Moment-Based Variational Inference for Markov Jump Processes

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Introduction

Model Class: Markov jump process / continuous time Markov chain

- Applications in many domains (finance, social networks, healthcare, systems biology, etc.)
- Data-driven modelling requires latent state estimation

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Proposed solution: new variational inference approach based on

- transition space partitioning
- gradient-based optimization

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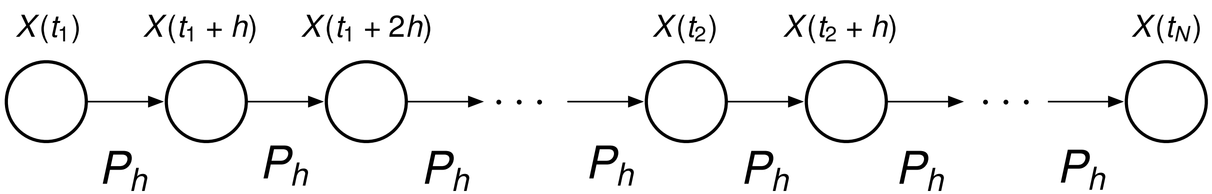
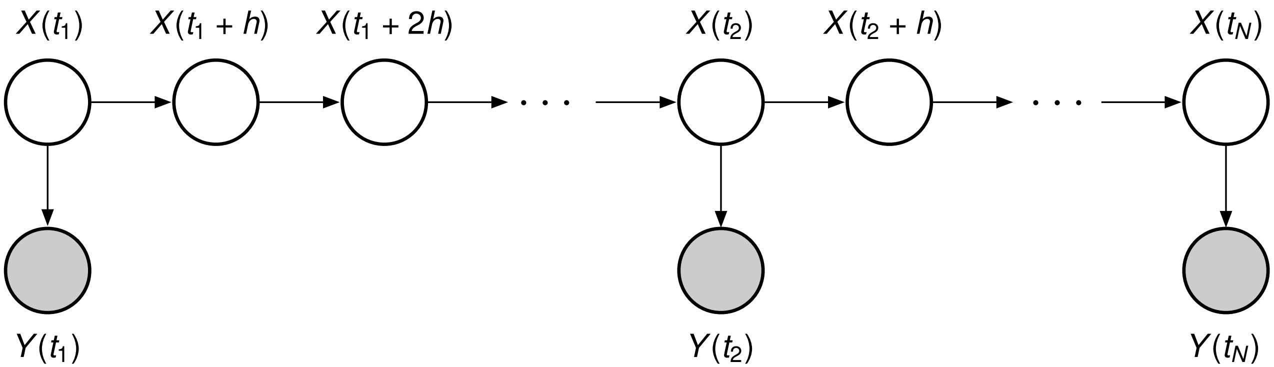


discretized representation of hidden MJP

Exact Inference

Goal: Compute posterior *path* distribution $P(X_{[0,T]} \mid Y_1, \ldots, Y_n)$



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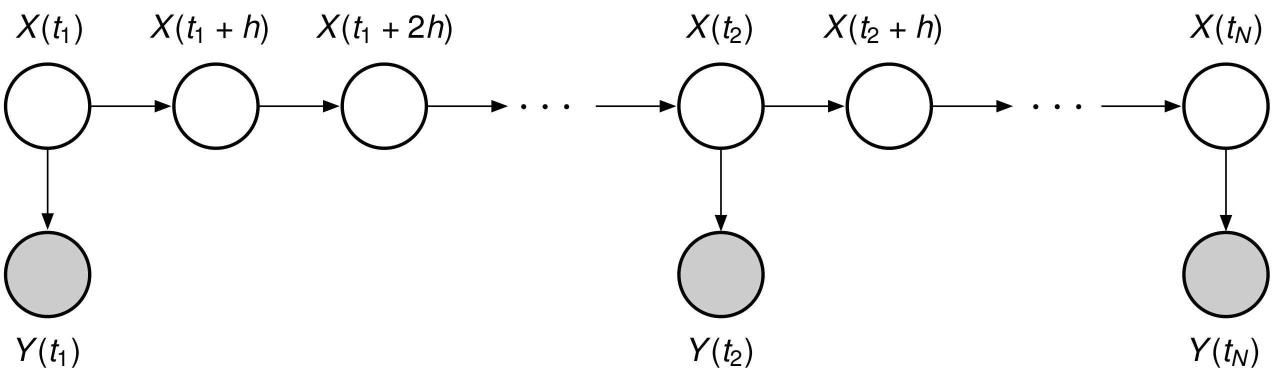

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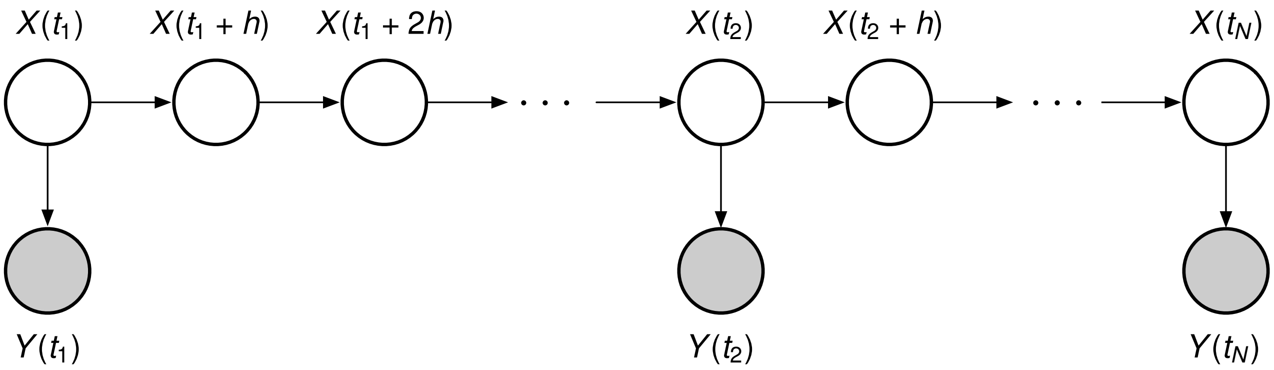

discretized representation of hidden MJP

hard to compute

Posterior paths are realized by smoothing process $\tilde{X}$ with modified transition function

$$\tilde{Q}(x, y, t) = \frac{\sigma(y, t)}{\sigma(x, t)} Q^X(x, y)$$

Variational Inference

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Minimize path level KL divergence $D_{KL}[P^{Z} || P^{\tilde{X}}]$

exact smoothing process

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negative ELBO

$$D_{KL}[P^Z || P^{\tilde{X}}] = \underbrace{D_{KL}[P^Z || P^X]}_{\text{variational to prior}} - \sum_{k=1}^{N} \mathrm{E}[\log p(y_k \mid Z(t_k)] + \underbrace{\log p(y_1, \ldots, y_n)}_{\text{marginal likelihood (evidence)}}$$

variational to prior

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Variational Inference

Minimize path level KL divergence $D_{KL}[P^Z || P^{\tilde{X}}]$ ← exact smoothing process

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Hard to construct suitable variational process class

Transition Space Partitioning

Smoothing process is in the class of controlled MJP with

$$Q^Z(x, y, t) = \underbrace{\lambda(x, y, t)}_{\text{time and state dependent control factor}} \underbrace{Q^X(x, y)}_{\text{prior transition function}}$$

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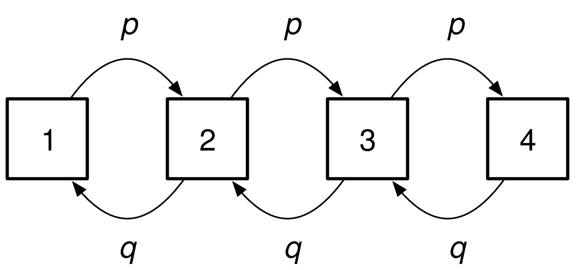
Example: random walk



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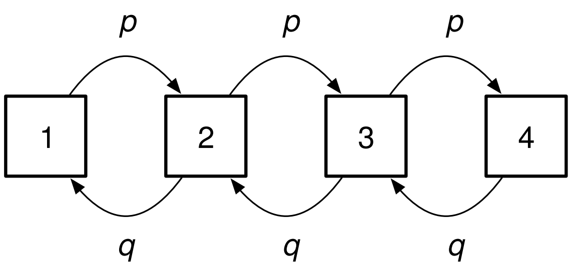

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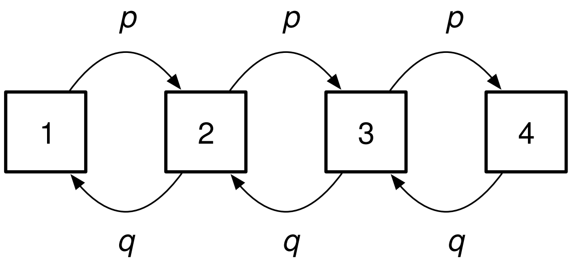

$$Q^X = \begin{pmatrix} -p & p & 0 & 0 \\ q & -(p+q) & p & 0 \\ 0 & q & -(p+q) & p \\ 0 & 0 & q & -q \end{pmatrix}$$

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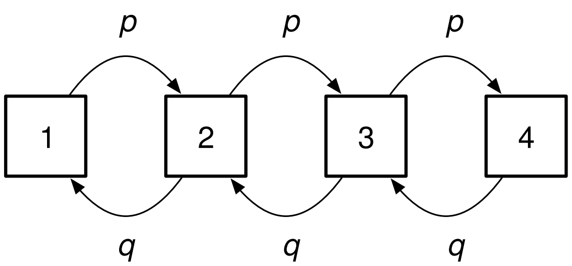

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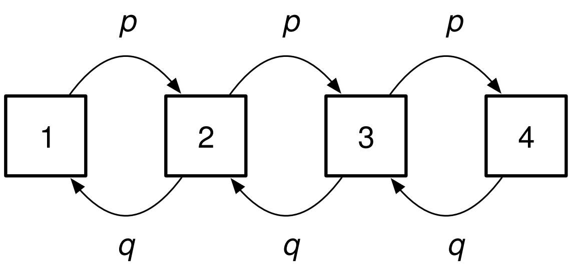

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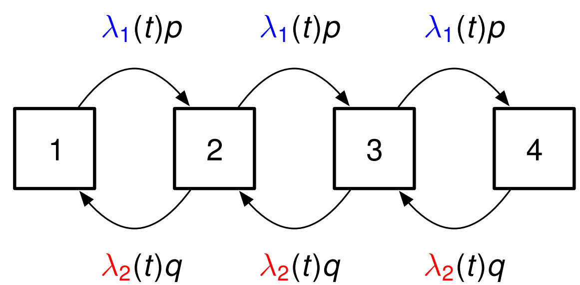

Complexity Reduction

$$D_{KL}[P^Z \,||\, P^X] = \int_0^T \sum_x p^Z(x,t) \sum_{y \neq x} \Big[Q^X(x,y) - Q^Z(x,y,t) - Q^Z(x,y,t) \log \left(\frac{Q^Z(x,y,t)}{Q^X(x,y)} \right) \Big] \, dt$$

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expected summary statistic

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Obtain non-linear, deterministic optimal control problem

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Solve via natural gradient descent in the controls $\lambda(t)$

Example Application

Scenario:

Stochastic gene expression

Studied by fluorescence microscopy

Goals:

Parameter estimation

Model comparison

Optimal experiment design