Hidden Markov state models

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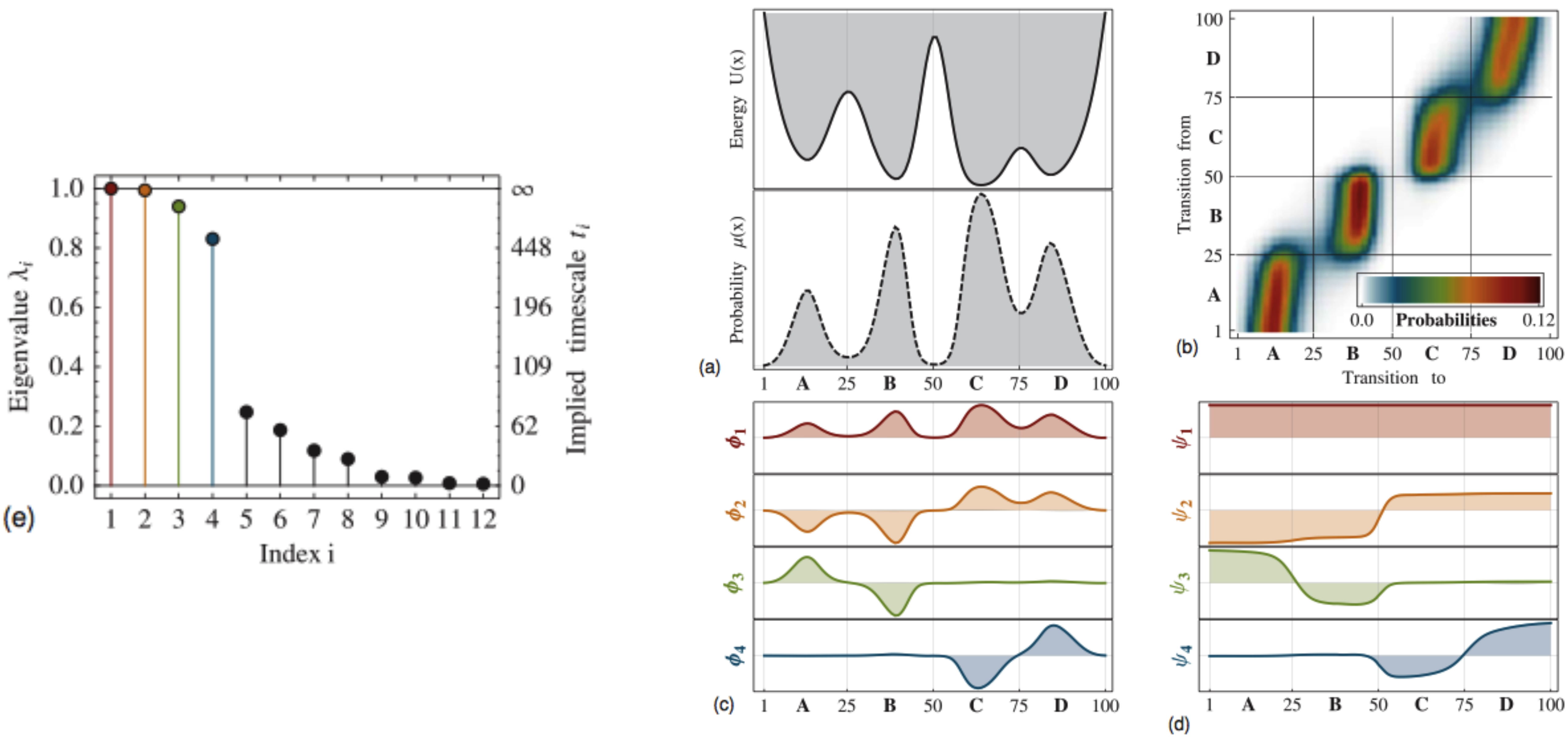
Discretization

Backward propagator

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

Spectral decomposition

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



Prinz et al, **JCP 134**, 174105 (2011)

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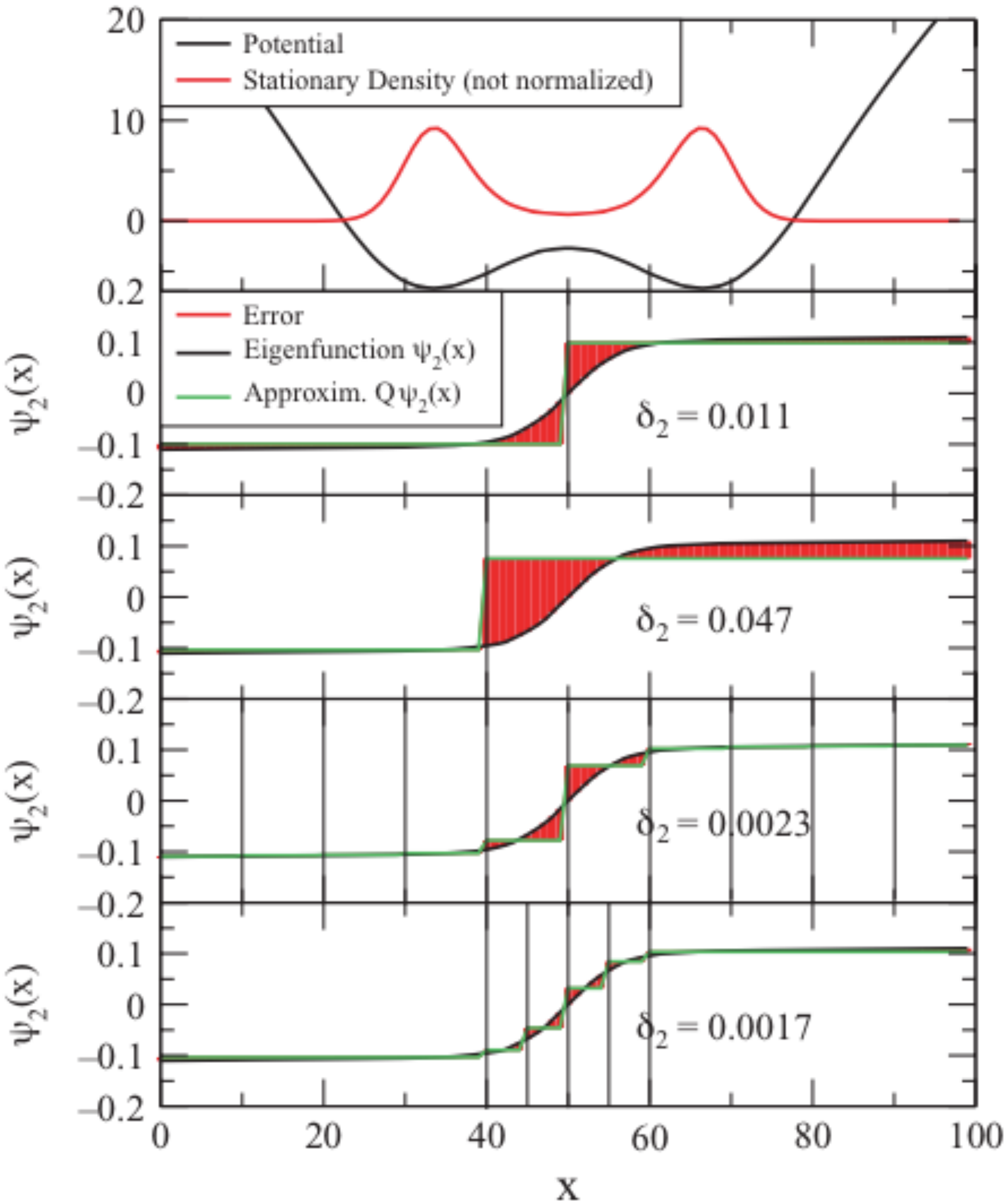

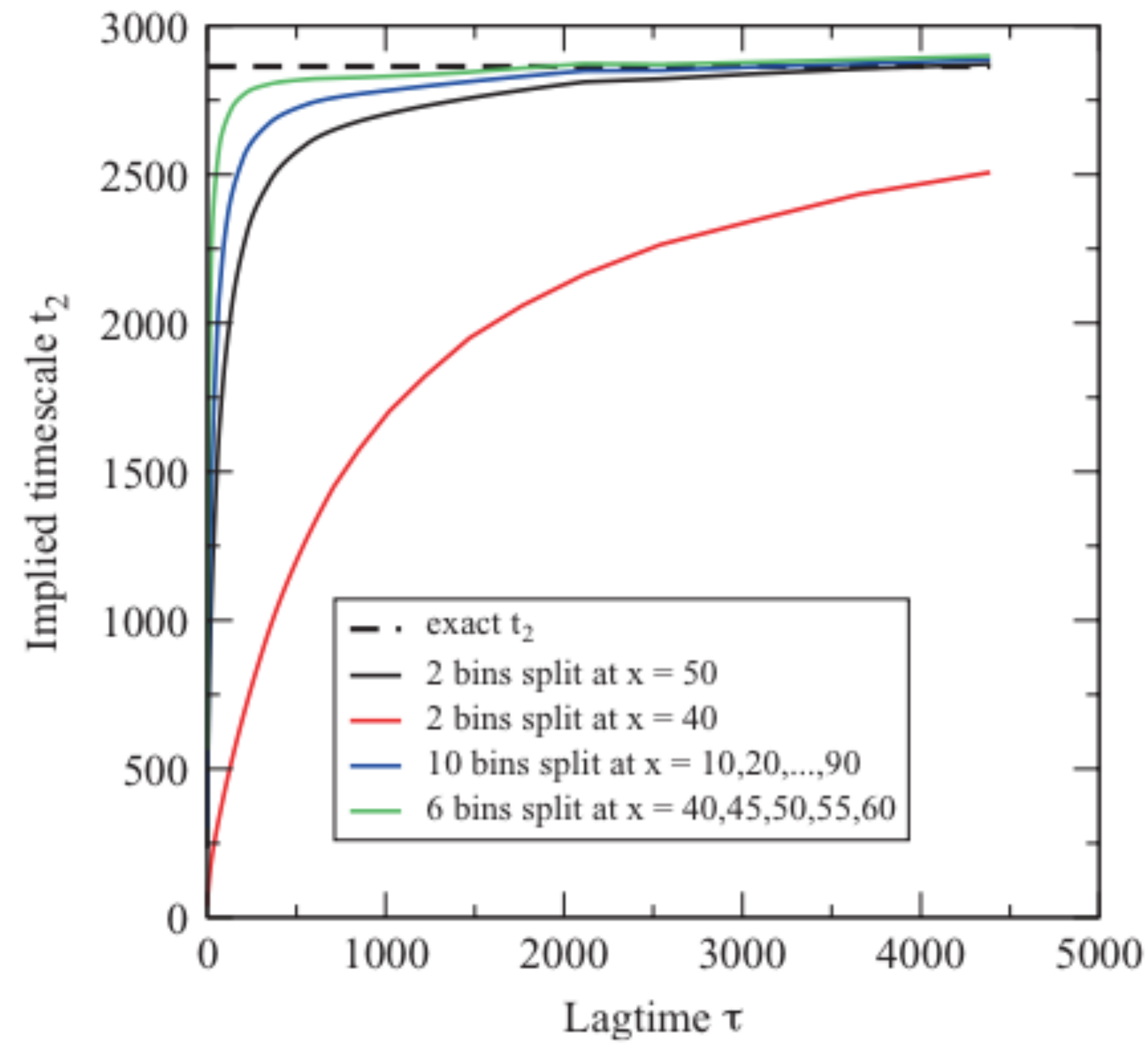

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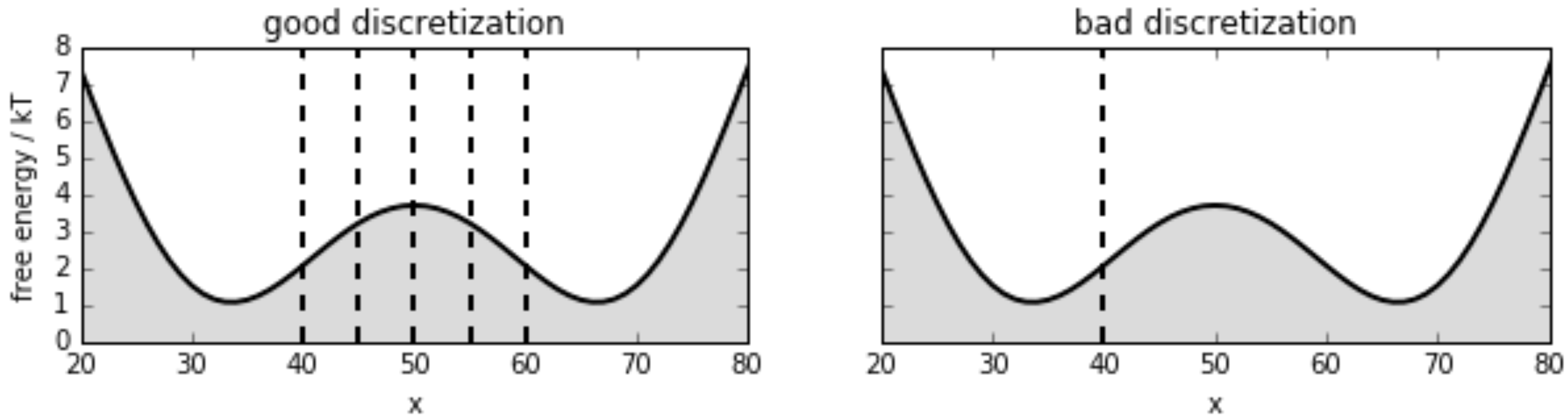
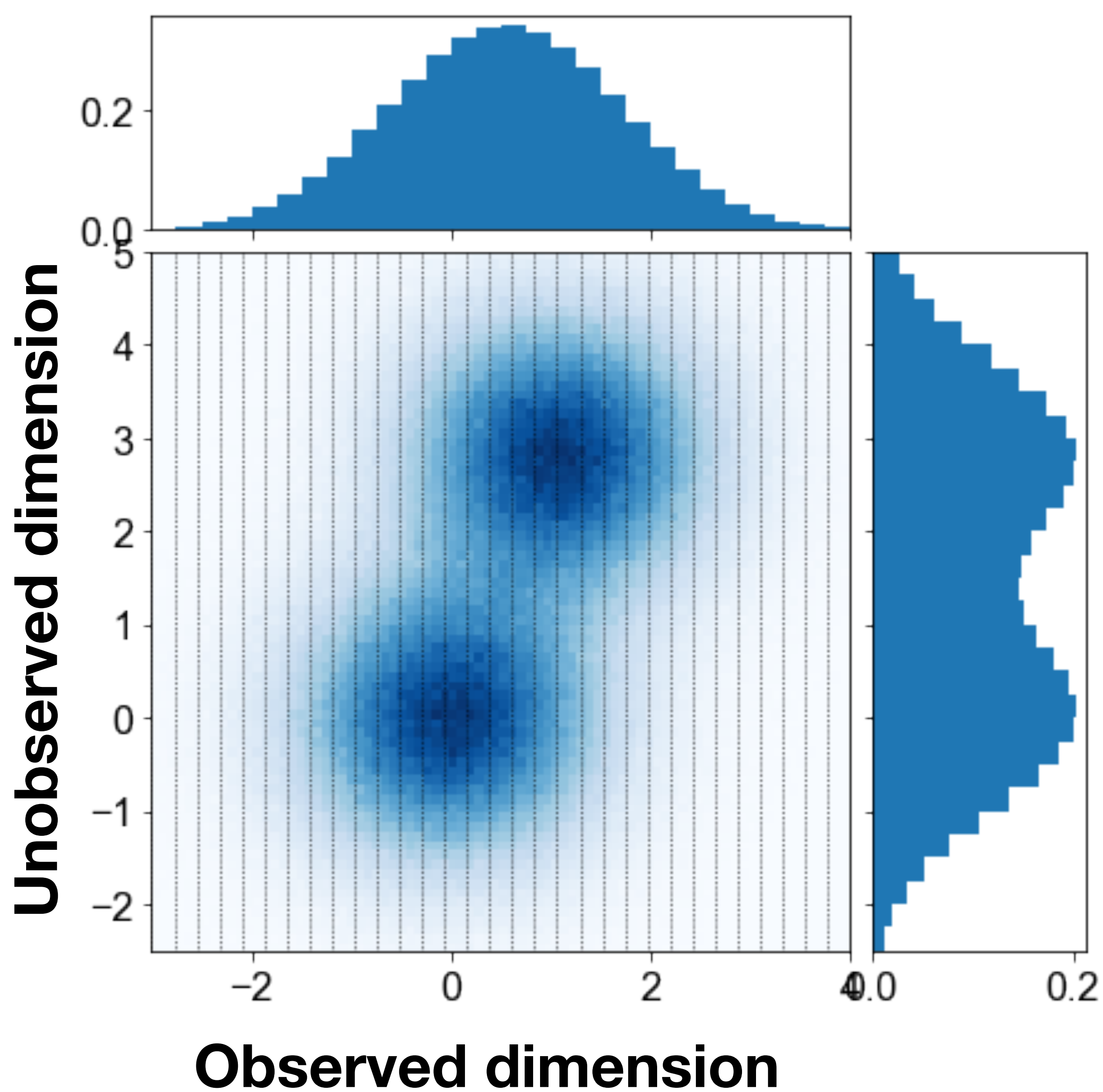
There are two flavors of discretization error





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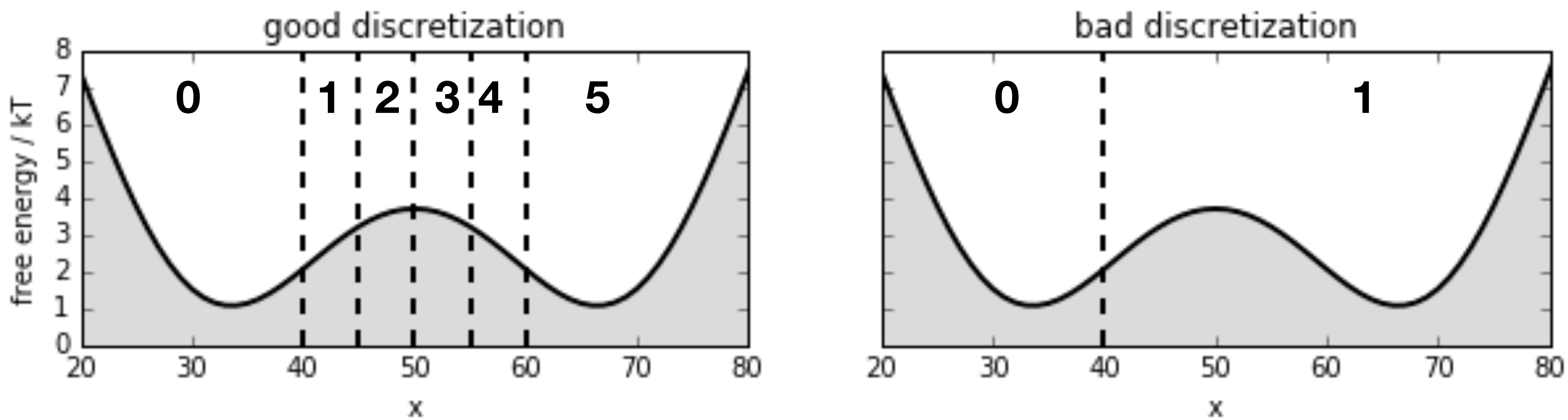

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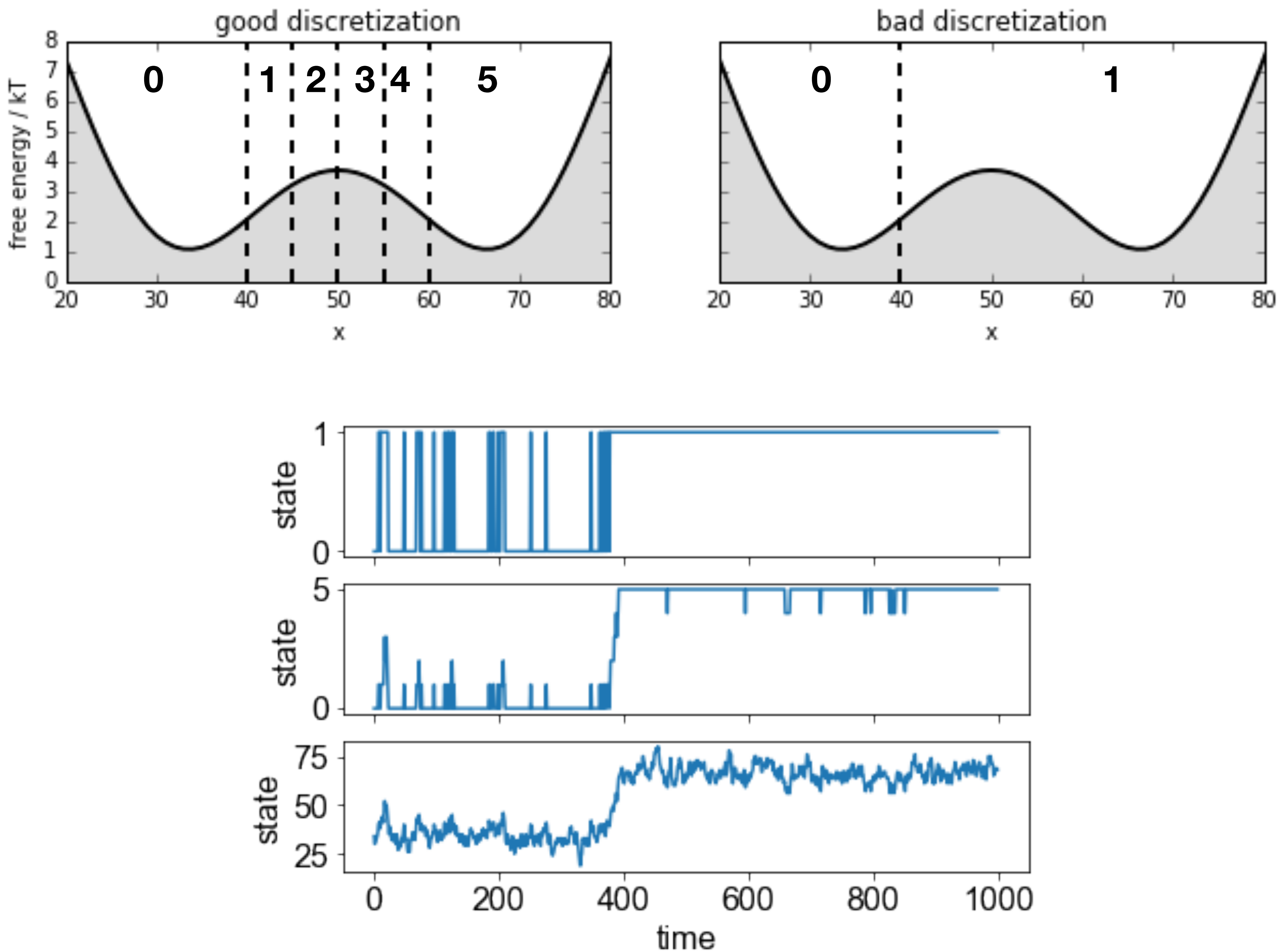

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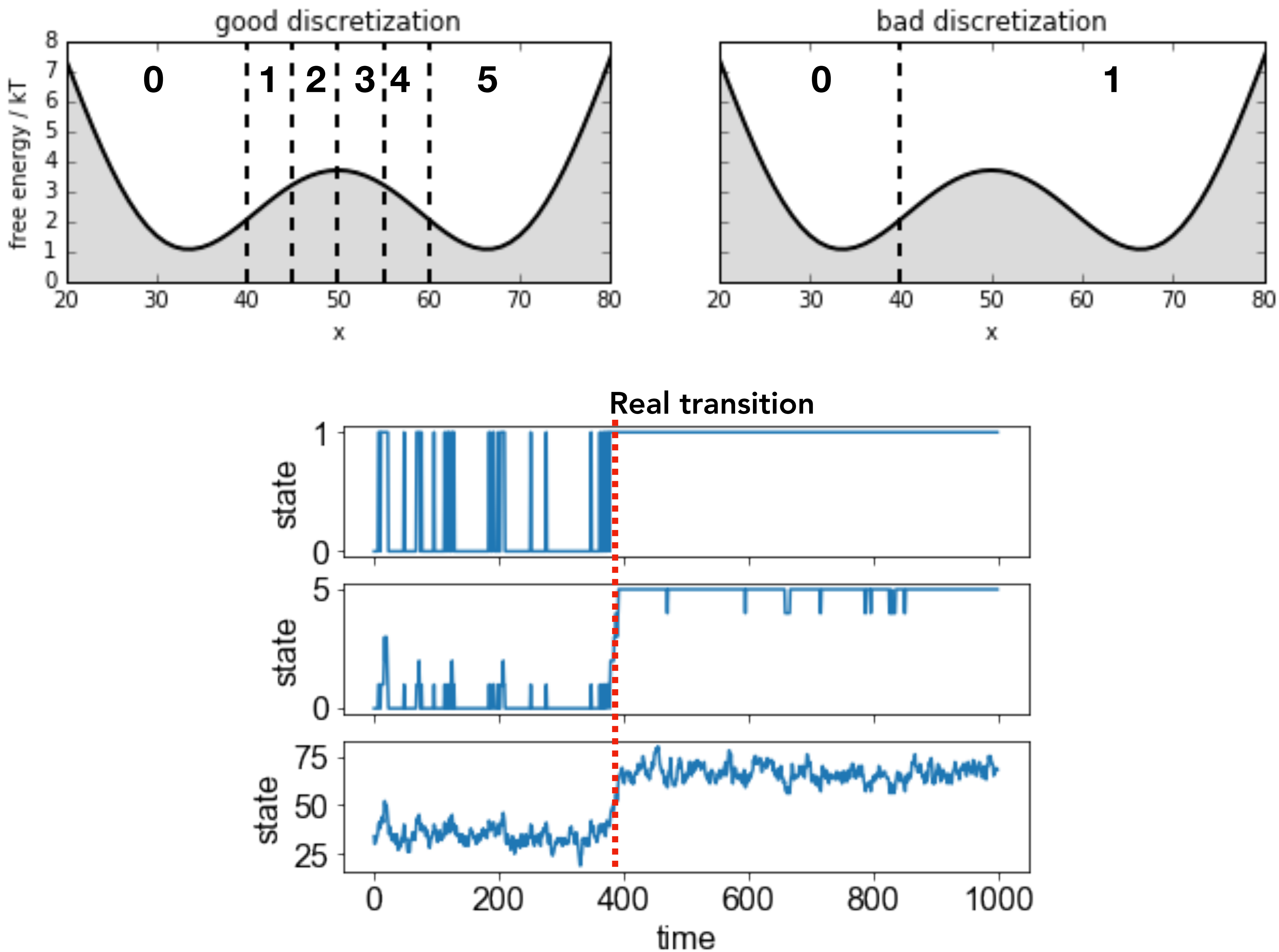

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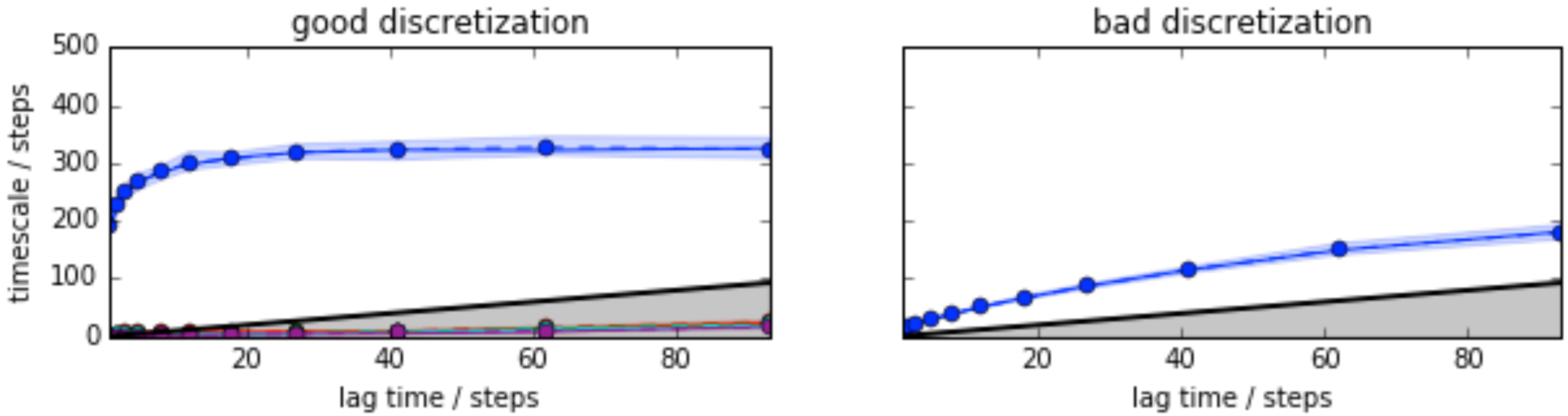

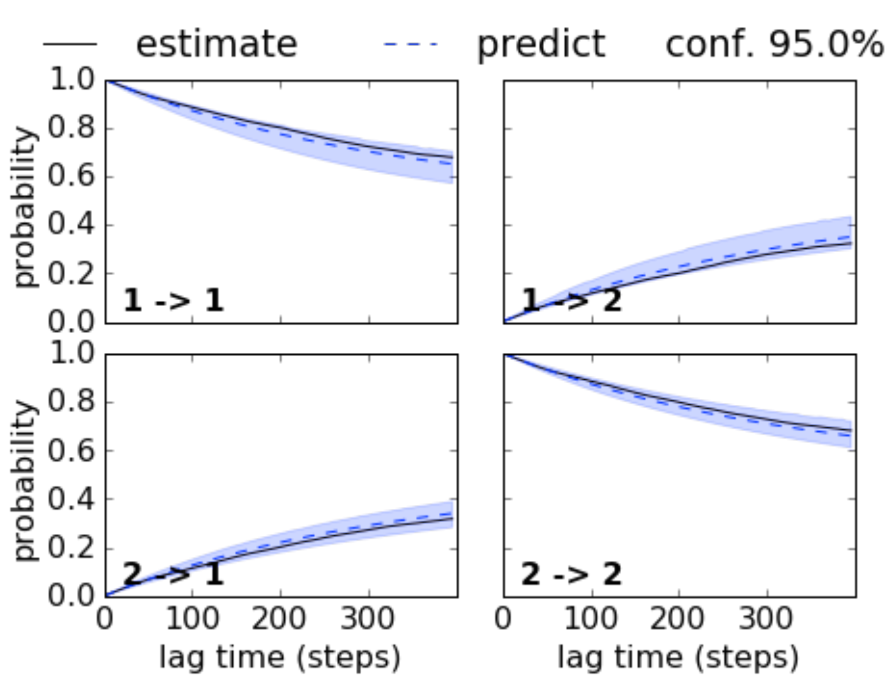

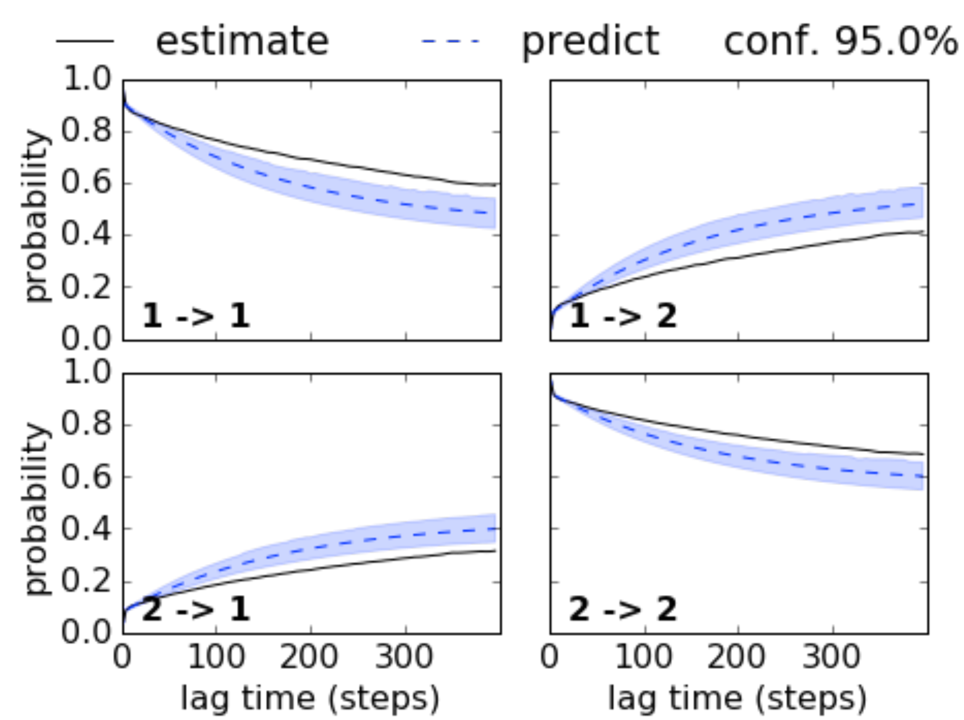

Projection/discretization error leads to systematic errors

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

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Remedies:

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- Improve featurization and clustering

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

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.

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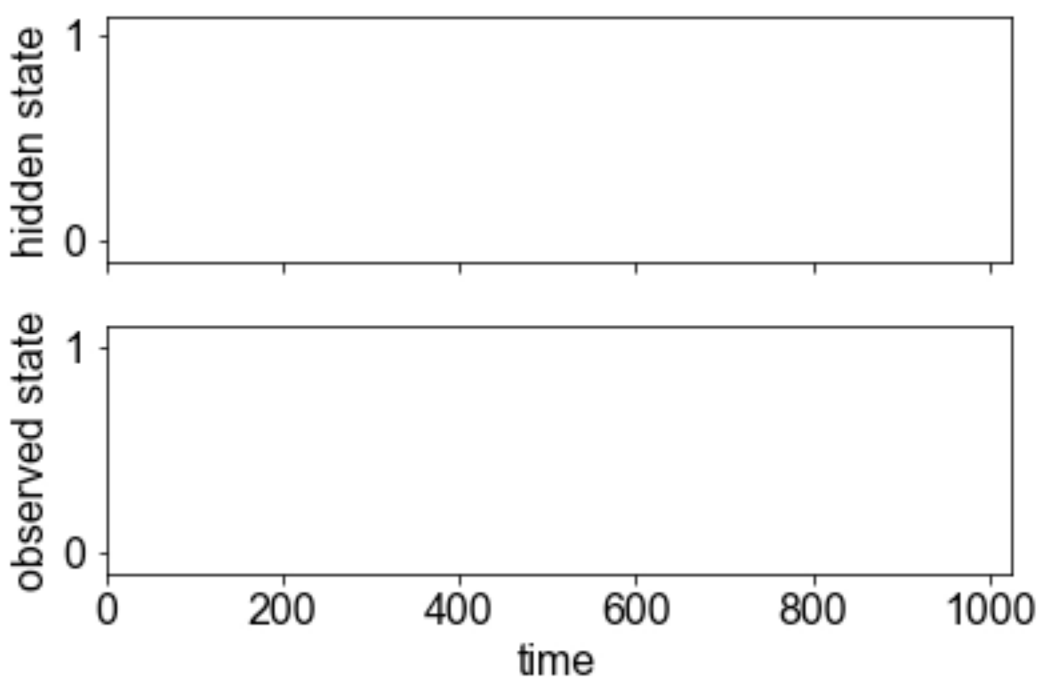

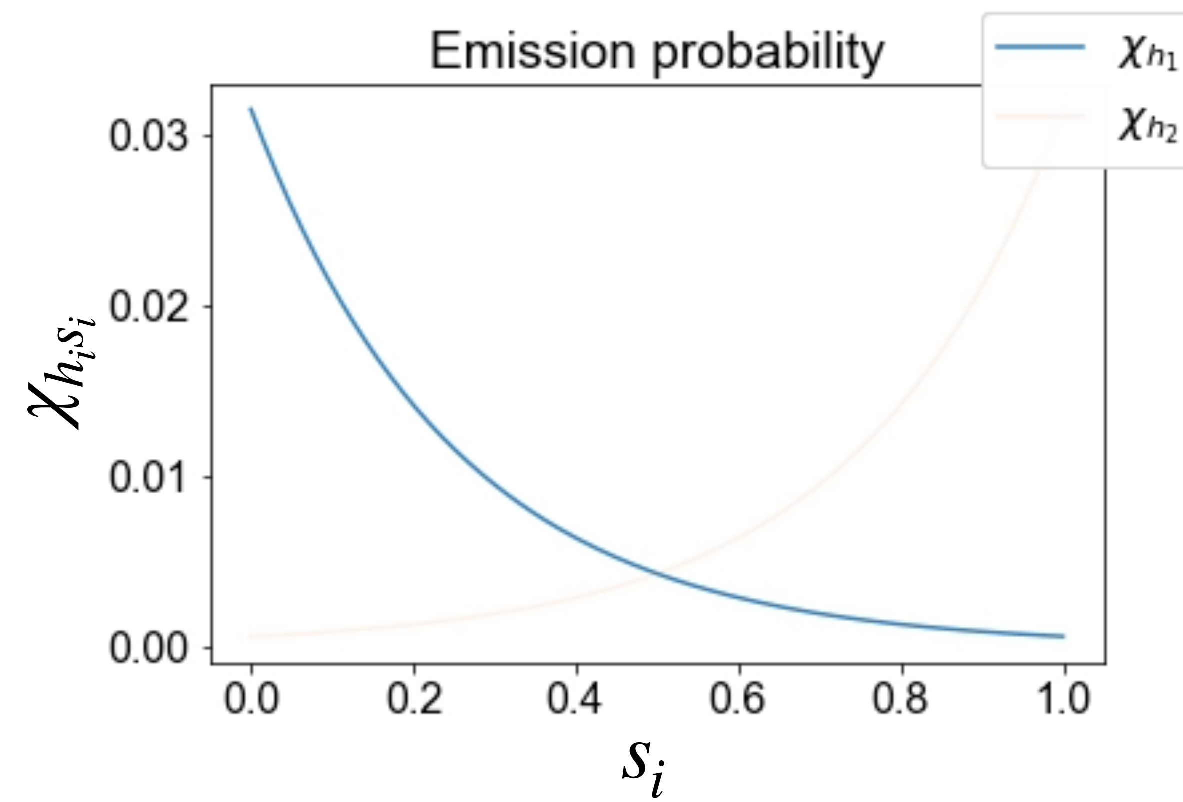

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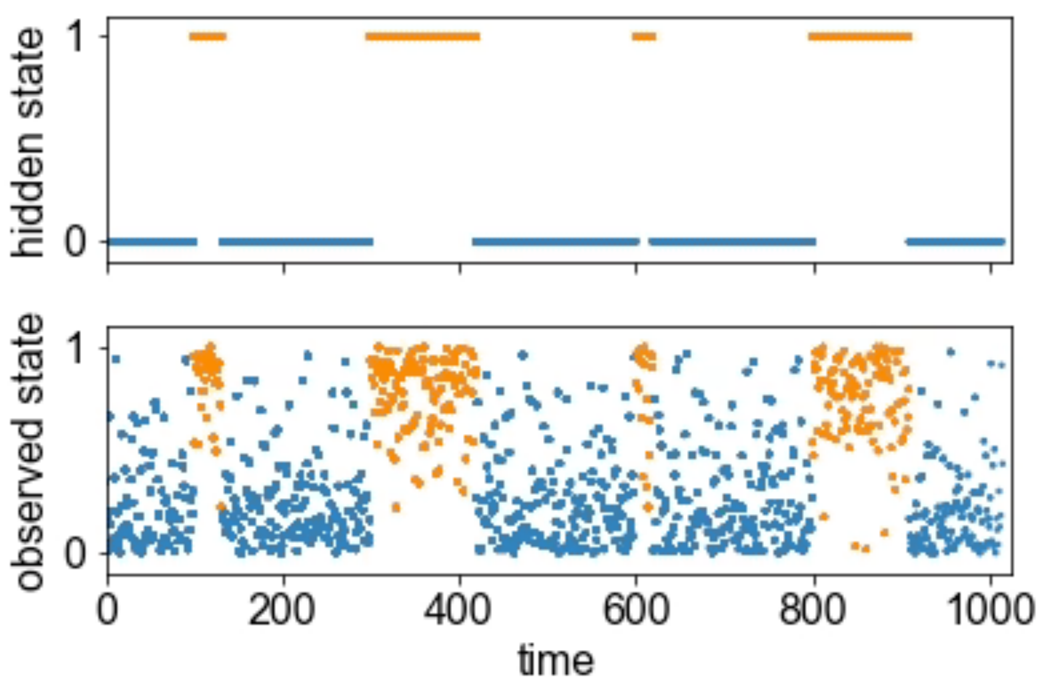

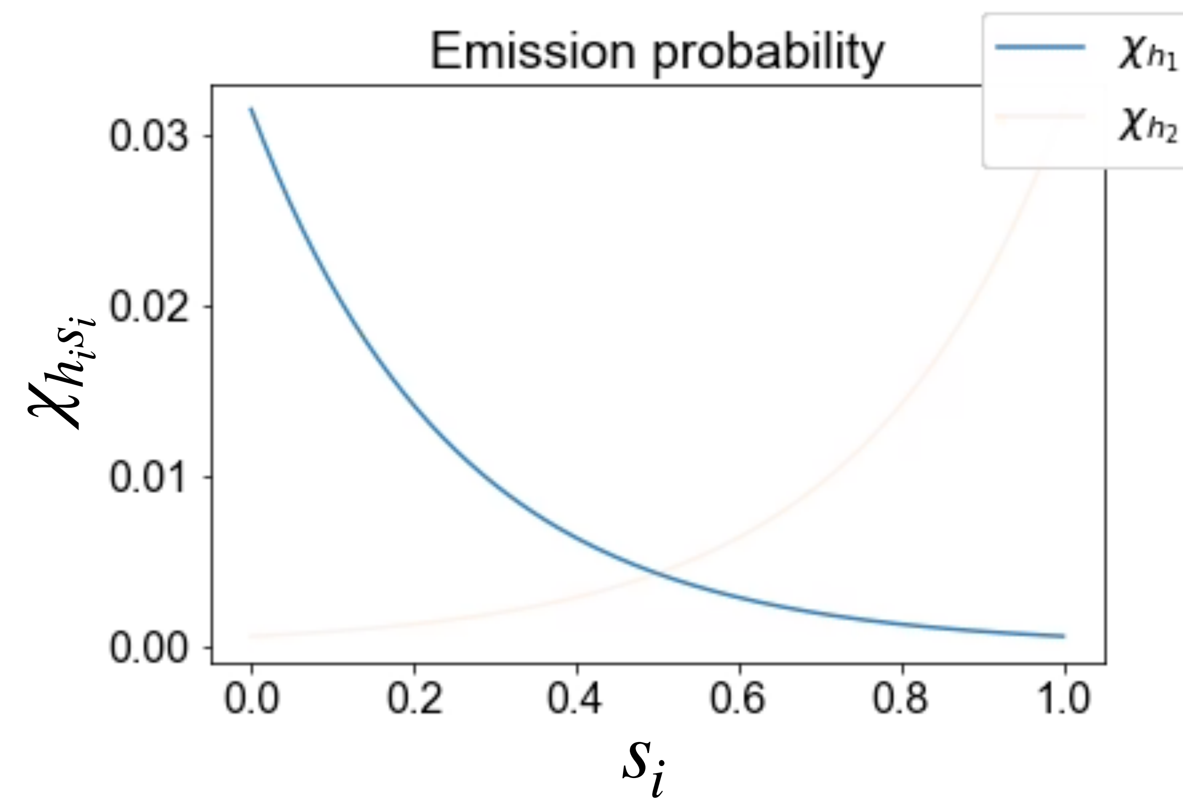

Maximum-Likelihood and Bayesian estimators are available:

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.
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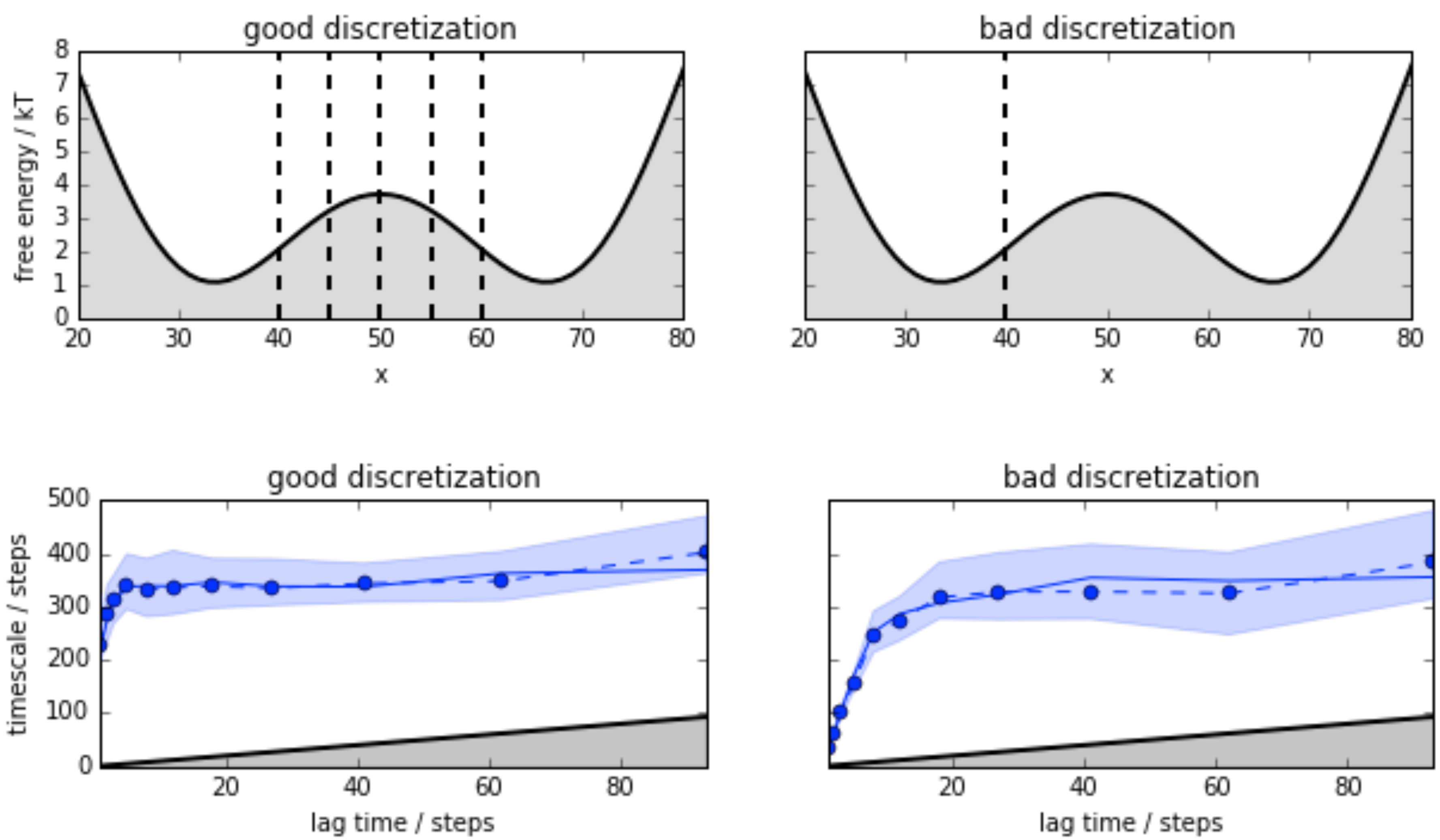

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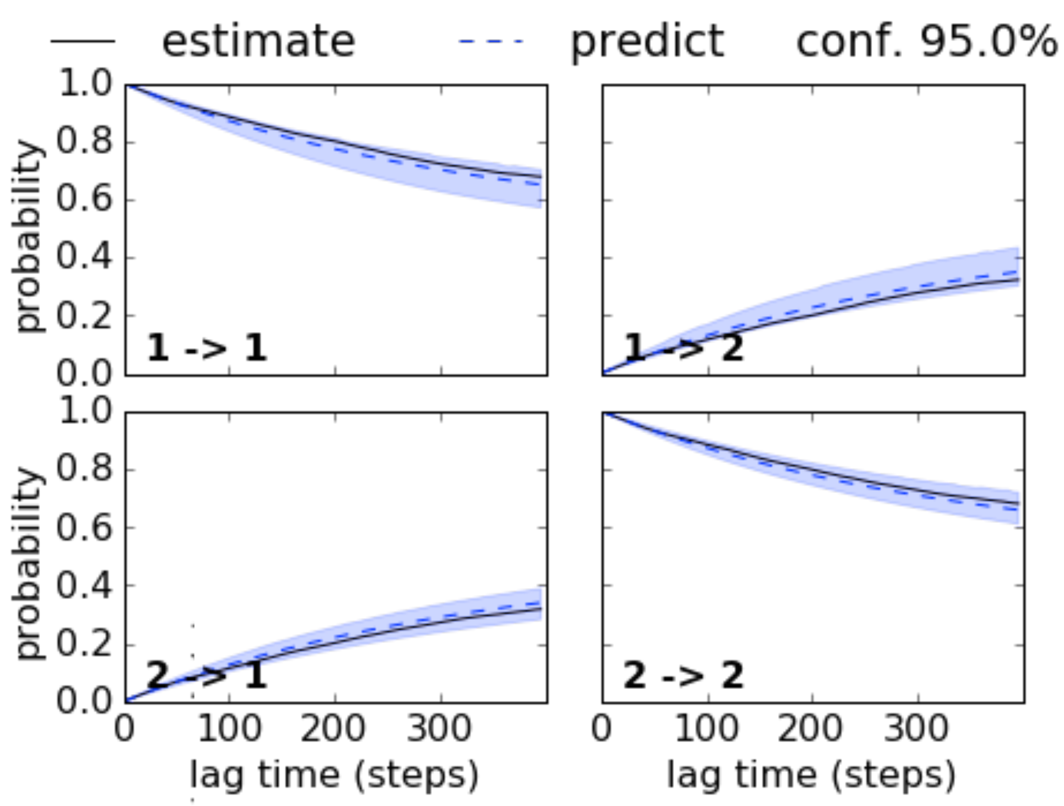

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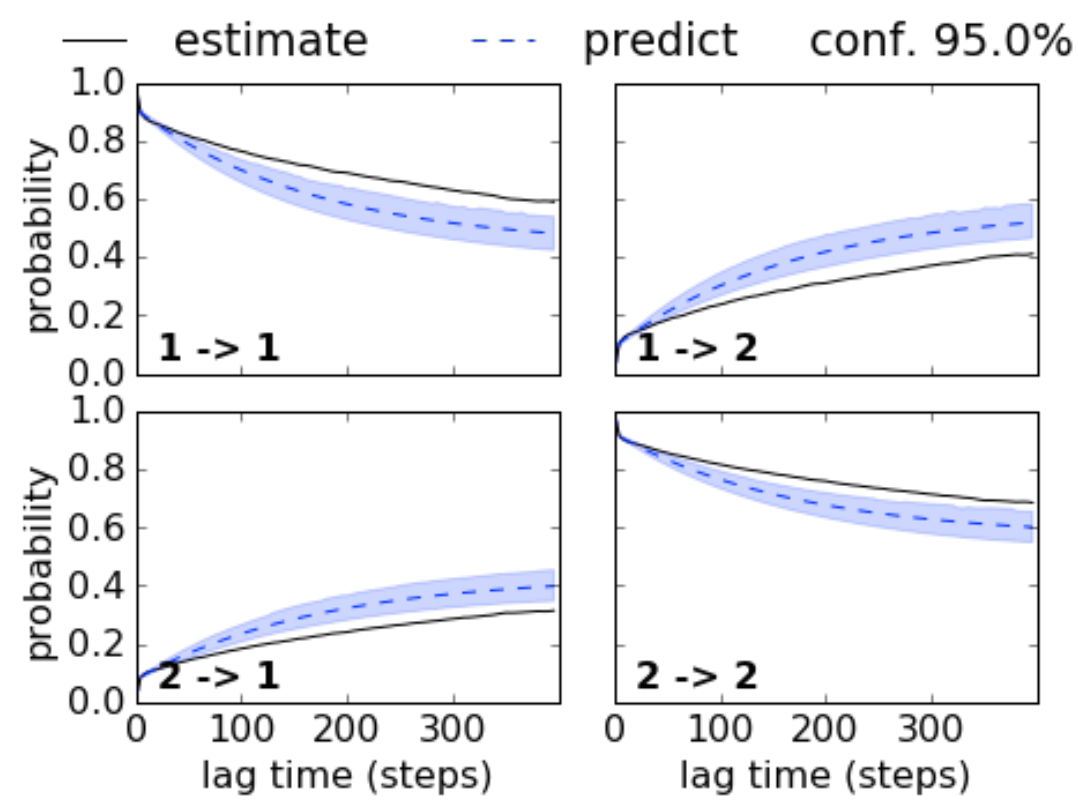

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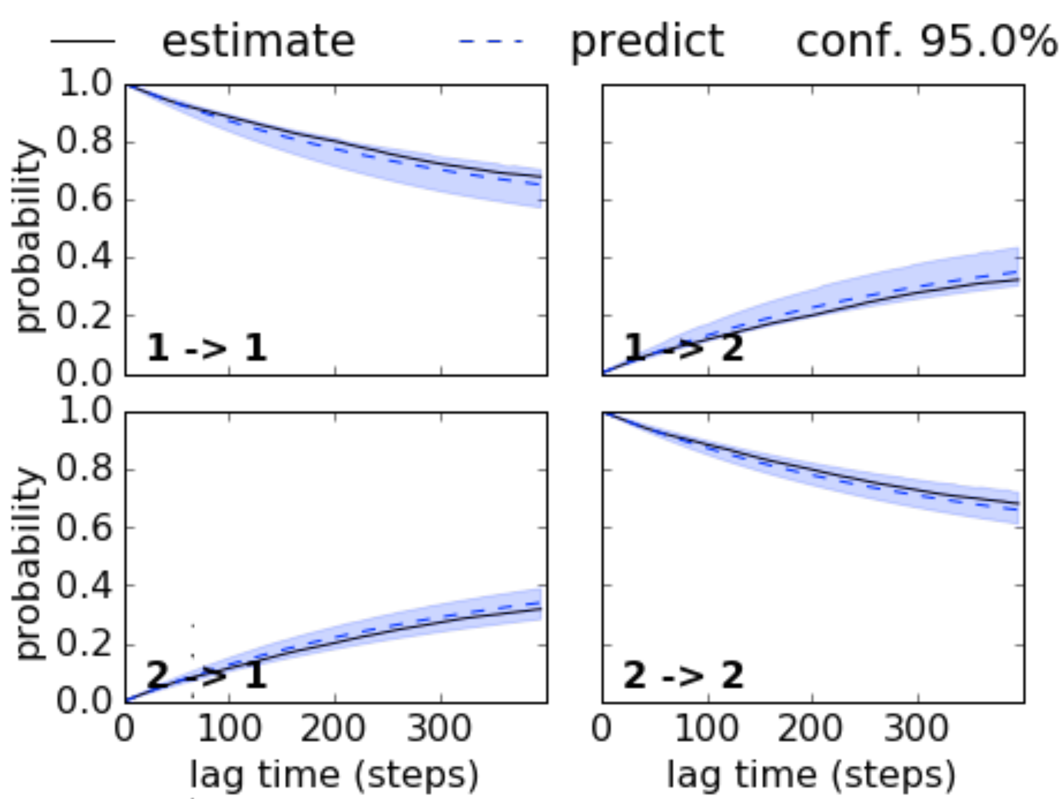

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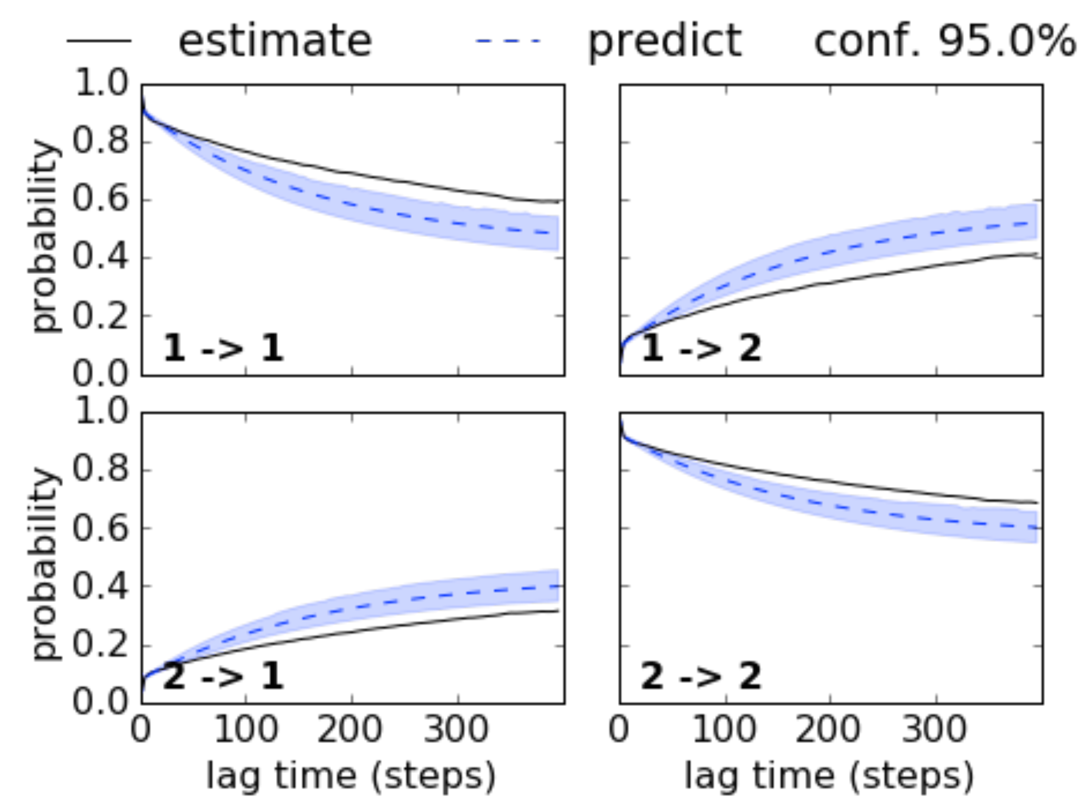

<u>We get a robust model of the dynamics which simultaneously resolves meta-stable states.</u>

Questions?

Notebook time