

Non-reversible samplers for mixture models

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Bayesian mixture models

$$Y_i \mid \boldsymbol{\theta}, \mathbf{w} \stackrel{\text{i.i.d.}}{\sim} \sum_{k=1}^K w_k f_{\theta_k}(\cdot) \quad i = 1, \dots, n$$

$$\theta_k \stackrel{\text{i.i.d.}}{\sim} p_{\theta}, \quad \mathbf{w} = (w_1, \dots, w_K) \sim p_{\mathbf{w}}.$$

f_{θ} = **parametric family**, K = **number of components** (finite or infinite)

¹Blei et al., 2004; Marin et al., 2005, McLachlan et al., 2019

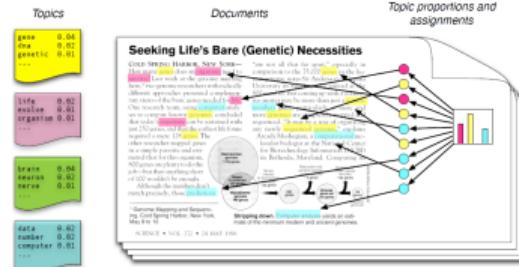
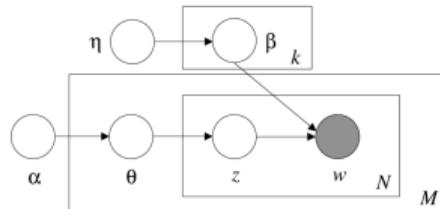
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- Very classical models. Applied in various fields in many variants¹
- Building block of larger probabilistic models (e.g. hierarchical, temporal, ...)
- Computationally challenging (i.e. algorithms slow for large $n!$)

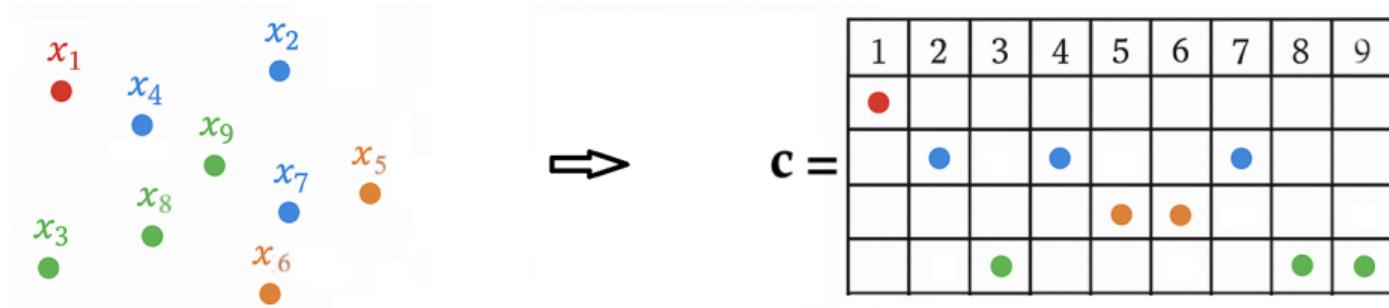


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Formulation with allocation variables

Introduce **allocation variables** $c = (c_1, \dots, c_n) \in [K]^n$. Assume K **fixed** for now!

$$Y_i \mid c, \theta, \mathbf{w} \stackrel{\text{i.i.d.}}{\sim} f_{\theta_{c_i}}(y), \quad c_i \mid \theta, \mathbf{w} \stackrel{\text{i.i.d.}}{\sim} \text{Mult}(\mathbf{w}), \quad \theta_k \stackrel{\text{i.i.d.}}{\sim} p_0, \quad \mathbf{w} \sim p_{\mathbf{w}}$$



Classical MCMC for (finite) mixture models

If $p_{\mathbf{w}} = \text{Dir}(\boldsymbol{\alpha})$, with $\boldsymbol{\alpha} = (\alpha, \dots, \alpha)$:

- **Conditional sampler:** updates $\mathbf{c} \sim \pi(\mathbf{c} | \boldsymbol{\theta}, \mathbf{w})$ and $(\boldsymbol{\theta}, \mathbf{w}) \sim \pi(\boldsymbol{\theta}, \mathbf{w} | \mathbf{c})$ with target

$$\pi(\mathbf{c}, \boldsymbol{\theta}, \mathbf{w}) \propto \prod_{k=1}^K w_k^{n_k(c) + \alpha - 1} \prod_{i: c_i = k} f_{\theta_k}(Y_i) p_{\theta}(\theta_k)$$

$$n_k(c) = \sum_{i=1}^n \mathbb{1}(c_i = k)$$

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- **Marginal sampler:** updates $c_i \sim \pi(c_i | c_{-i})$ for $i \in [n]$ with target

$$\pi(\mathbf{c}) \propto \prod_{k=1}^K \Gamma(\alpha + n_k(c)) \int_{\Theta} \prod_{i: c_i = k} f_{\theta_k}(Y_i) p_{\theta}(\theta_k) d\theta_k$$

Classical MCMC for (finite) mixture models

If $p_w = \text{Dir}(\alpha)$, with $\alpha = (\alpha, \dots, \alpha)$:

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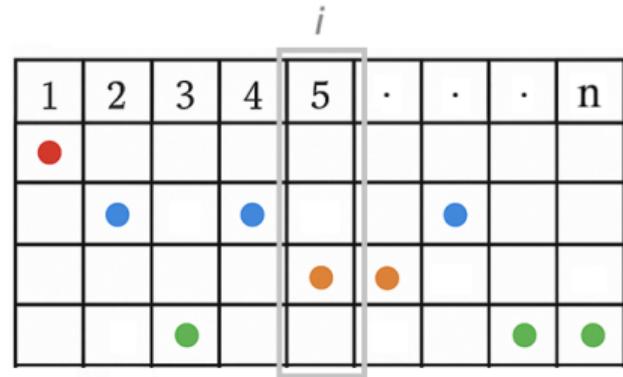
- Similarly happens with $K = \infty$ and p_w the GEM distribution \Rightarrow **Dirichlet process!**

Marginal (Gibbs) sampler

$\pi(c)$ -reversible Markov kernel P_{MG} on $[K]^n$

At each iteration:

1. Sample $i \sim \text{Unif}([n])$
2. Update $c_i \sim \pi(c_i \mid c_{-i})$

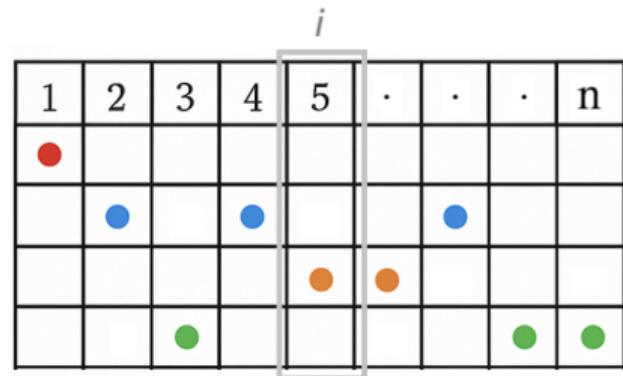


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- Arguably among the most popular MCMC schemes for mixture models.
- Simple to implement.
- $\mathcal{O}(K)$ cost per iteration.

How does it **scale** with n ?

Prior case: slow convergence

Consider the prior case: $f_\theta(y) = f(y)$ \Leftarrow limiting case of **weakly informative** data.

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Theorem (variation of Khare and Zou, 2009)

The L^2 -relaxation time of P_{MG} is

$$t_{\text{rel}} = \frac{n(n + K\alpha - 1)}{K\alpha} \approx n^2$$

- Related to Pólya urns and models in population genetics
- Implication: $\mathcal{O}(n^2)$ required for convergence
- Intuition: **random-walk behaviour** \Rightarrow see later!

Posterior case: slow convergence

Consider data generated as

$$Y_i \stackrel{\text{i.i.d.}}{\sim} 0.9N(y \mid 0.9, 1) + 0.1N(y \mid -0.9, 1), \quad i = 1, \dots, n = 2000$$

and consider $K = 2$ and $f_\theta(y) = N(y \mid \theta, 1)$ \Leftarrow “**easy**” problem.

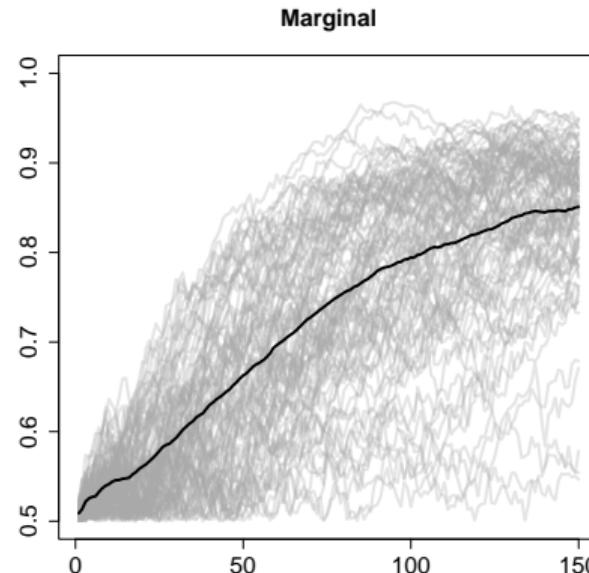
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- Traceplot of the **size of the largest cluster**.
- Initialized **uniformly at random**.
- Thinning of size $n = 2000$.
- We expect to be close to 0.9 **in stationarity**.



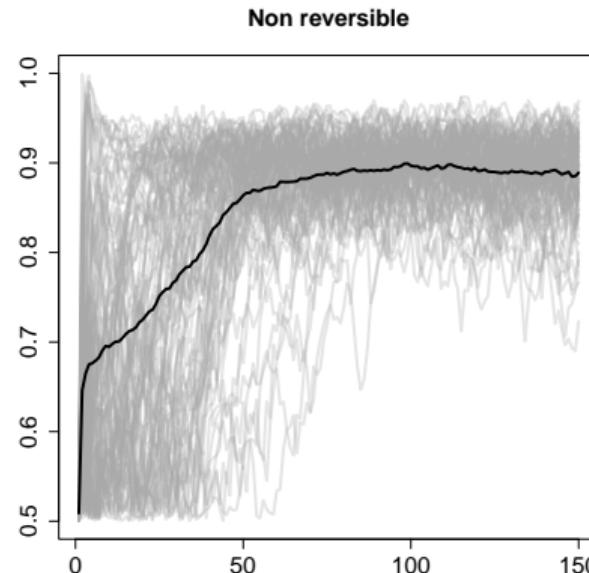
Posterior case: our proposal

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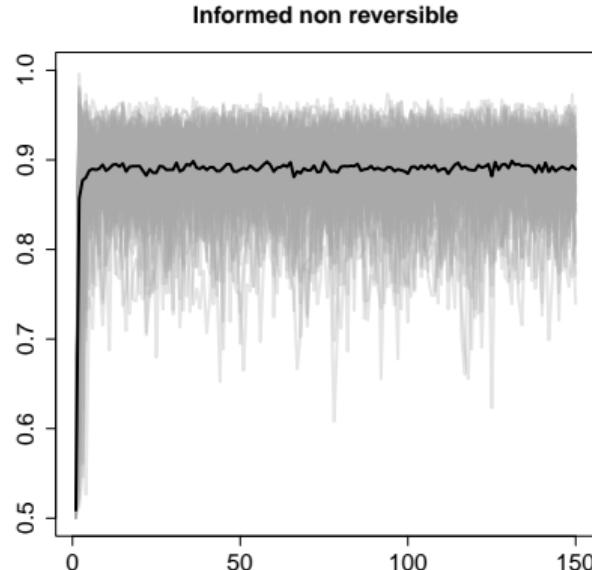
Posterior case: our proposal (advanced)

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- Traceplot of the **size of the largest cluster**.
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Goal of this talk

- The marginal sampler is **provably and empirically** slow under many scenarios of interest.
- Its issues **when n is large** have been known for a long time ².
- P_{MG} is arguably one of the most popular MCMC schemes for mixture models.

²Celeux et al. (2000)

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What's next?

- Understanding why P_{MG} is slow.
- Showing a **random-walk** behaviour of P_{MG} when n is large.
- Exploit recent literature on **non-reversible** sampler to devise a **simple and more efficient** MCMC scheme (scaling **linearly** with n in the prior case).

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A. F. and Zanella, G. (2026+) A fast non-reversible sampler for Bayesian finite mixture models.
Under review.

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Insight: scaling limit

$\{c^{(t)}\}_t$ Markov chain on $[K]^n$ with kernel P_{MG}

³Deinitializing Markov chain using the terminology of Roberts and Rosenthal (2001)

Insight: scaling limit

$\{c^{(t)}\}_t$ Markov chain on $[K]^n$ with kernel P_{MG}

Consider prior case: $f_\theta(y) = f(y)$. Define

$$X_{t,k}(c) = \frac{n_k(c^{(t)})}{n} = \frac{\text{multiplicity of component } k \text{ at iteration } t}{n}$$

By symmetry of $\pi(c)$ across $i \in [n]$, **convergence of $c^{(t)}$** fully determined³ by the Markov chain

$$\mathbf{X}_t = (X_{t,1}, \dots, X_{t,K}) \quad t = 0, 1, 2, \dots$$

³Deinitializing Markov chain using the terminology of Roberts and Rosenthal (2001)

Insight: scaling limit

Expected change **after one iteration**:

$$\begin{aligned}\mathbb{E}[X_{t+1,k} - x_k \mid \mathbf{X}_t = \mathbf{x}] &= \frac{1}{n} \left[(1 - x_k) \frac{\alpha + nx_k}{K\alpha + n - 1} - x_k \frac{K\alpha - \alpha + n(1 - x_k)}{K\alpha + n - 1} \right] \\ &= \frac{2}{n^2} \left[\frac{\alpha}{2} - K\alpha \frac{x_k}{2} + o(1) \right]\end{aligned}$$

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- We expect $\mathcal{O}(n^2)$ iterations are needed for $\mathcal{O}(1)$ distance.
- Intuition: **the two probabilities cancel!**
- This can be made more rigorous.

Insight: scaling limit

Let $Z_t^{(n)} = X_{\lceil n^2 t \rceil}$ \Leftarrow time **acceleration** by $\mathcal{O}(n^2)$.

Insight: scaling limit

Let $\boxed{\mathbf{Z}_t^{(n)} = \mathbf{X}_{\lceil n^2 t \rceil}}$ \Leftarrow time **acceleration** by $\mathcal{O}(n^2)$.

Theorem

$\{\mathbf{Z}_t^{(n)}\}_{t \in \mathbb{R}_+} \rightarrow \{\mathbf{Z}_t\}_{t \in \mathbb{R}_+}$ weakly as $n \rightarrow \infty$, where $\{\mathbf{Z}_t\}_{t \in \mathbb{R}_+}$ is a diffusion process with generator

$$Lg(\mathbf{x}) = \sum_{k=1}^K \alpha(1 - Kx_k) \frac{\partial}{\partial x_k} g(\mathbf{x}) + \sum_{k,k'=1}^K x_k (\delta_{kk'} - x_{k'}) \frac{\partial^2}{\partial x_k \partial x_{k'}} g(\mathbf{x}),$$

- Wright-Fisher process = **diffusion** on the unit simplex
- **Diffusive** behaviour **at the level of cluster sizes**.

Insight: scaling limit

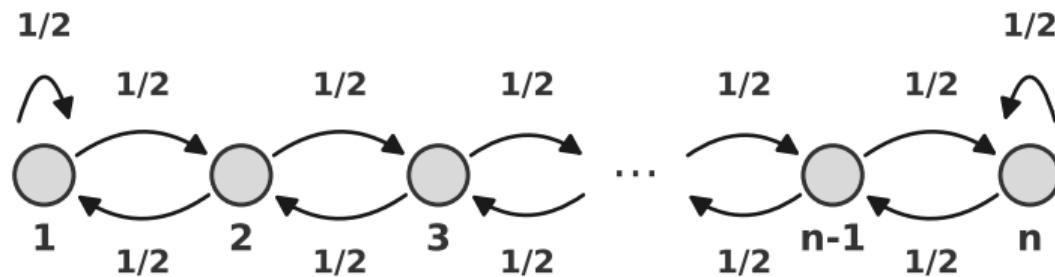
Main reason underlying **diffusive behaviour**:

$$\mathbb{P} \left(X_{t+1,k} - x_k = +\frac{1}{n} \mid \mathbf{X}_t = \mathbf{x} \right) \approx x_k(1 - x_k) \approx \mathbb{P} \left(X_{t+1,k} - x_k = -\frac{1}{n} \mid \mathbf{X}_t = \mathbf{x} \right).$$

- Almost **equally likely** to move along the two directions.
- The chain moves back and forth a lot!
- Reasonable that this happens also **a posteriori** (in weakly informative cases).
- How to solve this?

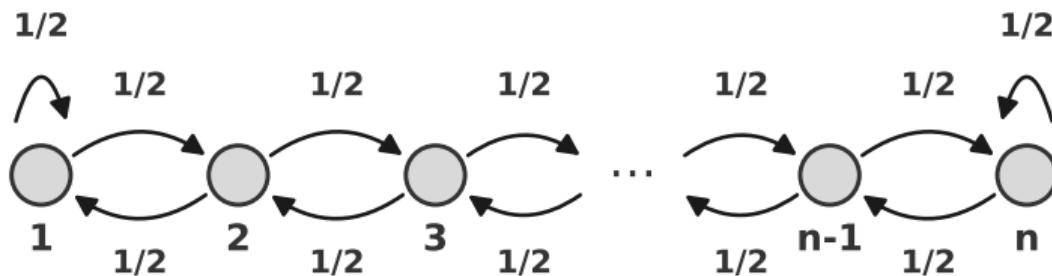
A simple example: problem

Chain in [Diaconis et al. \(2000\)](#).



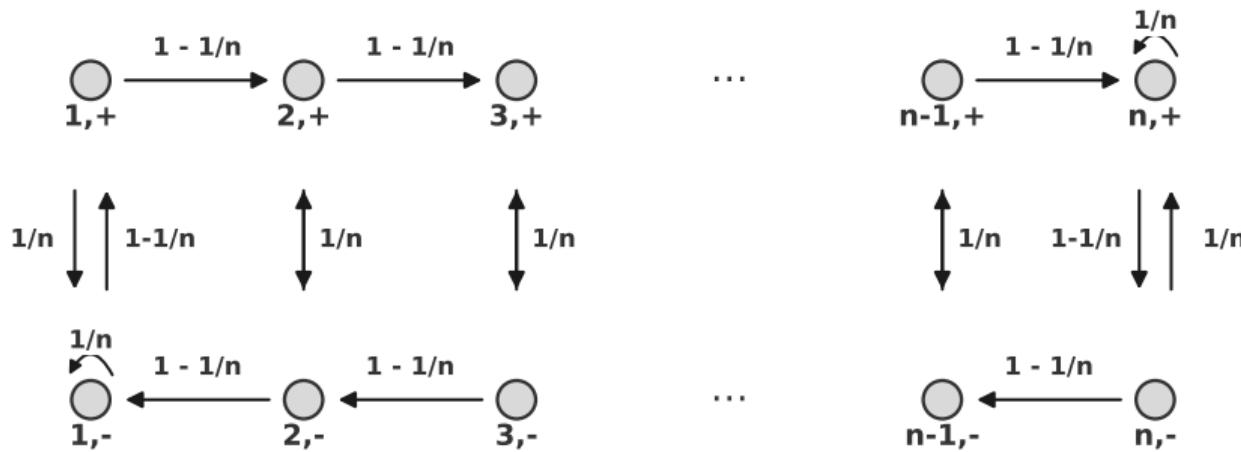
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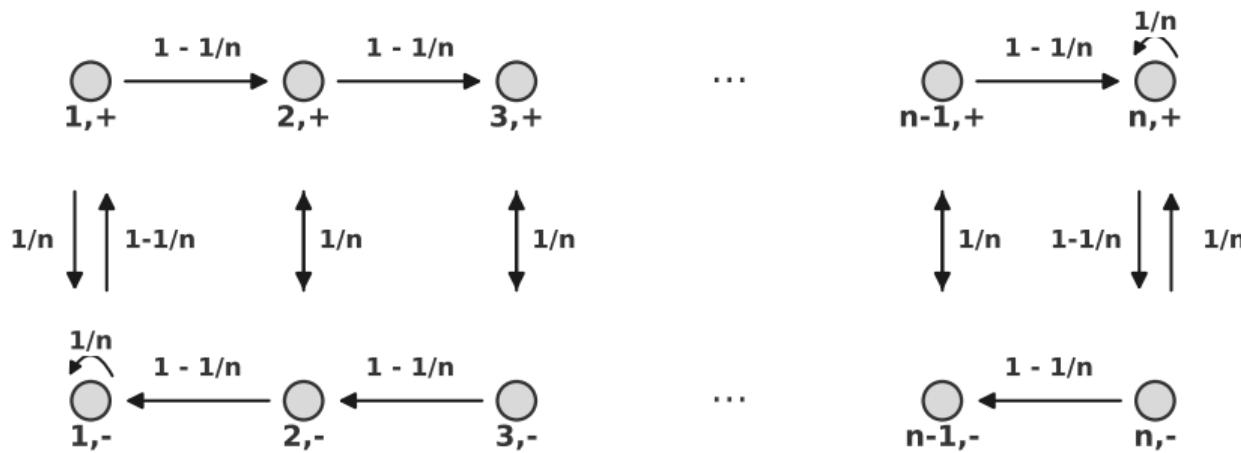


- Reversible chain with n **states**.
- $\mathcal{O}(n^2)$ iterations are needed to converge \Rightarrow similar to our case!

A simple example: solution



A simple example: solution



- Non-reversible (**lifted**) chain \Rightarrow we add a **direction**!
- $\mathcal{O}(n)$ iterations are needed to converge \Rightarrow fast!

Non-reversible sampler (informal)

Extended target: $\tilde{\pi}(c, v) = \pi(c) \left(\frac{1}{2}\right)^{K(K-1)/2}$ $c \in [K]^n$, $v = (v_{k,k'})_{k < k'} \in \{-1, +1\}^{K(K-1)/2}$

$v_{k,k'} =$ **direction across clusters k and k'**

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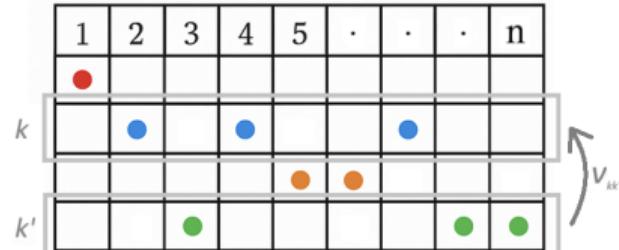
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$v_{k,k'} = \text{direction across clusters } k \text{ and } k'$

$\tilde{\pi}(c, v)$ -invariant **Markov kernel** P_{NR} :

1. Sample a pair of clusters $(k, k') \in [K]^2$.
2. Propose to **move a single observation according to** $v_{kk'}$.
3. Accept with usual Metropolis-Hastings ratio.
4. If rejected, **flip** $v_{kk'}$.



Non-reversible sampler

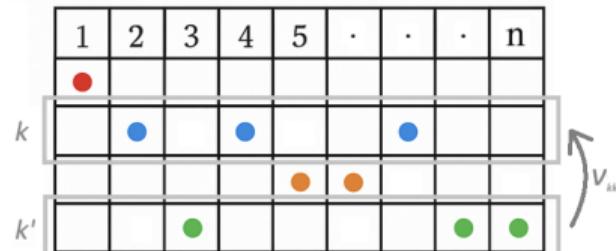
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$\tilde{\pi}(c, v)$ -invariant **Markov kernel** P_{NR} :

1. Sample $(k, k') \in [K]^2$ with probability $\frac{n_k(c) + n_{k'}(c)}{2(K-1)n} \mathbb{1}(k < k')$
2. Set $(k_-, k_+) = (k, k') \mathbb{1}(v_{k,k'} = +1) + (k', k) \mathbb{1}(v_{k,k'} = -1)$
3. Sample $i \sim \text{Unif}(\{i' : c_{i'} = k_-\})$ and set $c_i = k_+$ with prob.

$$\min \left\{ 1, \left(\frac{n_{k_-}(c)}{n_{k_+}(c) + 1} \right) \frac{\pi(c_i = k_+ | c_{-i})}{\pi(c_i = k_- | c_{-i})} \right\}.$$



If reject, flip $v_{kk'}$

Remarks

- P_{NR} is a **mixture of lifted kernels** with selection⁴ probabilities p_c :

$$P_{\text{NR}}(c, c') = \sum_{k < k'} p_c(k, k') P_{kk'}^{(\text{lift})}(c, c')$$

where $P_{kk'}^{(\text{lift})}$ is the MH-lift with **direction** $v_{kk'}$.

~ \rightsquigarrow **multiple velocity** components $(v_{kk'})_{k < k'}$. At each rejection, flip only one of them.

⁴Here $p_c(k, k') = \frac{n_k(c) + n_{k'}(c)}{2(K-1)n}$

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~~ **multiple velocity** components $(v_{kk'})_{k < k'}$. At each rejection, flip only one of them.

- For mixture models, **acceptance probability** becomes

$$\frac{n_{k_-}(c)}{n_{k_+}(c) + 1} \frac{\pi(c_i = k_+ \mid c_{-i})}{\pi(c_i = k_- \mid c_{-i})} = \underbrace{\frac{p(Y_i \mid Y_{-i}, c_{-i}, c_i = k_+)}{p(Y_i \mid Y_{-i}, c_{-i}, c_i = k_-)}}_{\text{likelihood ratio}} (1 + O(n^{-1}))$$

~~ proposal **matches the prior** to favour **long excursions!**

⁴Here $p_c(k, k') = \frac{n_k(c) + n_{k'}(c)}{2(K-1)n}$

Scaling limit

Again prior case $f_\theta(y) = f(y)$

$\mathbf{Z}_t^{(n)} = (\mathbf{X}_{\lceil nt \rceil}, \mathbf{V}_{\lceil nt \rceil}) \Leftarrow \text{time acceleration by } \mathcal{O}(n)$

Theorem

$\{\mathbf{Z}_t^{(n)}\}_{t \in \mathbb{R}_+} \rightarrow \{\mathbf{Z}_t\}_{t \in \mathbb{R}_+}$ weakly as $n \rightarrow \infty$, where $\{\mathbf{Z}_t\}_{t \in \mathbb{R}_+}$ is an (ergodic) piecewise deterministic Markov process

- **No diffusive** behaviour
- P_{NR} gives $\mathcal{O}(n)$ **speedup** relative to P_{MG} in prior case!

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What about more general π ?

Asymptotic variance comparisons

$$\text{Var}(g, P) := \lim_{T \rightarrow \infty} \text{Var} \left(\frac{1}{\sqrt{T}} \sum_{t=1}^T g(X_t) \right) \quad \text{for } X_0 \sim \pi, X_{t+1}|X_t \sim P(X_t, \cdot)$$

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Theorem

For every π on $[K]^n$ and $g : [K]^n \rightarrow \mathbb{R}$ we have

$$\text{Var}(g, P_{\text{NR}}) \leq 2(K-1) \text{Var}(g, P_{\text{MG}}) + (2K-3) \text{Var}_{\pi}(g)$$

and $\boxed{\text{Var}(g, P_{\text{MG}}) \leq \text{Var}(g, P_{\text{CD}})}$

P_{MG} = marginal sampler; P_{NR} = non-reversible sampler; P_{CD} = conditional sampler

Asymptotic variance comparisons

Theorem (Approximately)

For every π on $[K]^n$ and $g : [K]^n \rightarrow \mathbb{R}$ we have

$$\text{Var}(g, P_{\text{NR}}) \leq 2(K - 1) \text{Var}(g, P_{\text{MG}})$$

- $\text{Cost}(P_{\text{MG}}) = \mathcal{O}(K)$ and $\text{Cost}(P_{\text{NR}}) = \mathcal{O}(1) \rightsquigarrow \text{little to loose}$ by using P_{NR} instead of P_{MG} (typical feature of lifted schemes)

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- The conditional sampler is always **less efficient** than the marginal one.
- Do we gain much when targeting mixture model posteriors?

Bayesian discrete posteriors: does lifting help?

- Data often makes Bayesian posteriors with discrete parameters⁵ **sharply concentrated** and non-smooth
 - ~~ large ‘discrete gradients’ speed-up reversible samplers⁶ while reducing excursion lengths for lifted MCMC⁷

⁵e.g. variable selection, stochastic block model, graphical models

⁶Yang et al., 2016; Zhou et al., 2022; Zhou and Chang, 2023, ...

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 - ~~ large ‘discrete gradients’ speed-up reversible samplers⁶ while reducing excursion lengths for lifted MCMC⁷
- By contrast, mixture models have statistical features that are well-suited to lifted samplers, e.g.:
 1. **Lack of posterior concentration**
 2. **Flatness in the tails**
 3. **Overfitted regimes**

⁵e.g. variable selection, stochastic block model, graphical models

⁶Yang et al., 2016; Zhou et al., 2022; Zhou and Chang, 2023, ...

⁷different from, e.g., successful applications of lifting to Statistical Physics models

Posterior case: statistical features of mixture model

1. **Lack of posterior concentration for c :** for data (Y_1, \dots, Y_n) generated from mixture with true parameters (θ^*, \mathbf{w}^*) :⁸

$$\pi(\theta, \mathbf{w}) \rightarrow \delta_{(\theta^*, \mathbf{w}^*)} \quad \text{as } n \rightarrow \infty$$

$$\pi(c) \not\rightarrow \delta_{c^*} \quad \text{nor} \quad \pi(c_i) \not\rightarrow \delta_{c_i^*} \quad \text{as } n \rightarrow \infty$$

Intuition: only one observation per ‘parameter’ c_i

Contrast with Bayesian variable selection, stochastic block model, graphical models, where concentration in discrete model space occurs.

⁸with convergence to $\delta_{(\theta^*, \mathbf{w}^*)}$ in an appropriate sense, see e.g. Nguyen (2013); Guha et al. (2021)

Posterior case: statistical features of mixture model

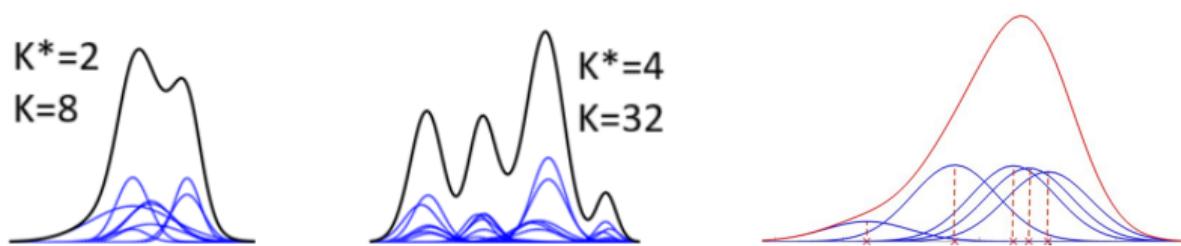
1. **Lack of posterior concentration**
2. **Flatness in the tails:** for random $c \sim \text{Unif}([K]^n)$

$$\frac{n_k(c)}{n_{k'}(c) + 1} \frac{\pi(c_i = k' \mid c_{-i})}{\pi(c_i = k \mid c_{-i})} = 1 + O(n^{-1/2})$$

~~ vanishing ‘discrete gradients’ in tails

Posterior case: statistical features of mixture model

1. Lack of posterior concentration
2. Flatness in the tails
3. Overfitted or misspecified regimes: mixture models often used in overfitted (i.e. K^* 'true' components with $K^* < K$; left figure) and misspecified (right figure) regimes



↔ weakly identifiable and strongly overlapping clusters with

$$\frac{p(Y_i | Y_{-i}, c_{-i}, c_i = k_+)}{p(Y_i | Y_{-i}, c_{-i}, c_i = k_-)} \approx 1$$

Numerics: set-up

- **Parametric family:** 1d Gaussian mixture model

$$f_\theta(y) = N(y \mid \theta, 1), \quad p_0(\theta) = N(\theta \mid 0, 1)$$

- **Data:** generate $n = 1000$ data points from mixture with K^* components. Fit mixture with K components

Numerics: set-up

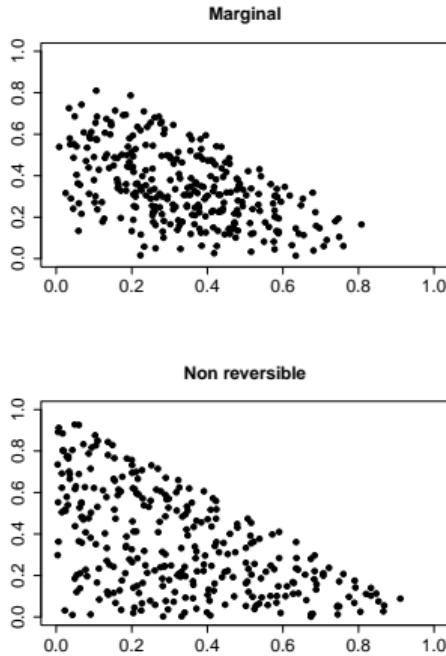
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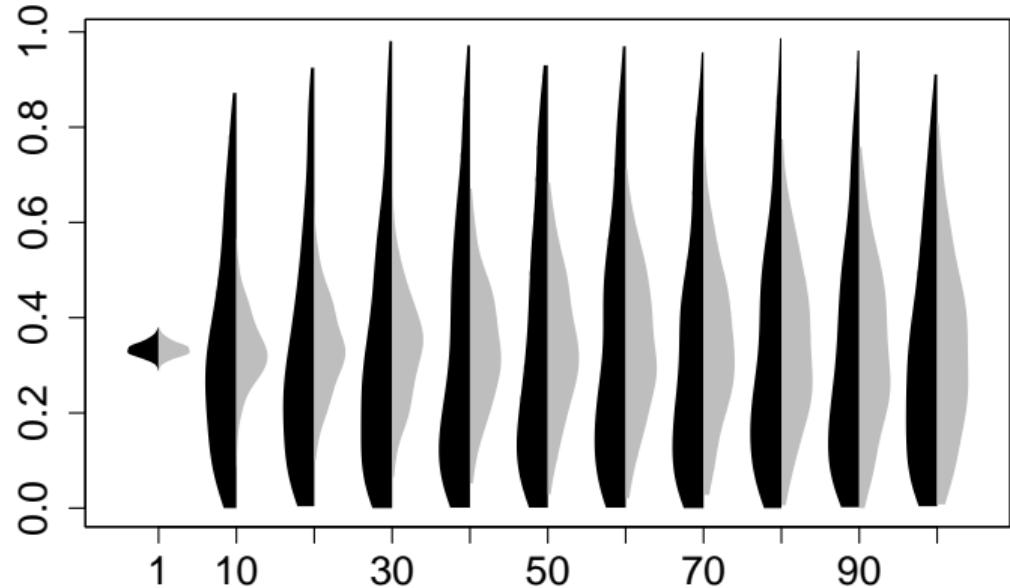
- **Data:** generate $n = 1000$ data points from mixture with K^* components. Fit mixture with K components
- Compare P_{MG} and P_{NR} through **prior-posterior check**:
 - Generate random datasets Y from the model distribution $p(Y)$
 - Sample from posterior $\pi(c) := p(c \mid Y)$ with MCMC
 - If chains reach convergence we **should recover the prior distribution** $p(c)$

First case: $K = K^* = 3, \alpha = 1$

Left: **final proportions** of the first two components after $100 \times n$ iterations \Rightarrow Dirichlet(1, 1, 1)
Right: **evolution over time** with thinning of size n . Gray = P_{MG} , Black = P_{NR}

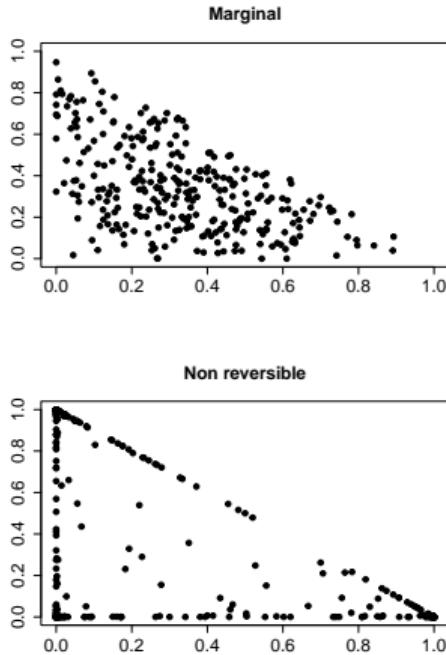


Marginal distribution of the chains

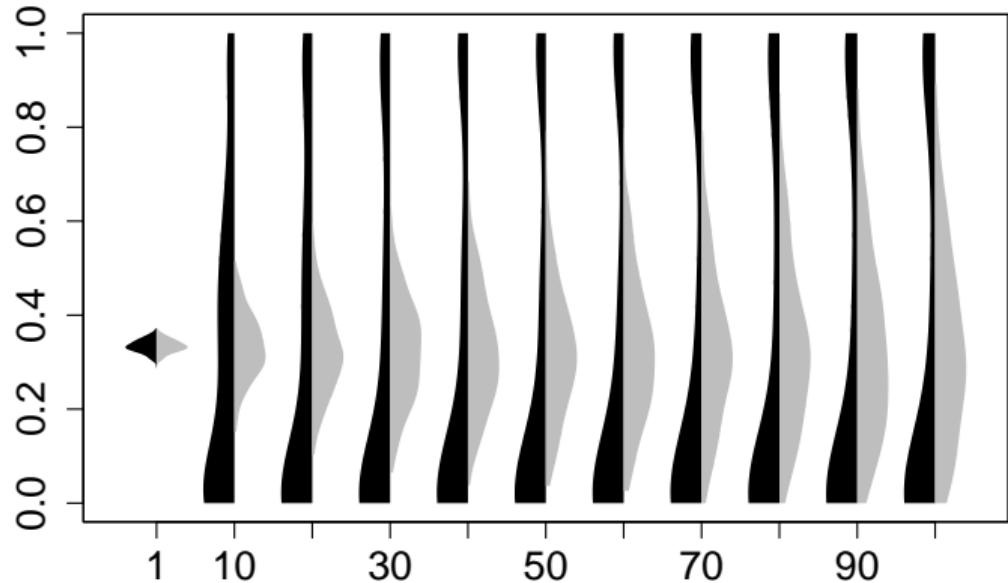


Second case: $K = K^* = 3, \alpha = 0.1$

Left: **final proportions** of the first two components after $100 \times n$ iterations \Rightarrow Dirichlet(0.1, 0.1, 0.1)
Right: **evolution over time** with thinning of size n . Gray = P_{MG} , **Black** = P_{NR}



Marginal distribution of the chains



Dirichlet process mixtures

$$Y_i \mid P \stackrel{\text{i.i.d.}}{\sim} Pf_{\theta}(\cdot) \quad i = 1, \dots, n \quad P \sim \text{DP}(\alpha, P_0).$$

$\text{DP}(\alpha, P_0)$ = **Dirichlet process**, α = **concentration** parameter, P_0 = **baseline** distribution.

⁹Ruggiero and Walker (2009)

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Similar situation as before!

- The marginal sampler is even **more popular** (and often slow to converge).
- The prior case still admits a **scaling limit** with $\mathcal{O}(n^2)$ scaling factor⁹.
- Wright-Fisher process → **Fleming-Viot process**.

⁹Ruggiero and Walker (2009)

Dirichlet process mixtures

The **non-reversible sampler** works as before! At each iteration:

1. Select a pair of clusters $(k, k') \leftarrow$ allowing to select a **new** one.
2. Propose a move **according to the direction** $v_{k,k'}.$
3. If rejected, flip $v_{k,k'}.$

Dirichlet process mixtures

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Not discussed in this talk:

- Adjusting the non-reversible sampler to the **space of partitions** is not trivial!
- We need to allow **creation** and **elimination** of clusters.
- The selection probabilities must be chosen to preserve ergodicity.

Numerics: set-up

- **Parametric family:** 1d Gaussian mixture model

$$f_\theta(y) = N(y \mid \theta, 1), \quad P_0(\theta) = N(\theta \mid 0, 1)$$

- **Data:** generate $n = 1000$ data points from the associated Dirichlet Process Mixture model.

Numerics: set-up

- **Parametric family:** 1d Gaussian mixture model

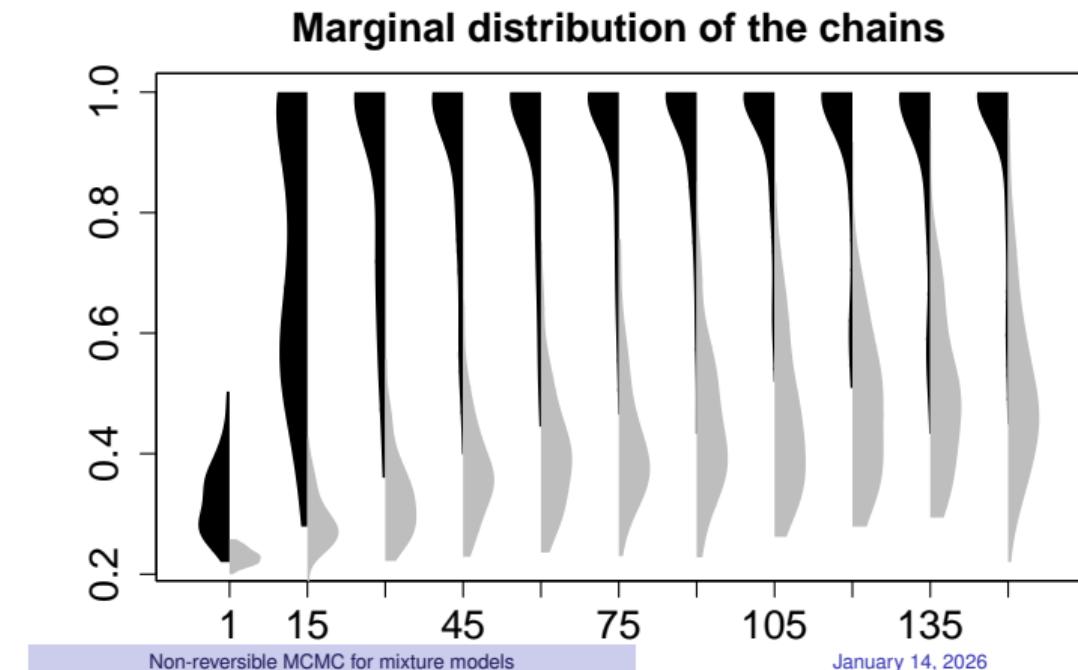
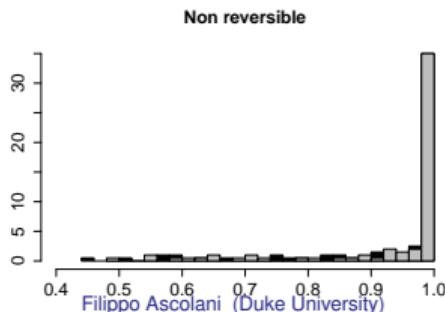
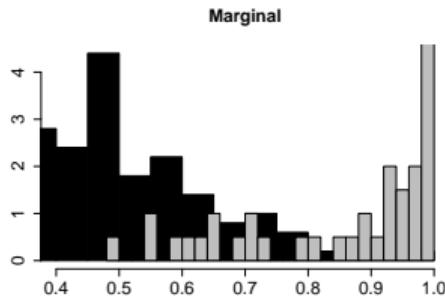
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 - Sample from posterior $\pi(c) := p(c \mid Y)$ with MCMC
 - If chains reach convergence we **should recover the prior distribution**.
 - We focus on the distribution of the **largest cluster**.

Dirichlet process mixtures with $\alpha = 0.1$

Left: histogram of the **proportion of the largest cluster** after $100 \times n$ iterations, compared with the prior distribution.

Right: **evolution over time** with thinning of size n . Gray = P_{MG} , **Black** = P_{NR}



Practical takeaways

When should lifting help for mixture model samplers?

- Components **not well-separated**
- During **convergence phase**
- **Overfitted case** with $K > K^*$

Practical takeaways

When should lifting help for mixture model samplers?

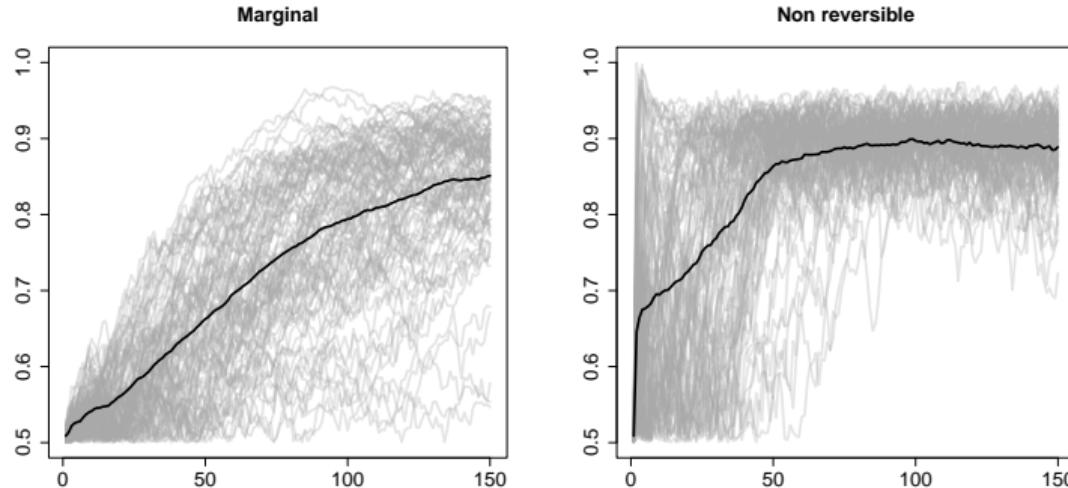
- Components **not well-separated**
- During **convergence phase**
- **Overfitted case** with $K > K^*$

Expect less improvement when

- Components are well-separated, $K = K^*$ and closer to convergence

Limitations (of methodology)

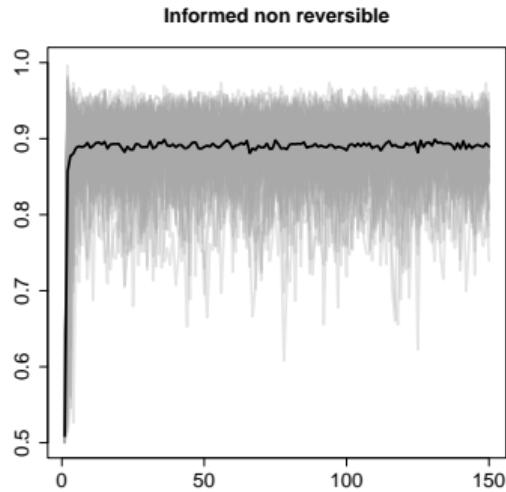
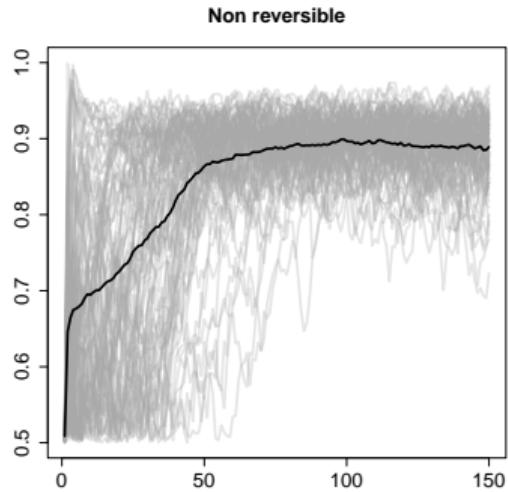
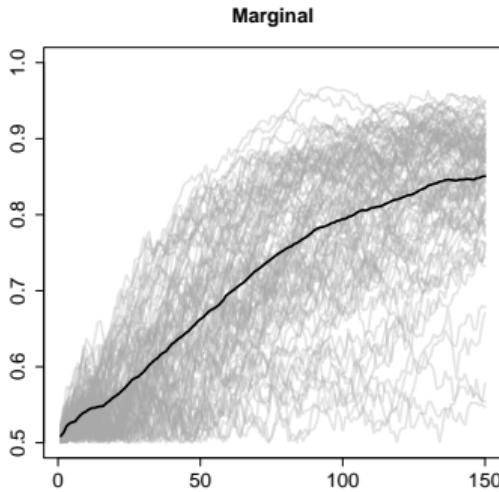
- For lifting to work well, **need to engineer directions with acceptance ≈ 1**
~~ not easy to do in general!
- Example: if $K = K^* = 2$ and components well-separated obtain



Can we improve?

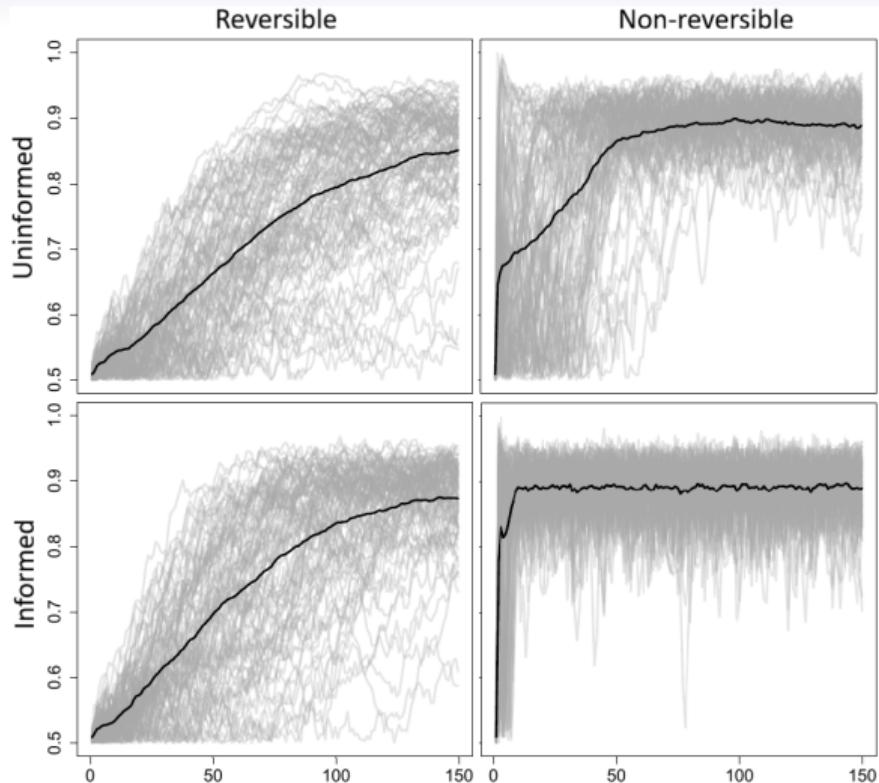
Informed versions

- Combining lifting with **informed proposals**¹⁰ leads to MH acceptance ≈ 1
~~ allows to preserve momentum!

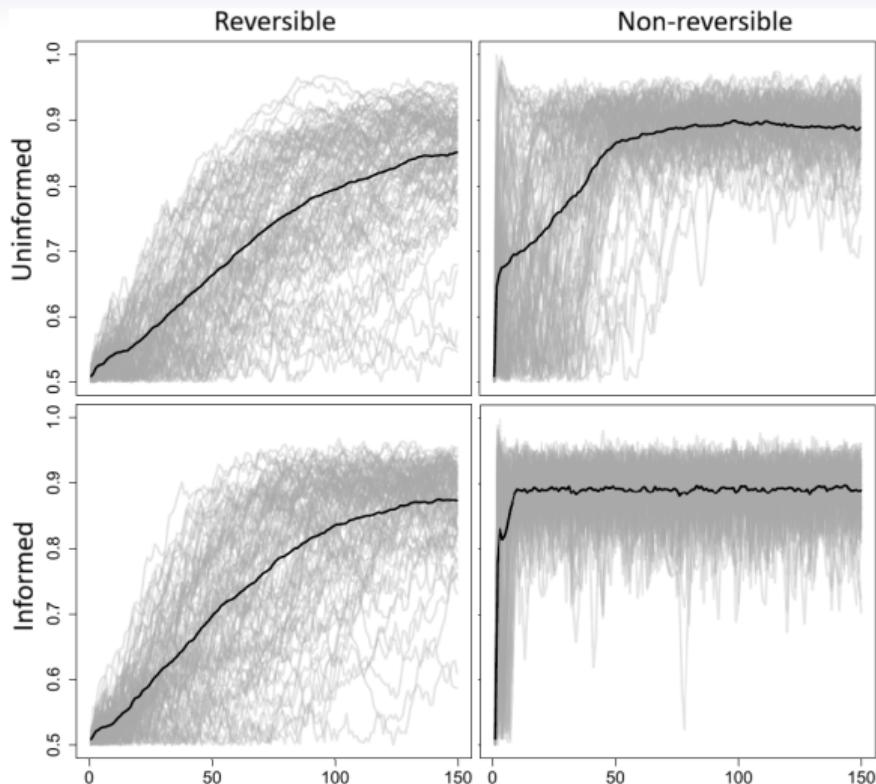


¹⁰Zanella (2020), Power and Goldman (2019), Gagnon and Maire (2024)

NB: here informed version only needed to increase acceptance and preserve momentum!



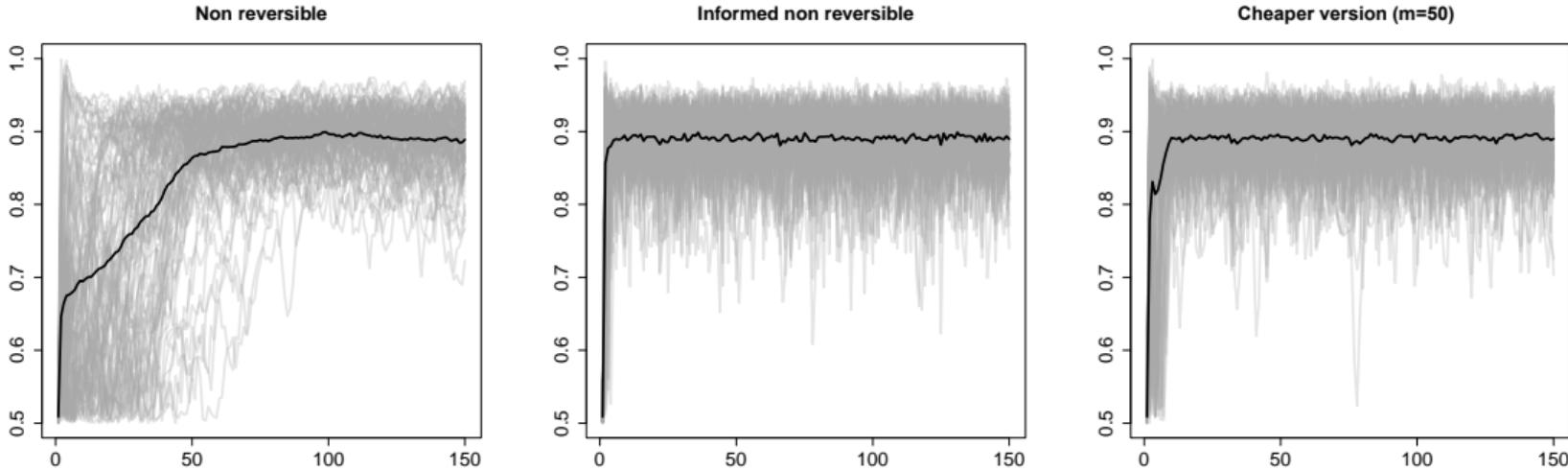
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Issue: in general $O(n)$ cost per iteration. Can we do something cheaper?

Cheaper informed versions

- Sample **random neighborhood** of size m and use informed proposal therein¹¹
- Moderate m (e.g. $m = 50$ with $n = 2000$) can be enough to make $\alpha \approx 1 \rightsquigarrow$ favourable trade-off



¹¹similar to random neighborhood approach of Liang et al (2022) or informed multiple-try of Gagnon et al (2023)

Limitations (of theory)

We have

- **non-deterioration results** for any target
- **$O(n)$ speedup** in prior case

We miss

- **quantify speedup in posterior case?**

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Current approach: scaling limits with data

\rightsquigarrow no exchangeability across $i \in [n]$ \rightsquigarrow **measure-valued diffusion limit**

Conclusions

Summary:

- Standard reversible algorithms for mixture models can be **slow**
- We introduce a **non-reversible version** (simple to implement, **no extra cost**)
- Theoretically: **never slower, $O(n)$ speed-up in prior case**
- Empirically: **large speed-ups in posterior case**

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Many open problems:

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- **More robust approaches** to preserve momentum in general discrete spaces?
- Comparison with **Split-and-Merge** schemes?

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Thanks for listening!