Augmented Ensemble MCMC with applications to Factorial HMMs

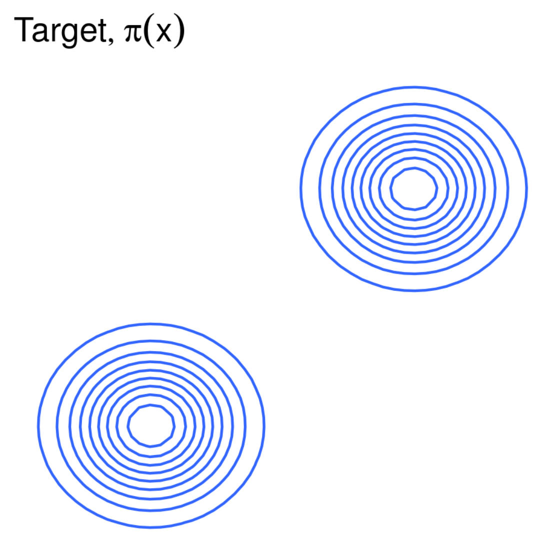
Kaspar Märtens, Michalis Titsias, Christopher Yau

UNIVERSITY OF OXFORD

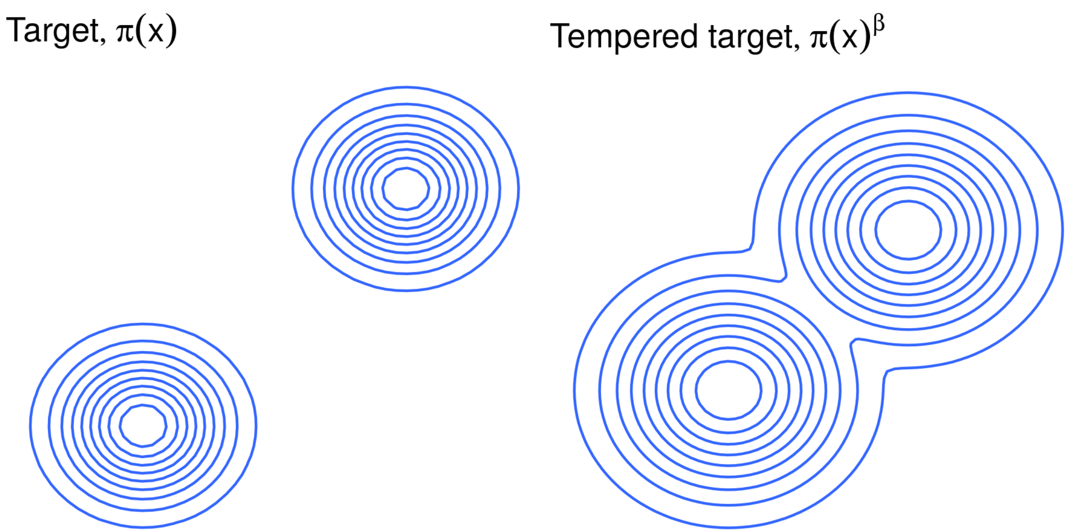
DEPARTMENT OF STATISTICS

Background

Bayesian inference for high-dimensional models is challenging: it is difficult to explore multimodal distributions.



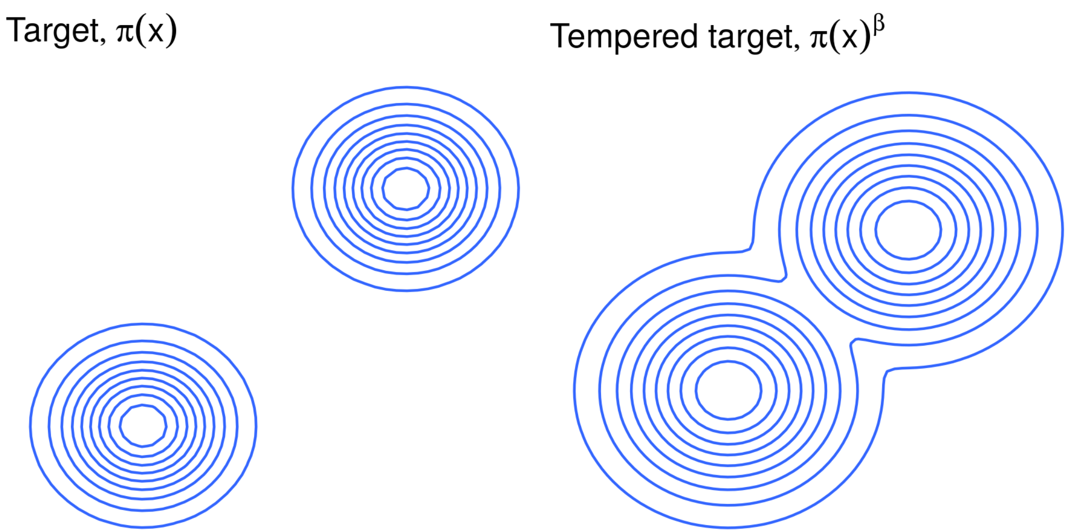
Parallel tempering



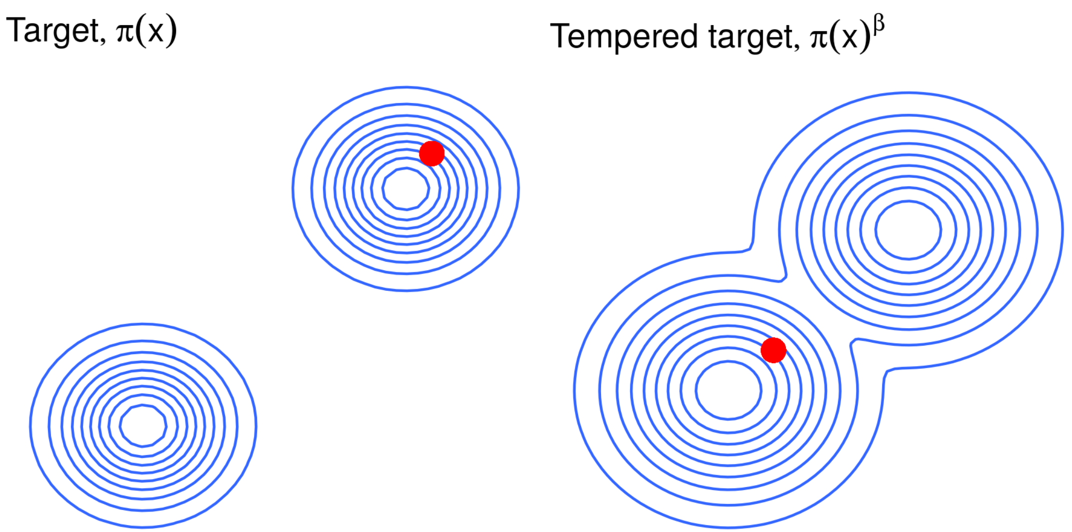
Parallel tempering

Instead of simply targeting $\pi(x)$, introduce a temperature ladder $T_1 < T_2 < \ldots < T_K$ and run multiple MCMC chains, with chain k targeting

$$\pi(x)^{\beta_k} \text{ where } \beta_k = 1/T_k$$



How to exchange information between an ensemble of chains



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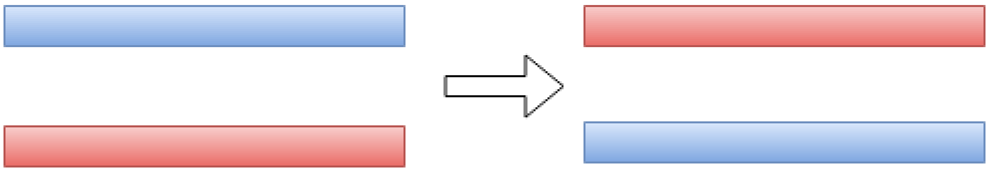
1. **Swap move**: Propose to swap (using Metropolis-Hastings to accept/reject)



Inefficient in a high-dimensional setting

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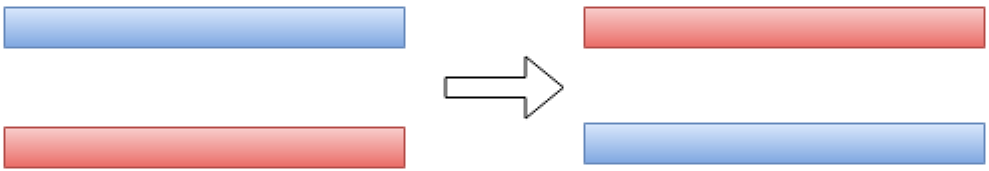
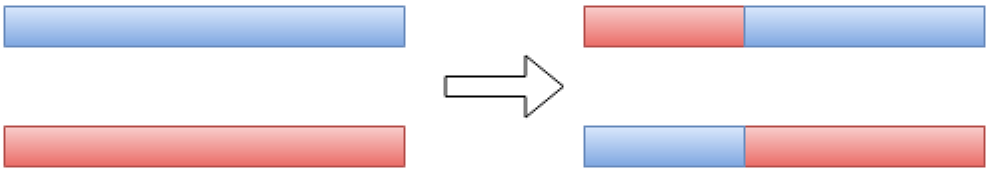


   Inefficient in a high-dimensional setting

2. **Genetic algorithms**:

   One-point **crossover** (using Metropolis-Hastings to accept/reject)



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1. Generate auxiliary $(\mathbf{u}, \mathbf{v}) \sim p(\mathbf{u}, \mathbf{v} | \mathbf{x}_i, \mathbf{x}_j)$
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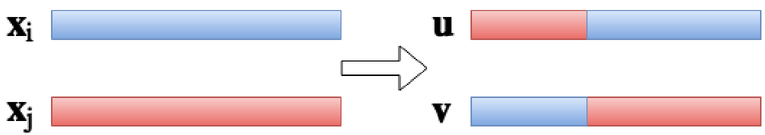

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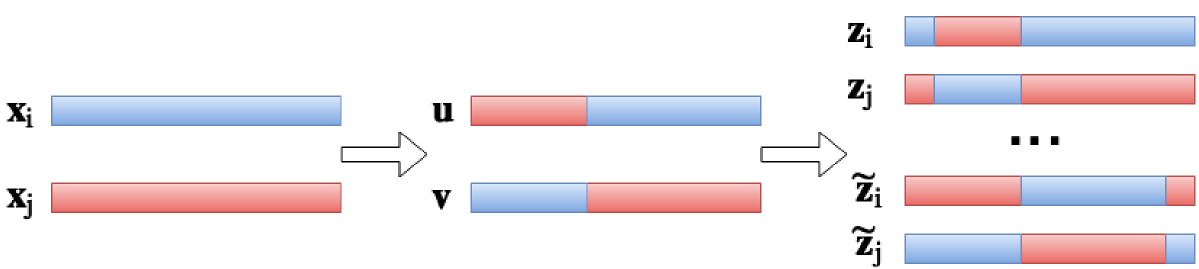
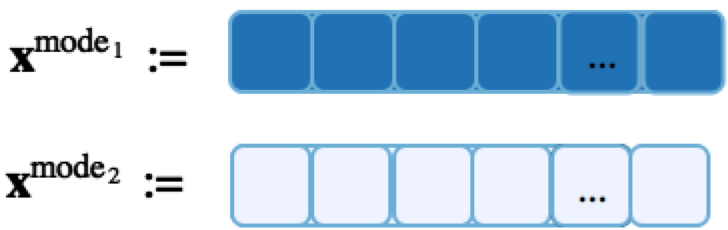
2. Generate $(\mathbf{x}_i, \mathbf{x}_j) \sim p(\mathbf{x}_i, \mathbf{x}_j | \text{rest})$, where

$$\begin{aligned} p(\mathbf{x}_i, \mathbf{x}_j | \text{rest}) &= \frac{1}{Z} \pi_i(\mathbf{x}_i) \pi_j(\mathbf{x}_j) p(\mathbf{u}, \mathbf{v} | \mathbf{x}_i, \mathbf{x}_j) \\ &= \frac{1}{Z} \pi_i(\mathbf{x}_i) \pi_j(\mathbf{x}_j) p(\mathbf{x}_i, \mathbf{x}_j | \mathbf{u}, \mathbf{v}) \\ &= \frac{1}{Z} \pi_i(\mathbf{x}_i) \pi_j(\mathbf{x}_j) I((\mathbf{x}_i, \mathbf{x}_j) \in \text{Crossover}(\mathbf{u}, \mathbf{v})) \end{aligned}$$



Toy example

Consider the following distribution over binary vectors with two separated modes:



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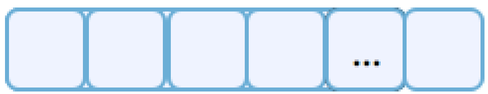
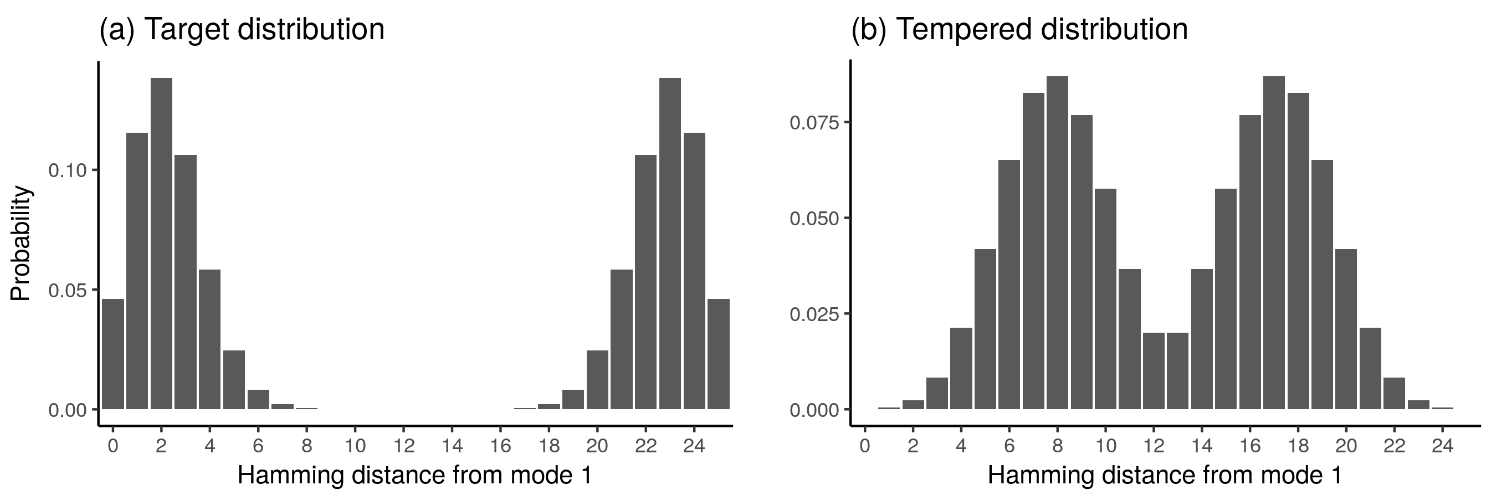
$\mathbf{x}^{\text{mode}_1} :=$

$\mathbf{x}^{\text{mode}_2} :=$

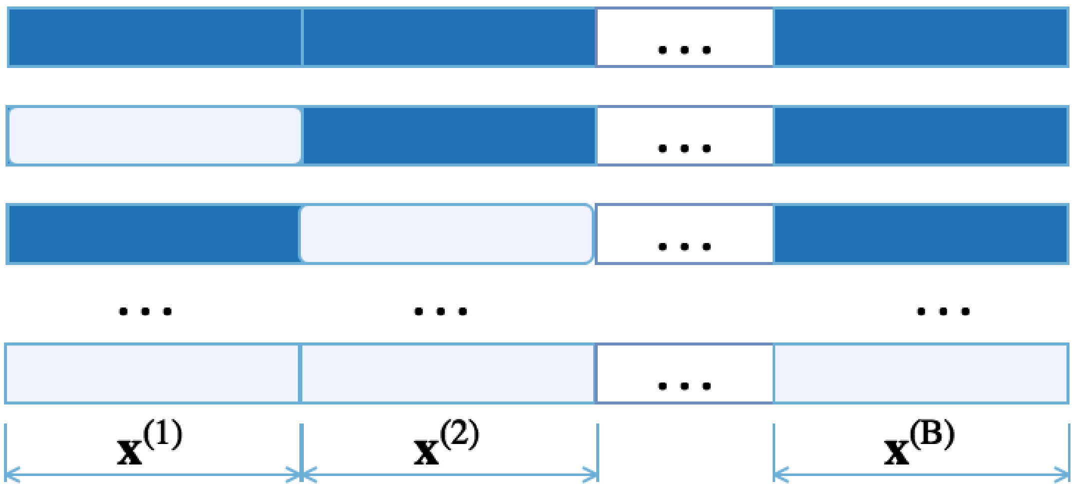




Toy example extended

Divide $\mathbf{x}$ into B blocks, within each block bimodal distribution.

Results in a total of 2^B modes:



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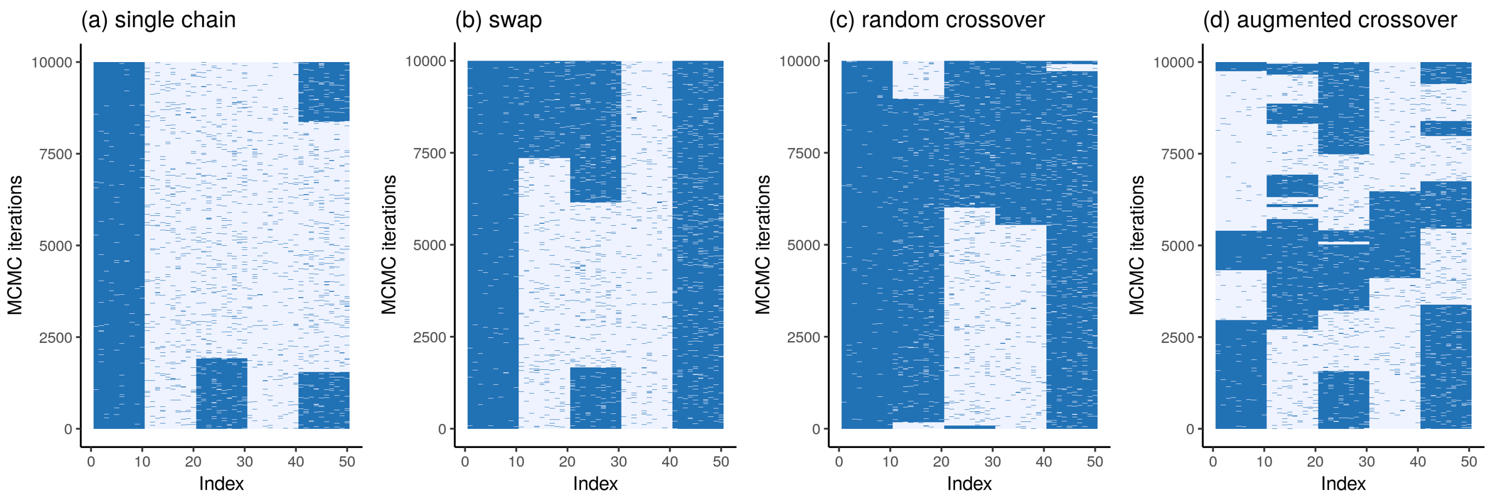
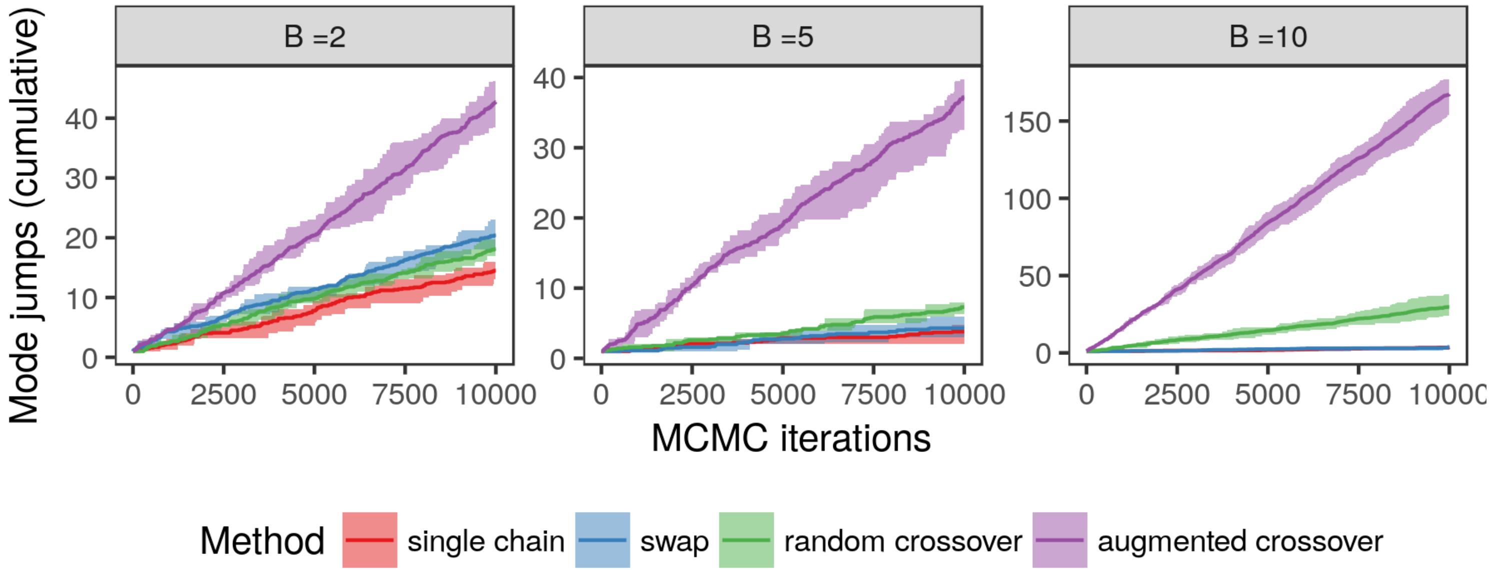


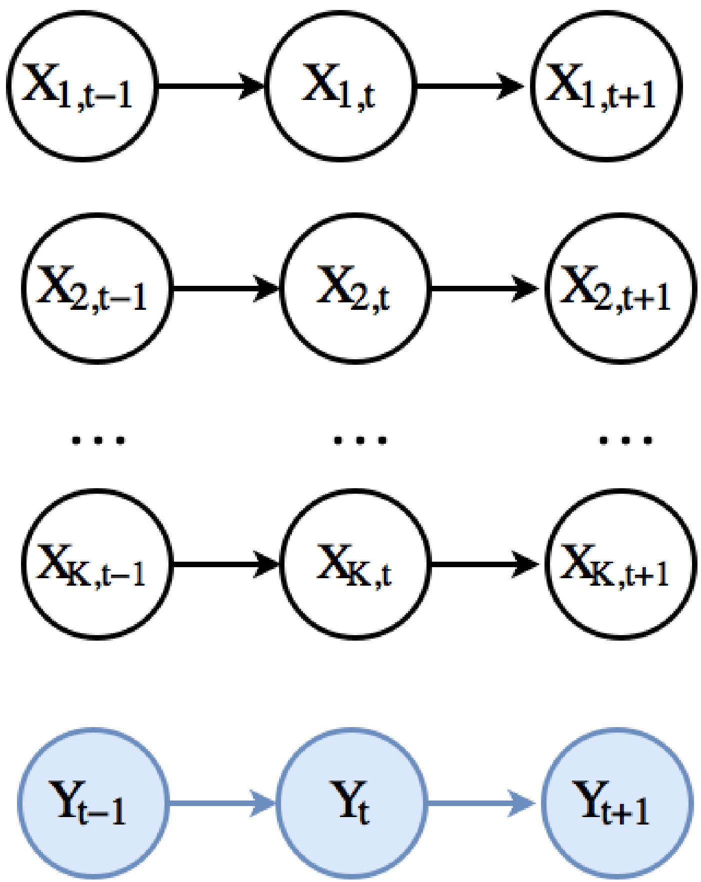
Toy example: comparison of samplers

Number of mode jumps (cumulative)

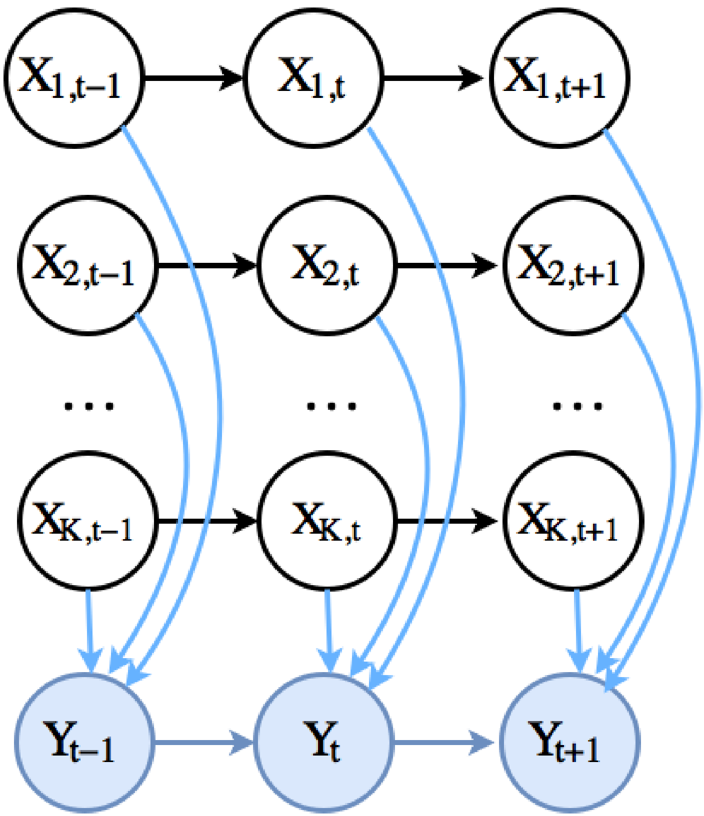


Factorial HMM

Extension of HMM: multiple latent sequences



Factorial HMM



$$(w_1, \ldots, w_K) \sim \mathrm{Dir}(\alpha, \ldots, \alpha)$$

$$Y_t | X_{:,t}, w \sim \mathcal{N}\left(\sum_{k=1}^{K} w_k X_{k,t},\ \sigma^2\right)$$

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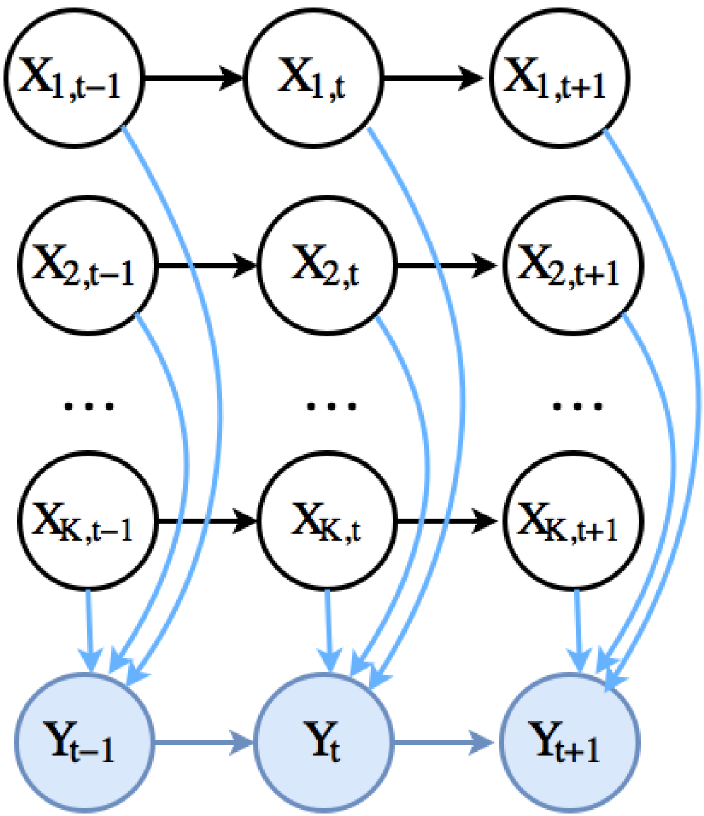

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Inference by Gibbs sampling:

1. Sample $\mathbf{w}|Y, X$
   - e.g. by random walk MH
2. Sample $X|\mathbf{w}, Y$
   - Full FB recursion becomes quickly infeasible, due to complexity $O(2^{2K}T)$
   - Solutions:
     - Update one row of X conditional on the rest
     - Hamming Ball sampling (Titsias and Yau 2016)

Factorial HMM example

Motivated by a cancer genomics application.

Consider the following example ($K = 3$) with multiple underlying explanations, where $w_1 + w_2 \approx w_3$

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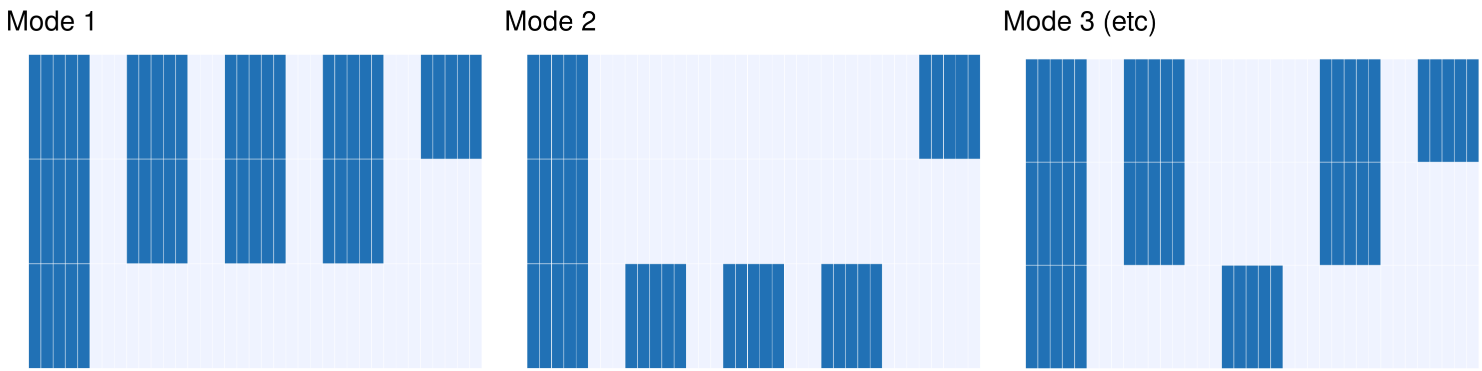

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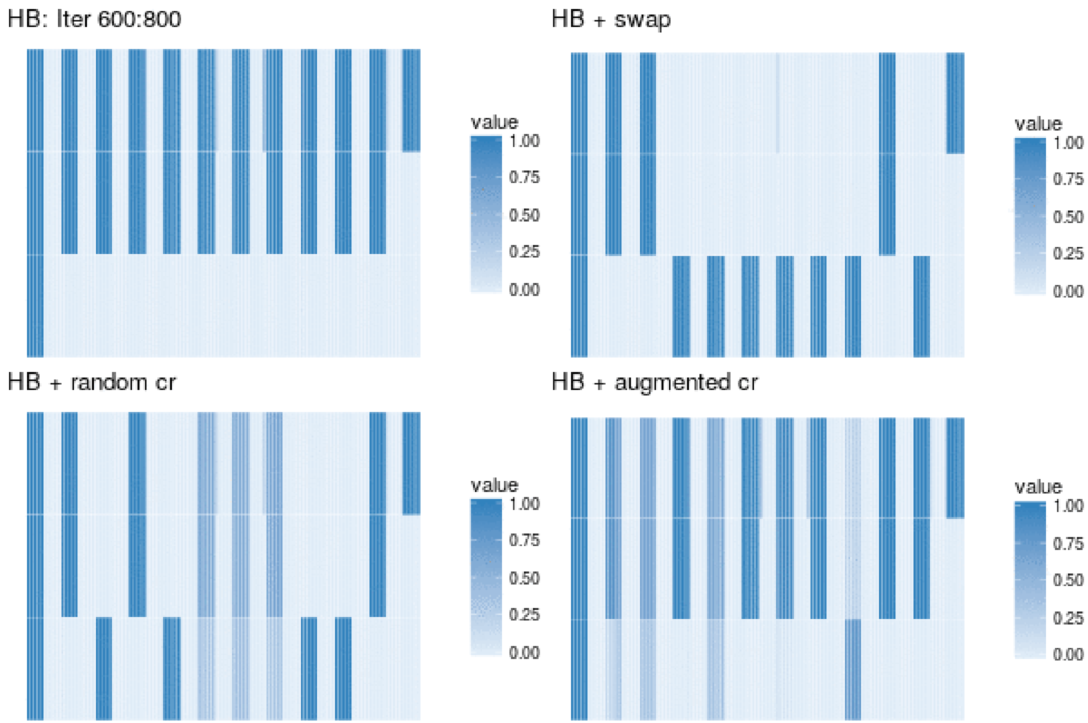

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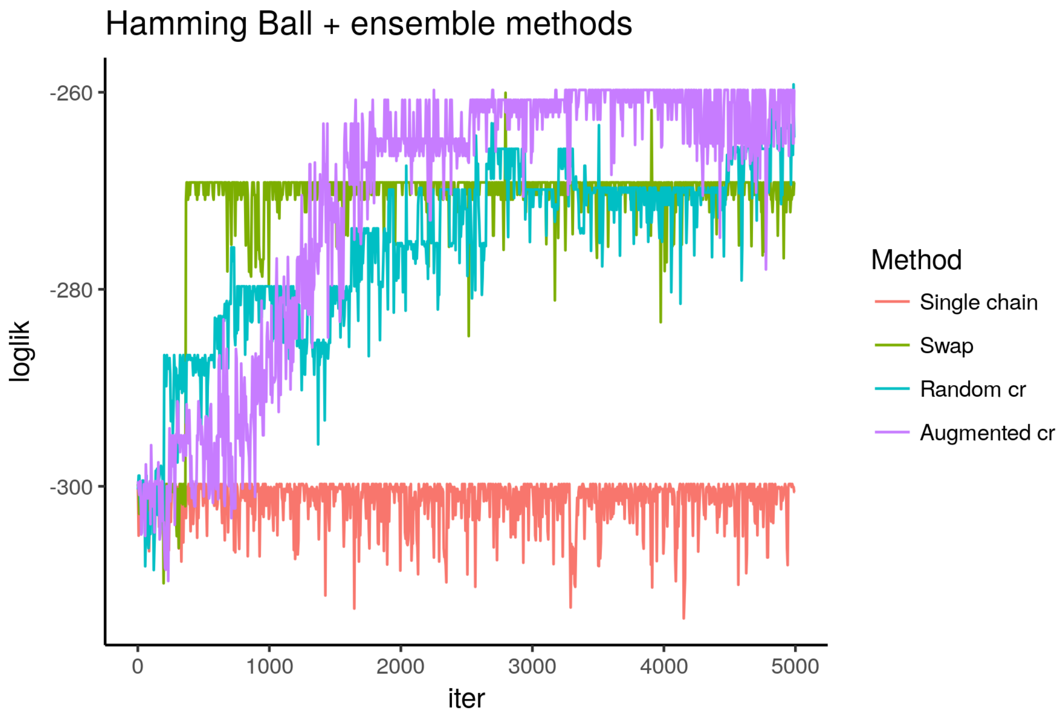

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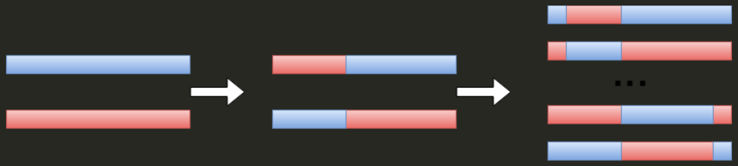
https://arxiv.org/abs/1703.08520



kaspar.martens@gmail.com

@kasparmartens