Probabilistic Graphical Models

Brown University CSCI 2950-P, Spring 2013

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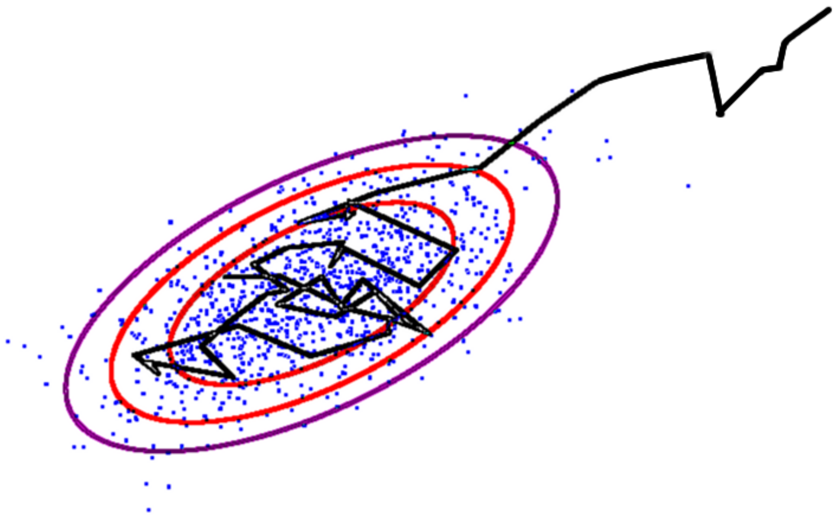
Lecture 17:
Collapsed Gibbs Samplers, MCMC Mixing and Diagnostics

Some slides and figures courtesy Iain Murray's tutorial,
Markov Chain Monte Carlo, MLSS 2009

Review: MCMC Methods

Construct a biased random walk that explores a target dist.



Markov steps, $x^{(s)} \sim T\big(x^{(s)} \leftarrow x^{(s-1)}\big)$

MCMC gives approximate,
correlated samples

$$\mathbb{E}_P[f] \approx \frac{1}{S}\sum_{s=1}^{S} f(x^{(s)})$$

Example transitions:

Metropolis–Hastings: $T(x' \leftarrow x) = Q(x'; x)\, \min\left(1,\ \frac{P(x')\, Q(x; x')}{P(x)\, Q(x'; x)}\right)$

Gibbs sampling: $T_i(\mathbf{x}' \leftarrow \mathbf{x}) = P(x_i' \,|\, \mathbf{x}_{j\neq i})\, \delta(\mathbf{x}'_{j\neq i} - \mathbf{x}_{j\neq i})$

Combining MCMC Transition Proposals

A sequence of operators, each with $P^\star$ invariant:

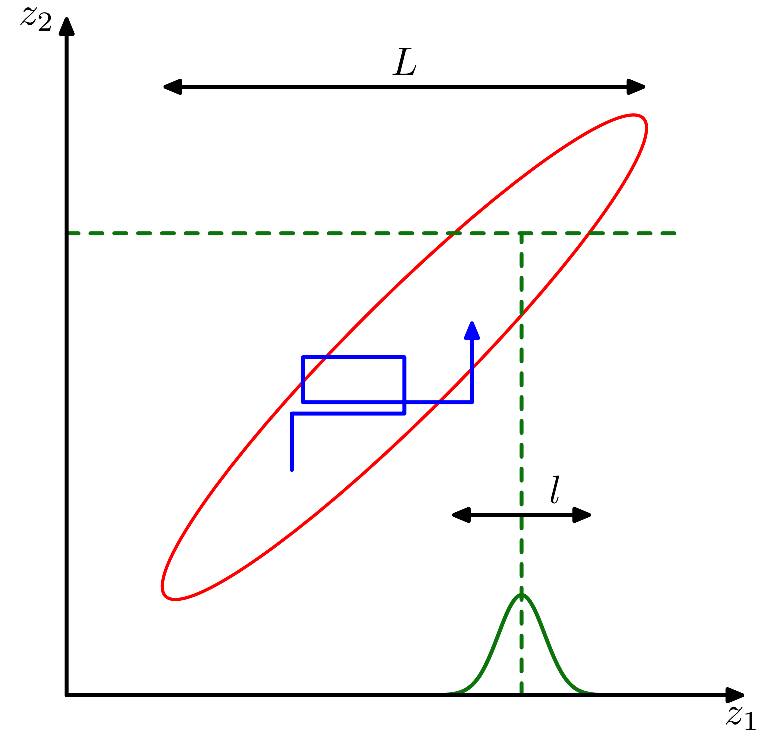
$$
\begin{aligned}
&x_0 \sim P^\star(x) \\
&x_1 \sim T_a(x_1 \leftarrow x_0) && P(x_1) = \textstyle\sum_{x_0} T_a(x_1 \leftarrow x_0) P^\star(x_0) = P^\star(x_1) \\
&x_2 \sim T_b(x_2 \leftarrow x_1) && P(x_2) = \textstyle\sum_{x_1} T_b(x_2 \leftarrow x_1) P^\star(x_1) = P^\star(x_2) \\
&x_3 \sim T_c(x_3 \leftarrow x_2) && P(x_3) = \textstyle\sum_{x_1} T_c(x_3 \leftarrow x_2) P^\star(x_2) = P^\star(x_3) \\
&\quad \cdots && \cdots
\end{aligned}
$$

— Combination $T_c T_b T_a$ leaves $P^\star$ invariant

— If they can reach any x, $T_c T_b T_a$ is a valid MCMC operator

— Individually T_c, T_b and T_a need not be ergodic

Gibbs Samplers



A method with no rejections:

– Initialize $\mathbf{x}$ to some value

– Pick each variable in turn or randomly and resample $P(x_i|\mathbf{x}_{j\neq i})$

At equilibrium can assume $\mathbf{x} \sim P(\mathbf{x})$

Figure from PRML, Bishop (2006)

Consistent with $\mathbf{x}_{j\neq i} \sim P(\mathbf{x}_{j\neq i}), \quad x_i \sim P(x_i\,|\,\mathbf{x}_{j\neq i})$

Proof of validity: **a)** check detailed balance for component update.
b) Metropolis–Hastings 'proposals' $P(x_i|\mathbf{x}_{j\neq i}) \Rightarrow$ accept with prob. 1
Apply a series of these operators. Don't need to check acceptance.

Gibbs Sampling Implementation

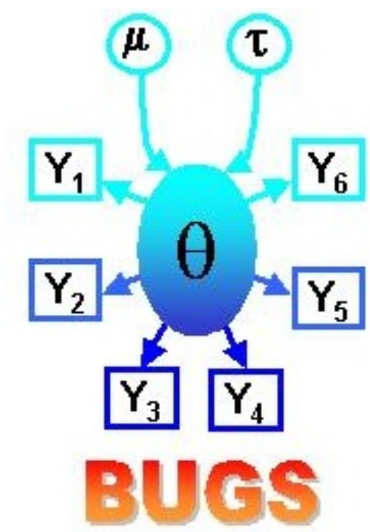
Gibbs sampling benefits from few free choices and convenient features of conditional distributions:

- Conditionals with a few discrete settings can be explicitly normalized:

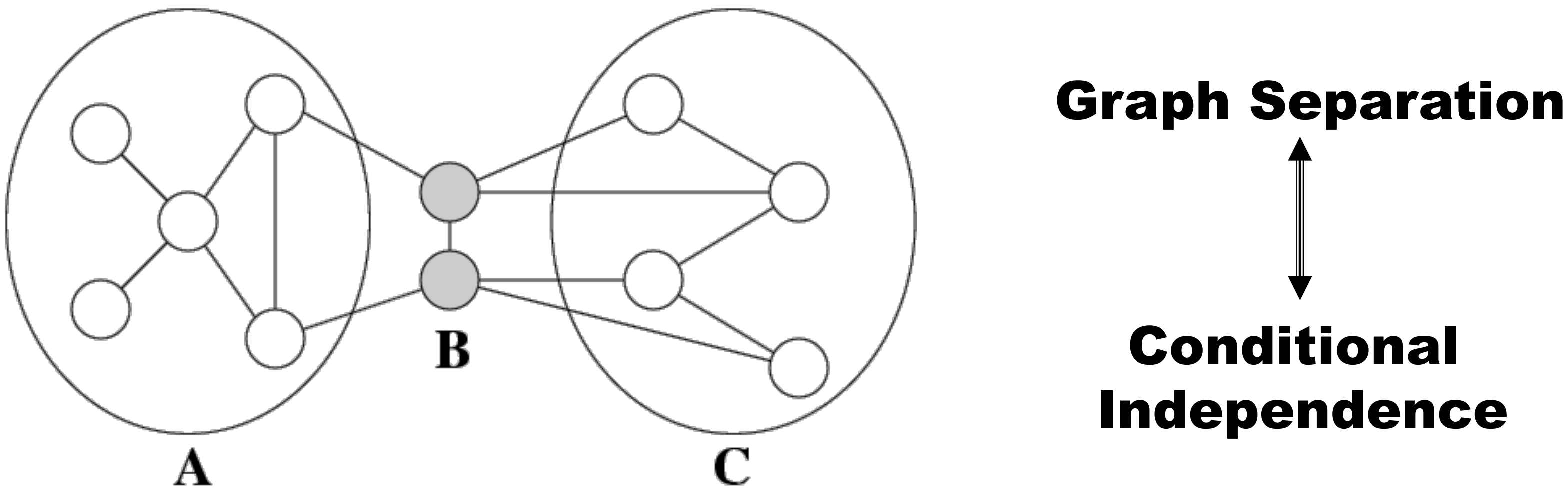
$$P(x_i|\mathbf{x}_{j\neq i}) \propto P(x_i, \mathbf{x}_{j\neq i})$$
$$= \frac{P(x_i, \mathbf{x}_{j\neq i})}{\sum_{x_i'} P(x_i', \mathbf{x}_{j\neq i})} \leftarrow \text{this sum is small and easy}$$

- Continuous conditionals only univariate
  $\Rightarrow$ amenable to standard sampling methods.

  - Inverse CDF sampling
  - Rejection sampling
  - Slice sampling
  - …



Undirected Graphical Models



$$p(x_A, x_C \mid x_B) = p(x_A \mid x_B) p(x_C \mid x_B)$$

- This global Markov property implies a local Markov property:

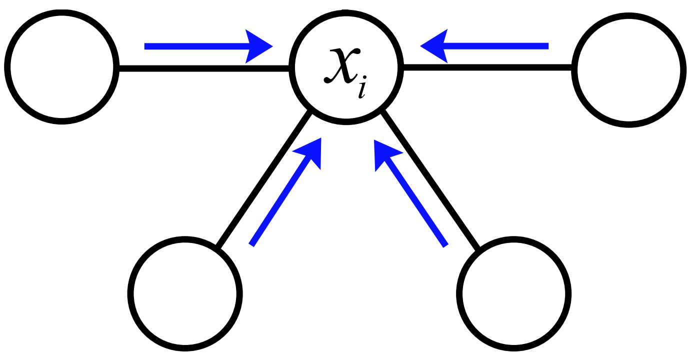
$$p\left(x_i \mid x_{\mathcal{V} \setminus i}\right) = p\left(x_i \mid x_{\Gamma(i)}\right)$$

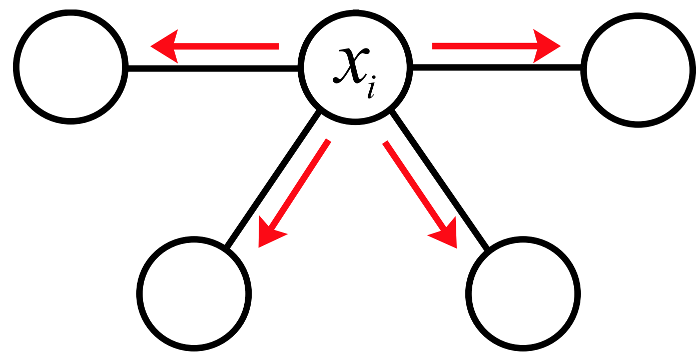
- Practical benefits of Gibbs sampling algorithm:
  - ➢ Model and algorithm have same modular structure
  - ➢ Conditionals can often be evaluated quickly, because they depend only on the neighboring nodes
  - ➢ Exponential families offer further efficiency improvements, by caching and recursively updating sufficient statistics

Gibbs Sampling as Message Passing

- Consider a pairwise undirected graphical model:

$$p(x) = \frac{1}{Z} \prod_{(s,t) \in \mathcal{E}} \psi_{st}(x_s, x_t) \prod_{s \in \mathcal{V}} \psi_s(x_s)$$





$$q_i(x_i) \propto \psi_i(x_i) \prod_{j \in \Gamma(i)} m_{ji}(x_i)$$

$$m_{ij}(x_j) \propto \psi_{ij}(\hat{x}_i, x_j)$$

$$\hat{x}_i \sim q_i(x_i)$$

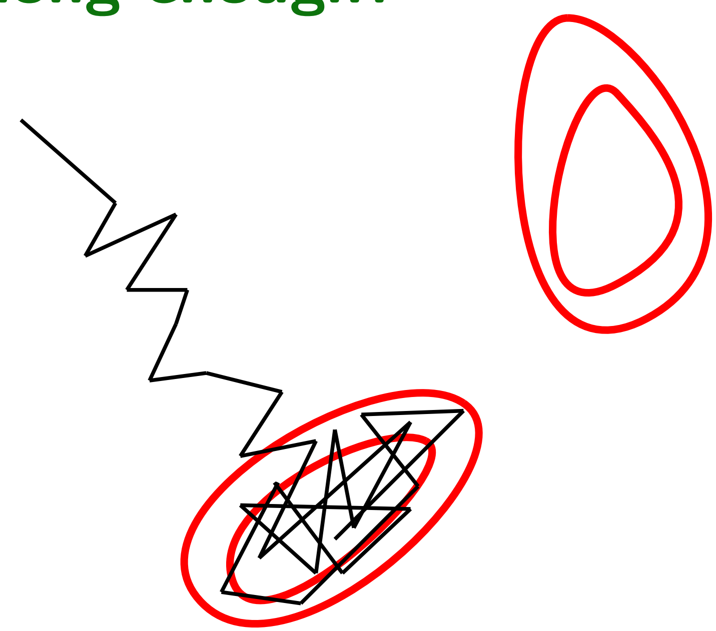
Draw single sample from marginal

Use sample to extract a "slice" of pairwise potential

- Valid for discrete and continuous variables, although sampling step may be harder for continuous models
- General factor graphs have similar form

MCMC Implementation & Application

- The samples aren't independent. Should we **thin**, only keep every Kth sample?
- Arbitrary initialization means starting iterations are bad. Should we discard a **"burn-in" period**?
- Maybe we should perform **multiple runs?**
- How do we know if we have run for **long enough?**



Estimating Moments from Samples

Approximately independent samples can be obtained by *thinning*.
However, **all the samples can be used.**

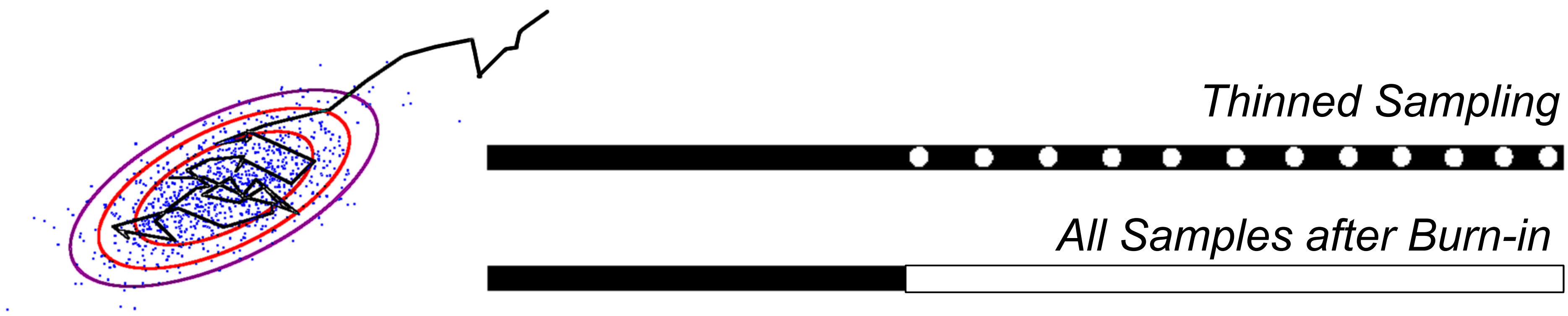
Use the simple Monte Carlo estimator on MCMC samples. It is:

— consistent

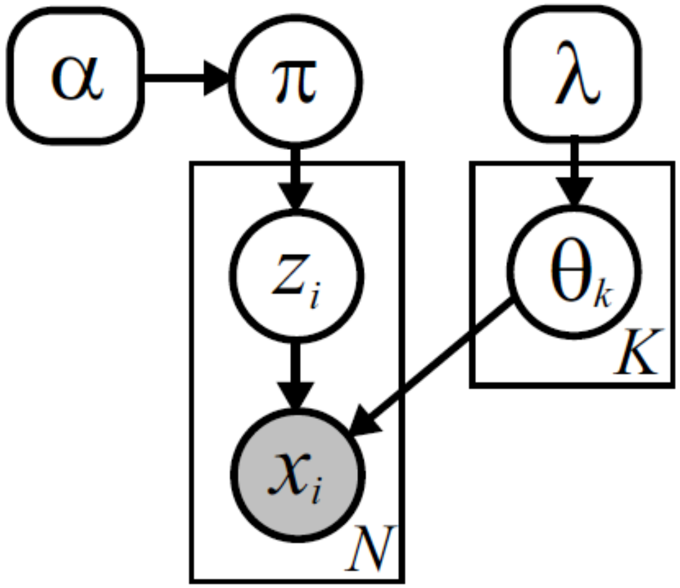
— unbiased if the chain has "burned in"

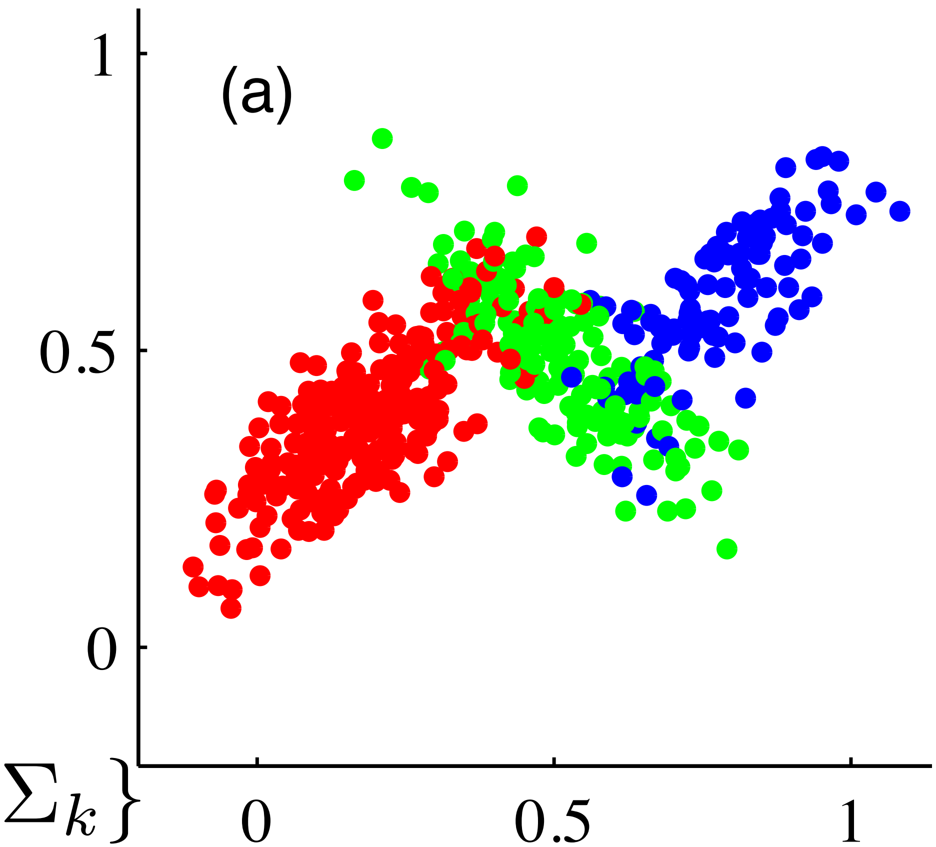
$$\mathbb{E}_P[f] \approx \frac{1}{S} \sum_{s=1}^{S} f(x^{(s)})$$

The correct motivation to thin: if computing $f(\mathbf{x}^{(s)})$ is expensive



Probabilistic Mixture Models





$$\pi \sim \text{Dir}(\alpha)$$

$$\theta_k \sim H(\lambda) \qquad \theta_k = \{\mu_k, \Sigma_k\}$$

$$p(z_i \mid \pi) = \text{Cat}(z_i \mid \pi)$$

$$p(x_i \mid z_i, \mu, \Sigma) = \mathcal{N}(x_i \mid \mu_{z_i}, \Sigma_{z_i})$$

Mixture Sampler Pseudocode

Given mixture weights $\pi^{(t-1)}$ and cluster parameters $\{\theta_k^{(t-1)}\}_{k=1}^K$ from the previous iteration, sample a new set of mixture parameters as follows:

1. Independently assign each of the N data points x_i to one of the K clusters by sampling the indicator variables $z = \{z_i\}_{i=1}^N$ from the following multinomial distributions:

$$z_i^{(t)} \sim \frac{1}{Z_i} \sum_{k=1}^K \pi_k^{(t-1)} f(x_i \mid \theta_k^{(t-1)})\, \delta(z_i, k) \qquad Z_i = \sum_{k=1}^K \pi_k^{(t-1)} f(x_i \mid \theta_k^{(t-1)})$$

2. Sample new mixture weights according to the following Dirichlet distribution:

$$\pi^{(t)} \sim \mathrm{Dir}(N_1 + \alpha/K, \ldots, N_K + \alpha/K) \qquad N_k = \sum_{i=1}^N \delta(z_i^{(t)}, k)$$

3. For each of the K clusters, independently sample new parameters from the conditional distribution implied by those observations currently assigned to that cluster:

$$\theta_k^{(t)} \sim p(\theta_k \mid \{x_i \mid z_i^{(t)} = k\}, \lambda)$$

   When λ defines a conjugate prior, this posterior distribution is given by Prop. 2.1.4.

Proposition 2.1.4. *Let $p(x \mid \theta)$ denote an exponential family with canonical parameters θ, and $p(\theta \mid \lambda)$ a family of conjugate priors defined as in eq. (2.28). Given L independent samples $\{x^{(\ell)}\}_{\ell=1}^L$, the posterior distribution remains in the same family:*

For each mixture component, posterior given assigned data

$$p(\theta \mid x^{(1)}, \ldots, x^{(L)}, \lambda) = p(\theta \mid \bar{\lambda}) \tag{2.31}$$

$$\bar{\lambda}_0 = \lambda_0 + L \qquad \bar{\lambda}_a = \frac{\lambda_0 \lambda_a + \sum_{\ell=1}^L \phi_a(x^{(\ell)})}{\lambda_0 + L} \qquad a \in \mathcal{A} \tag{2.32}$$

Mixture Sampler Pseudocode

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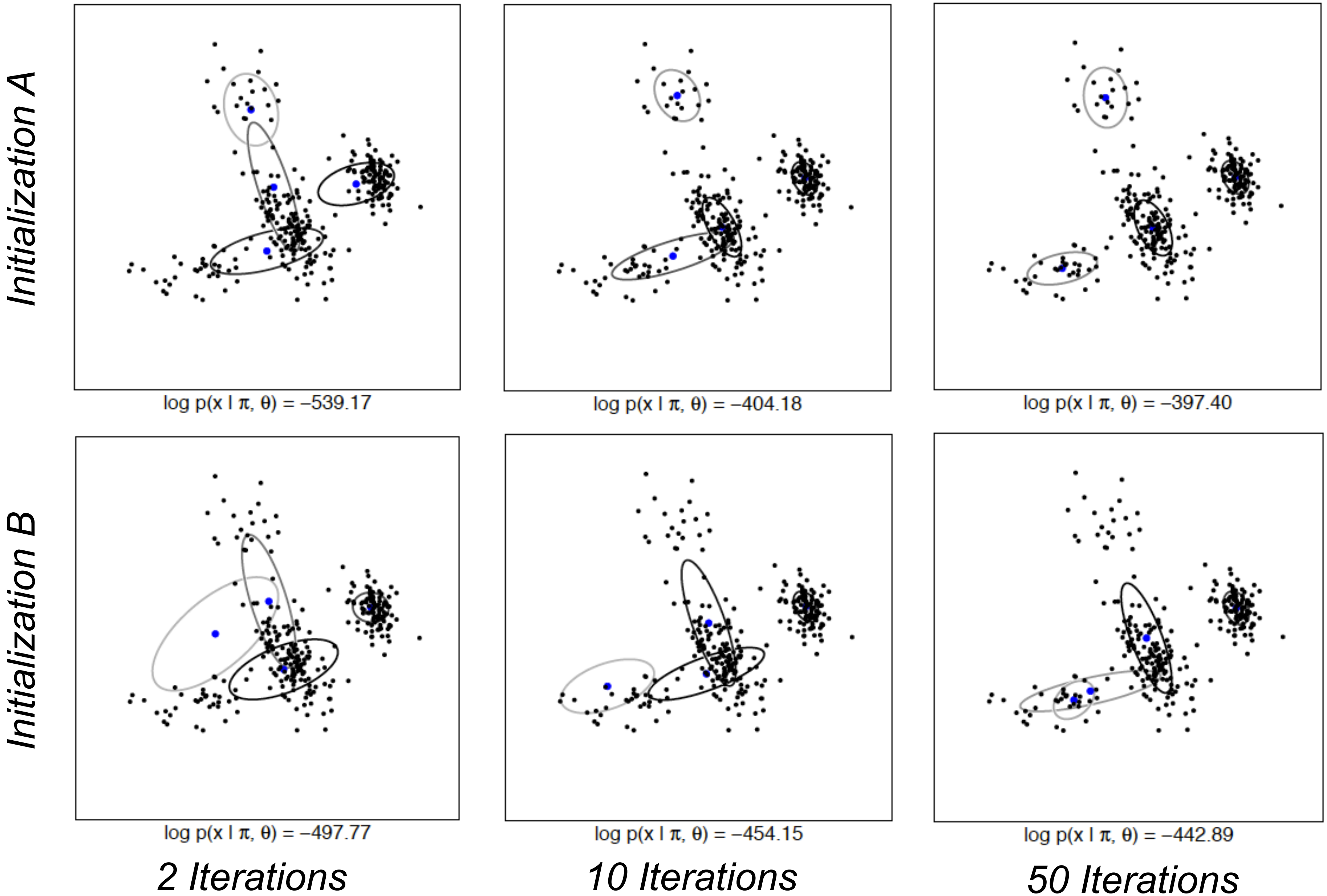
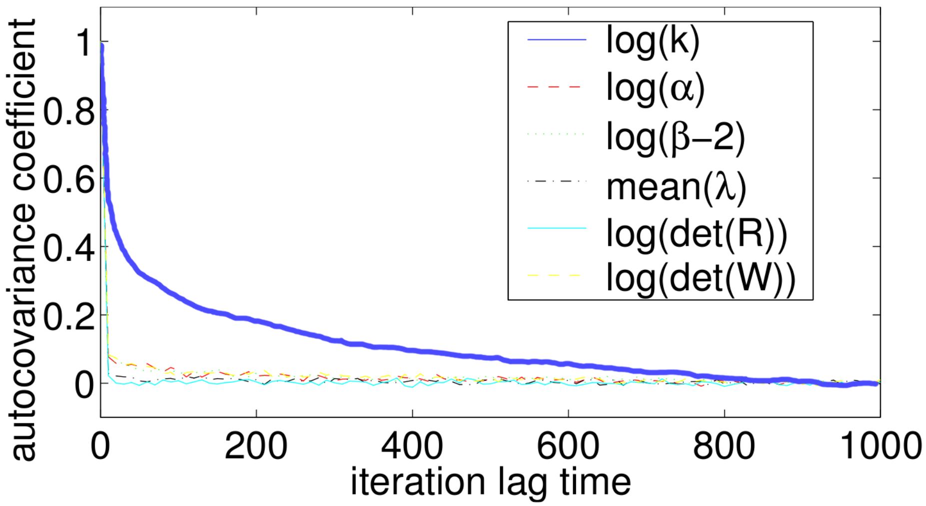
Compared to the EM algorithm for finite mixture models:

- Form same assignment indicator distributions as in E-step, but then draw a single sample from each distribution
- Sample, rather than taking mode, of parameter distributions

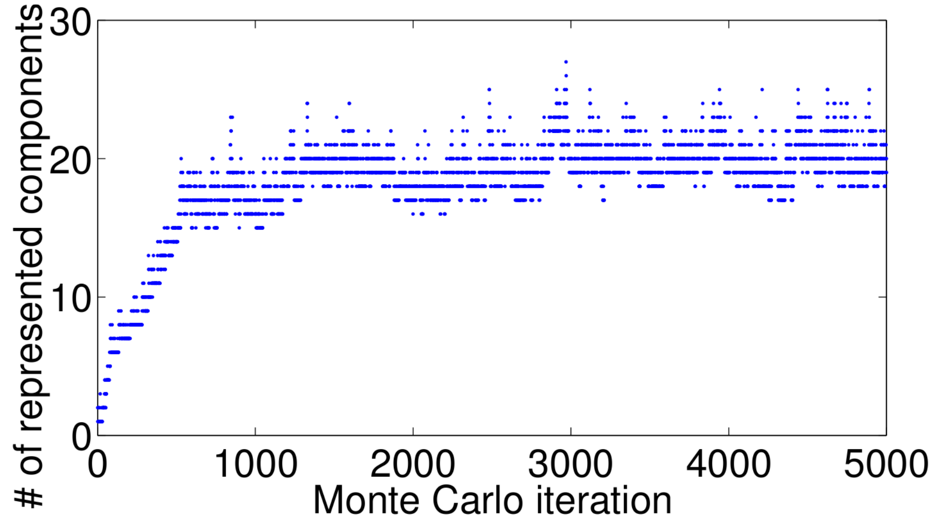
Snapshots of Mixture Gibbs Sampler



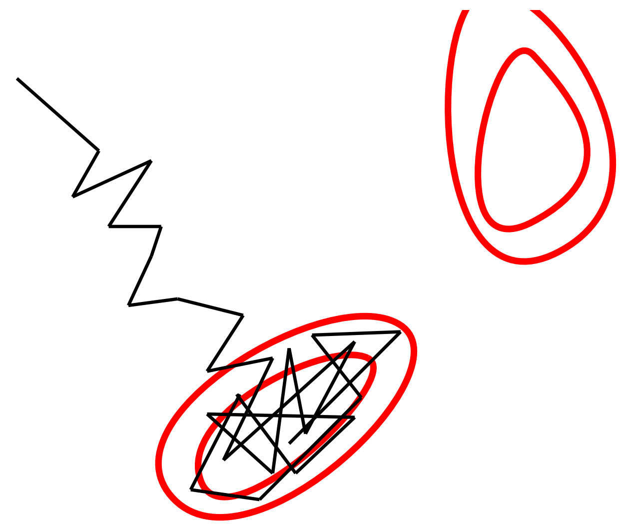
MCMC: Mixing Diagnostics



Autocovariance: Empirical covariance of values produced by MCMC method, versus iteration lag (spacing)

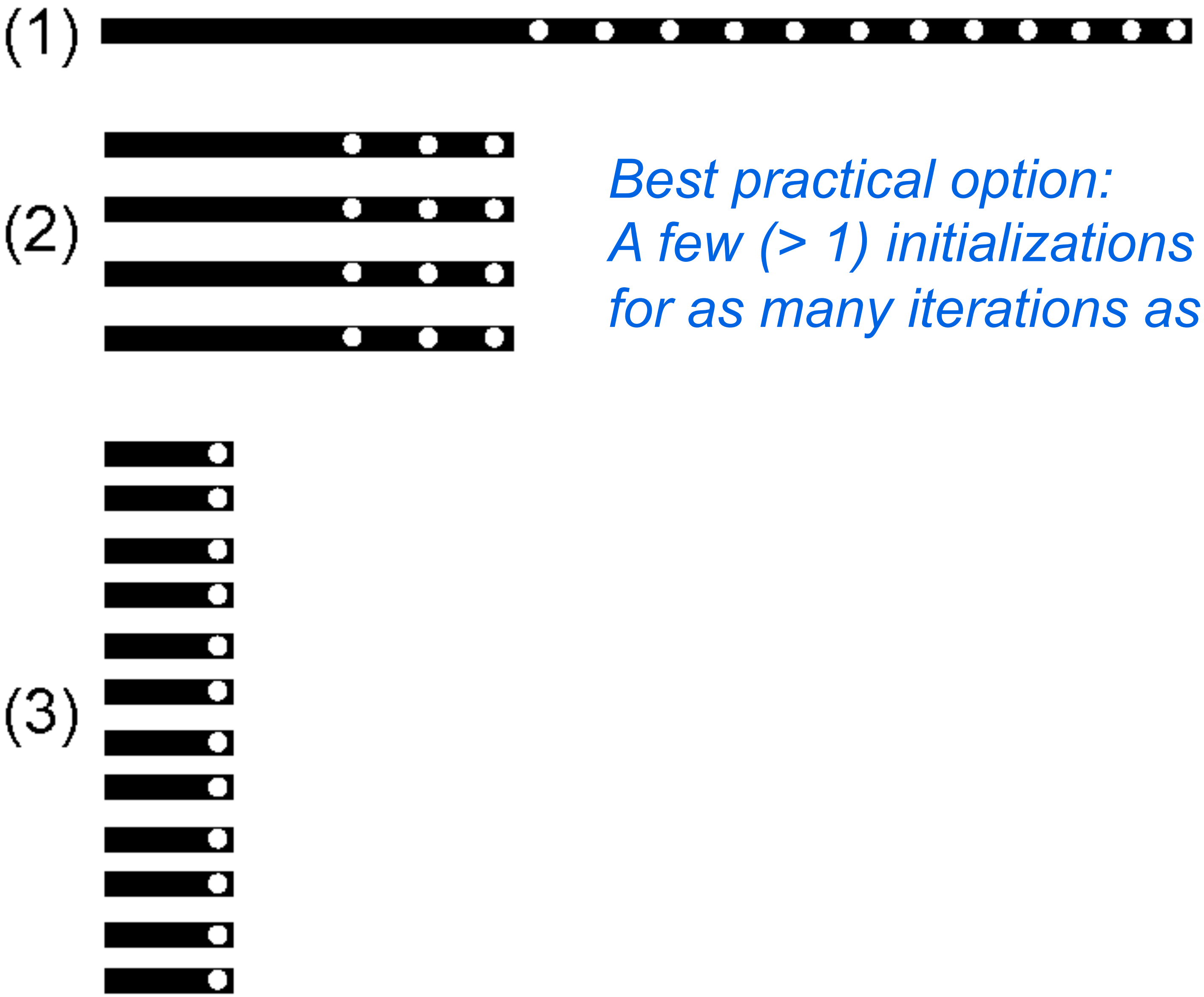


Trace Plot: Value of some "interesting" summary statistic, versus MCMC iteration



- Small autocovariances are necessary, but not sufficient, to demonstrate mixing to the target distribution
- Fairly reliable for unimodal posteriors, but *very misleading more generally*

MCMC & Computational Resources



Best practical option:
A few (> 1) initializations
for as many iterations as possible

Rao-Blackwellized Estimation

- Basic Monte Carlo estimation for joint distribution of *x, z*:

$$(x^{(\ell)}, z^{(\ell)}) \sim p(x, z) \qquad \ell = 1, 2, \ldots, L$$

$$\mathbb{E}_p[f(x,z)] = \int_{\mathcal{Z}} \int_{\mathcal{X}} f(x,z) p(x,z)\, dx\, dz \;\approx \frac{1}{L} \sum_{\ell=1}^{L} f(x^{(\ell)}, z^{(\ell)}) = \mathbb{E}_{\tilde{p}}[f(x,z)]$$

- But suppose that the conditional distribution $p(x \mid z)$ is tractable:

$$\begin{aligned}
\mathbb{E}_p[f(x,z)] &= \int_{\mathcal{Z}} \int_{\mathcal{X}} f(x,z) p(x \mid z)\, p(z)\, dx\, dz \\
&= \int_{\mathcal{Z}} \left[\int_{\mathcal{X}} f(x,z) p(x \mid z)\ dx \right] p(z)\, dz \\
&\approx \frac{1}{L} \sum_{\ell=1}^{L} \int_{\mathcal{X}} f(x, z^{(\ell)}) p(x \mid z^{(\ell)})\ dx = \mathbb{E}_{\tilde{p}}[\mathbb{E}_p[f(x,z) \mid z]]
\end{aligned}$$

- Should we expect this estimator to be more accurate?

Conditional vs Unconditional Variance

- The Rao-Blackwell Theorem, which was classically used to reduce the variance of estimators, is based on this identity:

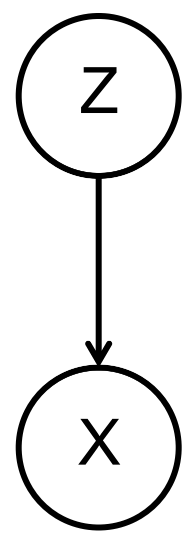
Theorem 2.4.1 (Rao-Blackwell). *Let x and z be dependent random variables, and $f(x,z)$ a scalar statistic. Consider the marginalized statistic $\mathbb{E}_x[f(x,z) \mid z]$, which is a function solely of z. The unconditional variance $\mathrm{Var}_{xz}[f(x,z)]$ is then related to the variance of the marginalized statistic as follows:*

$$\mathrm{Var}_{xz}[f(x,z)] = \mathrm{Var}_z[\mathbb{E}_x[f(x,z) \mid z]] + \mathbb{E}_z[\mathrm{Var}_x[f(x,z) \mid z]] \tag{2.159}$$

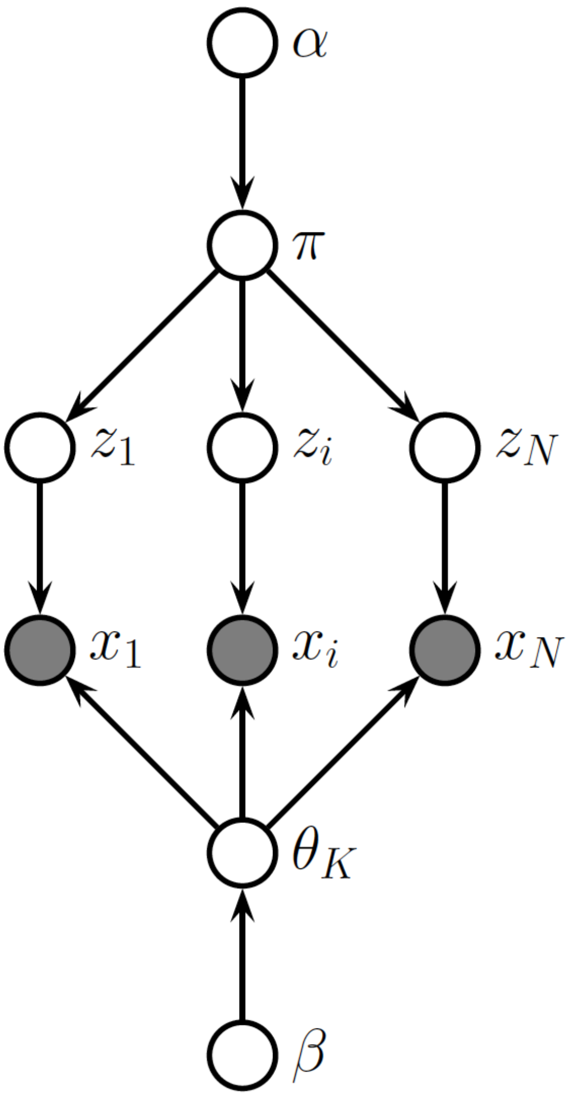
$$\geq \mathrm{Var}_z[\mathbb{E}_x[f(x,z) \mid z]] \tag{2.160}$$

Basic estimator *RB estimator* *non-negative*

- Applications in Monte Carlo methods:
  - Given output of any "standard" MCMC method, process to produce more efficient estimators
  - Analytically marginalize, or *collapse*, some variables from the model and derive Gibbs sampler for this collapsed representation



Collapsed Sampling Algorithms

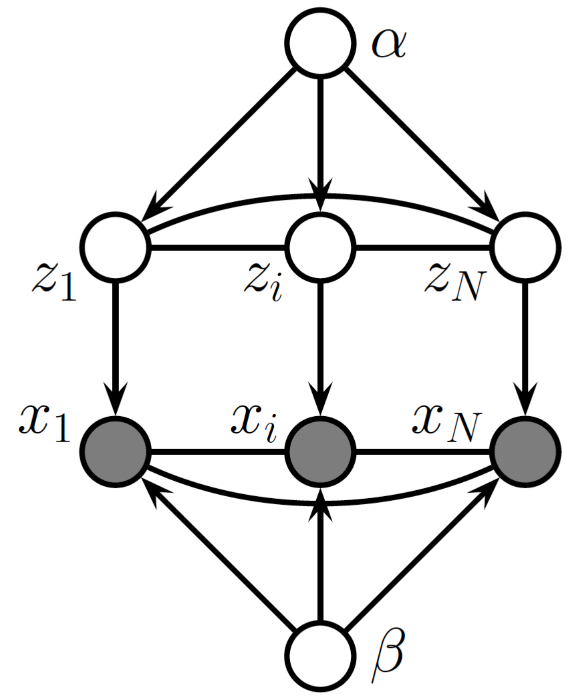


$$\pi \sim \mathrm{Dir}(\alpha)$$

$$z_i \sim \mathrm{Cat}(\pi)$$

$$x_i \sim F(\theta_{z_i})$$

$$\theta_k \sim G(\beta)$$



Conjugate priors allow exact marginalization of parameters, to make an equivalent model with fewer variables

Mixture Sampler Pseudocode

Given previous cluster assignments $z^{(t-1)}$, sequentially sample new assignments as follows:

1. Sample a random permutation $\tau(\cdot)$ of the integers $\{1, \ldots, N\}$.
2. Set $z = z^{(t-1)}$. For each $i \in \{\tau(1), \ldots, \tau(N)\}$, sequentially resample z_i as follows:
   (a) For each of the K clusters, determine the predictive likelihood
   $$f_k(x_i) = p(x_i \mid \{x_j \mid z_j = k, j \neq i\}, \lambda)$$
   This likelihood can be computed from cached sufficient statistics via Prop. 2.1.4.
   (b) Sample a new cluster assignment z_i from the following multinomial distribution:
   $$z_i \sim \frac{1}{Z_i} \sum_{k=1}^{K} (N_k^{-i} + \alpha/K) f_k(x_i) \delta(z_i, k) \qquad Z_i = \sum_{k=1}^{K} (N_k^{-i} + \alpha/K) f_k(x_i)$$
   N_k^{-i} is the number of other observations assigned to cluster k (see eq. (2.162)).
   (c) Update cached sufficient statistics to reflect the assignment of x_i to cluster z_i.
3. Set $z^{(t)} = z$. Optionally, mixture parameters may be sampled via steps 2–3 of Alg. 2.1.

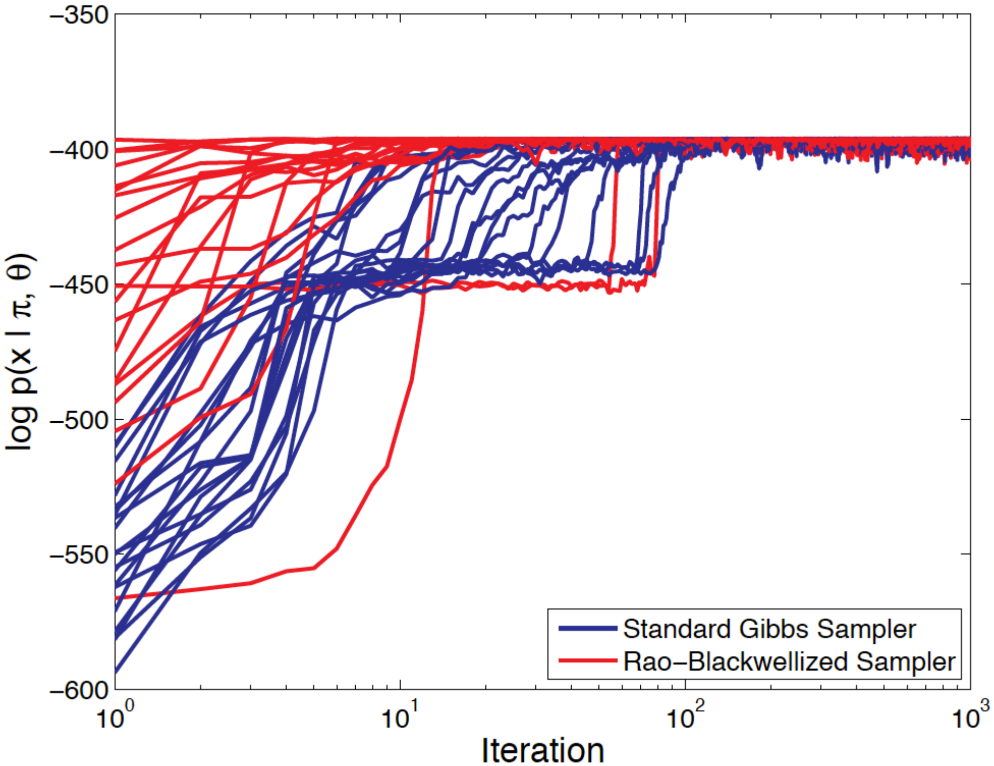
$$p(\theta \mid x^{(1)}, \ldots, x^{(L)}, \lambda) = p(\theta \mid \bar{\lambda}) \tag{2.31}$$

$$\bar{\lambda}_0 = \lambda_0 + L \qquad \bar{\lambda}_a = \frac{\lambda_0 \lambda_a + \sum_{\ell=1}^{L} \phi_a(x^{(\ell)})}{\lambda_0 + L} \qquad a \in \mathcal{A} \tag{2.32}$$

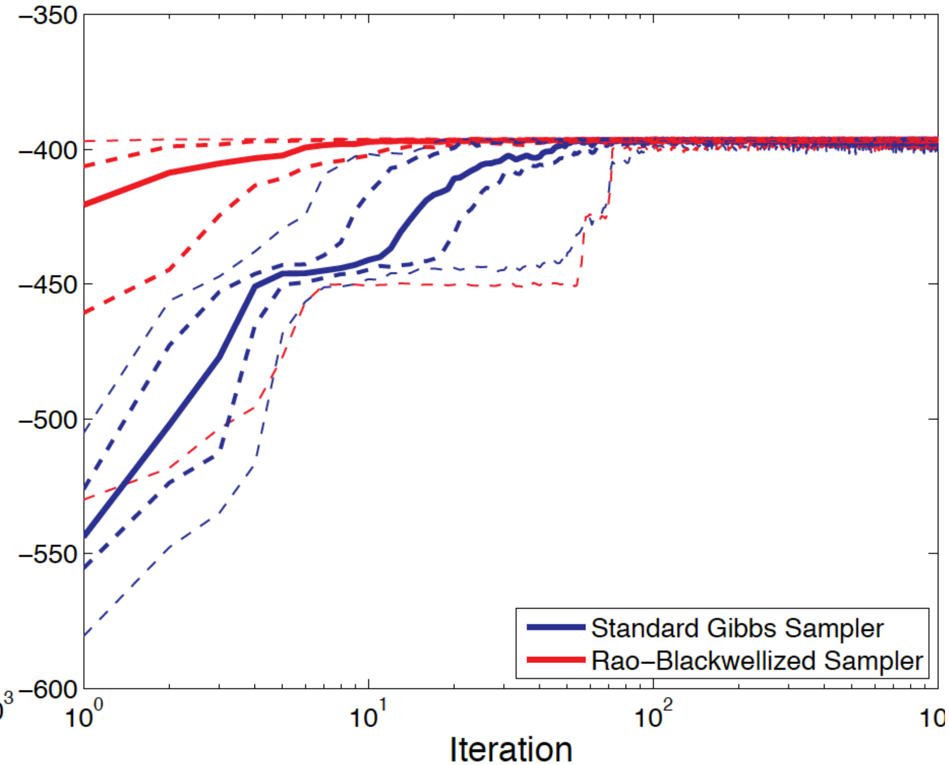
Integrating over Θ, the log-likelihood of the observations can then be compactly written using the normalization constant of eq. (2.29):

$$\log p(x^{(1)}, \ldots, x^{(L)} \mid \lambda) = \Omega(\bar{\lambda}) - \Omega(\lambda) + \sum_{\ell=1}^{L} \log \nu(x^{(\ell)}) \tag{2.33}$$

Gibbs: Representation and Mixing



Multiple Initializations



Quantiles of 100 Chains

Standard Gibbs: Alternatively sample assignments, parameters

Collapsed Gibbs: Marginalize parameters, sample assignments