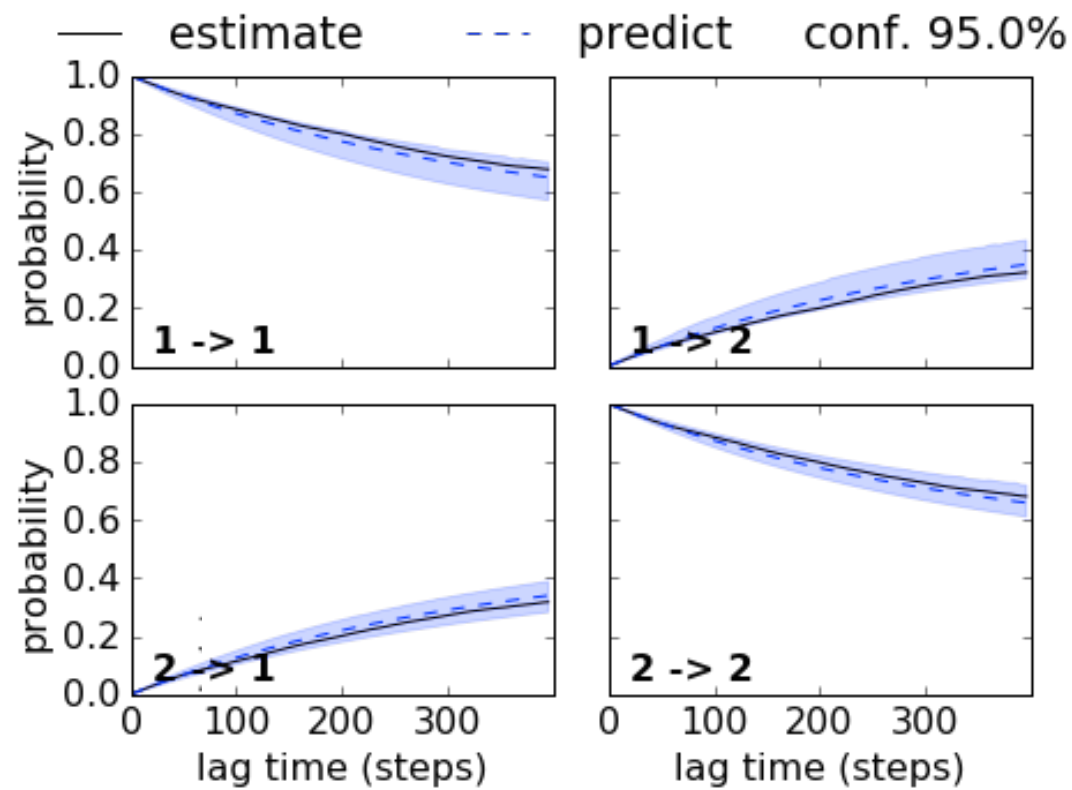


# Hidden Markov state models — an alternative to MSMs

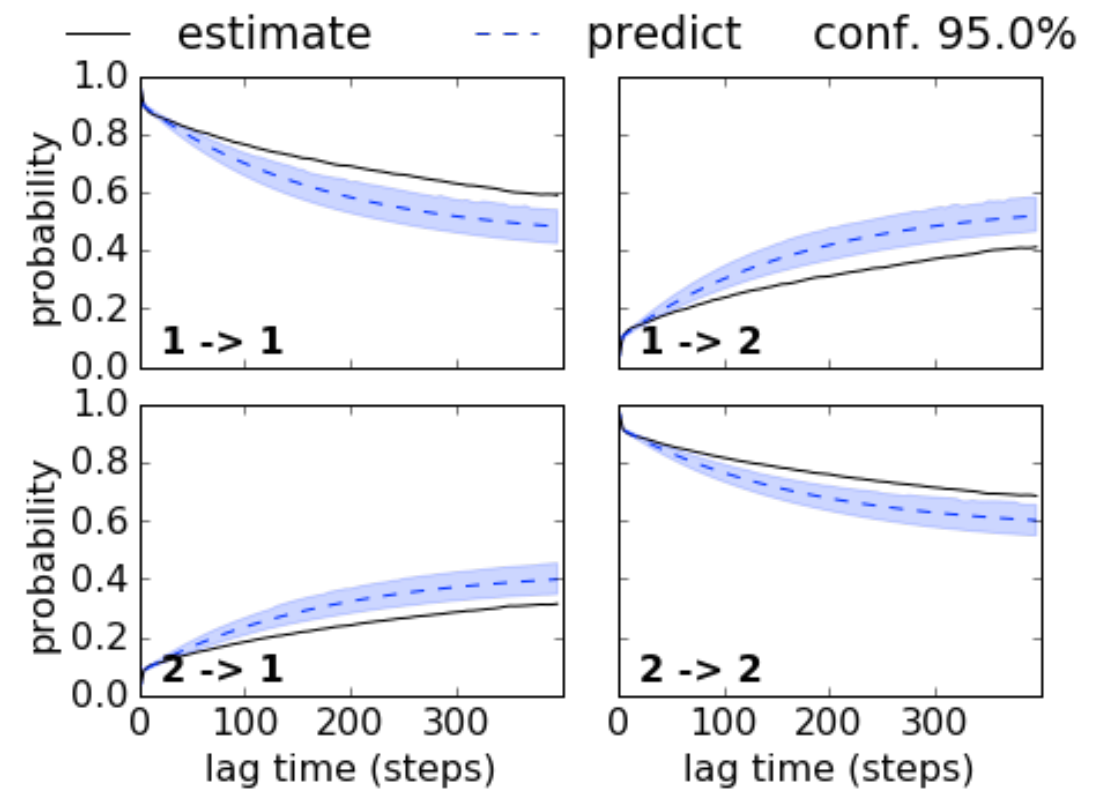
- Models the system dynamics by estimation of transition probabilities of hidden Markov process, and emission probability distributions.
- We need to decide the number of states of the hidden Markov process a priori (the number of meta-stable states)

Let's revisit our two well potential from before:

**Good discretization**



**Bad discretization**

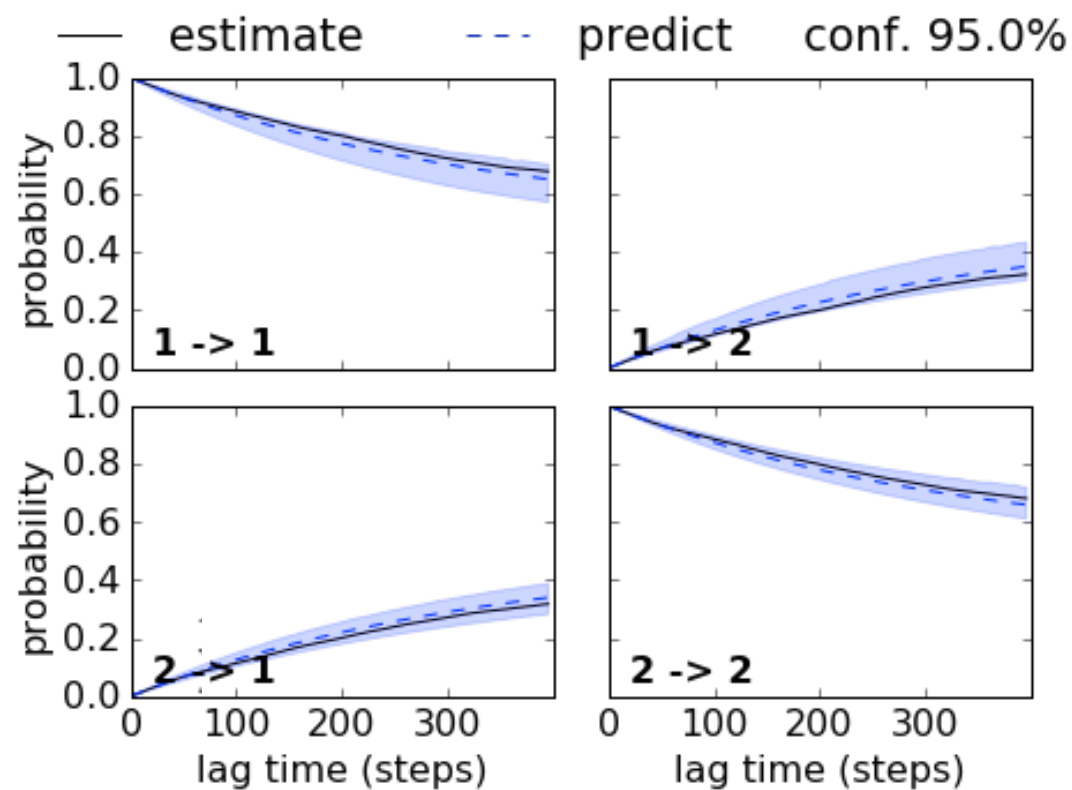


# Hidden Markov state models — an alternative to MSMs

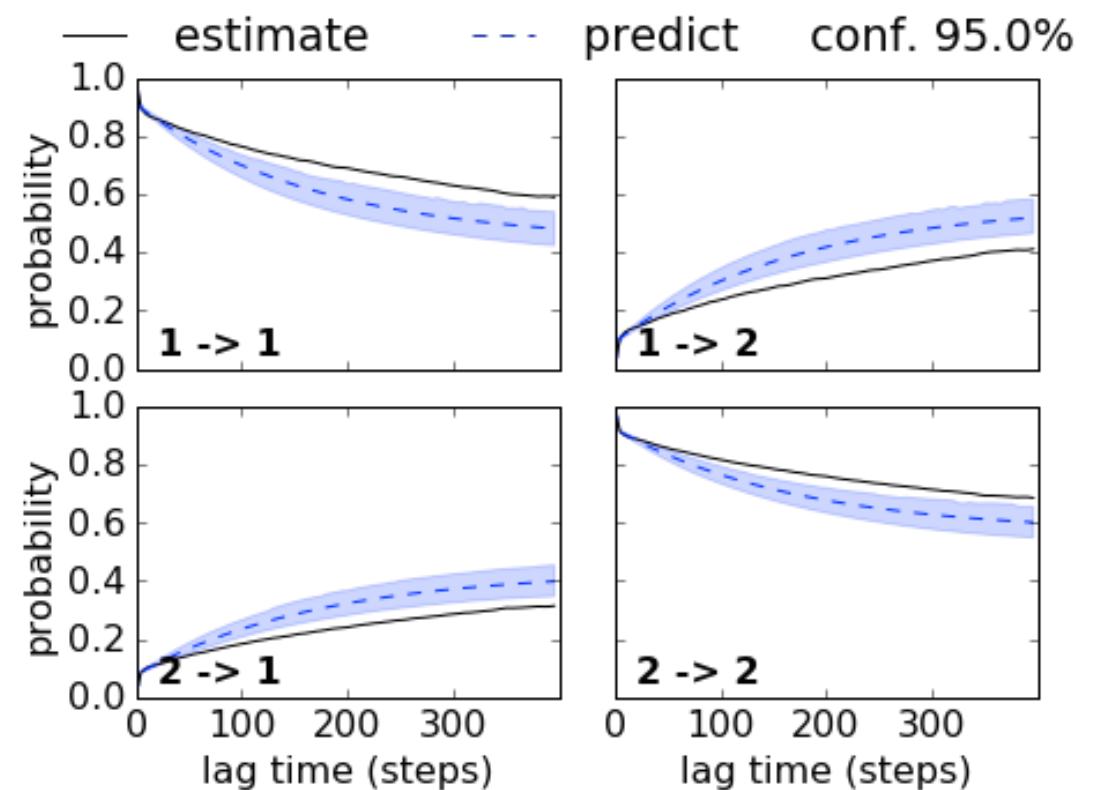
- Models the system dynamics by estimation of transition probabilities of hidden Markov process, and emission probability distributions.
- We need to decide the number of states of the hidden Markov process a priori (the number of meta-stable states)

Let's revisit our two well potential from before:

**Good discretization**



**Bad discretization**



We get a robust model of the dynamics which simultaneously resolves meta-stable states.

**Questions?**