CS242: Probabilistic Graphical Models

Lecture 19: Collapsed & Blocked Gibbs Samplers

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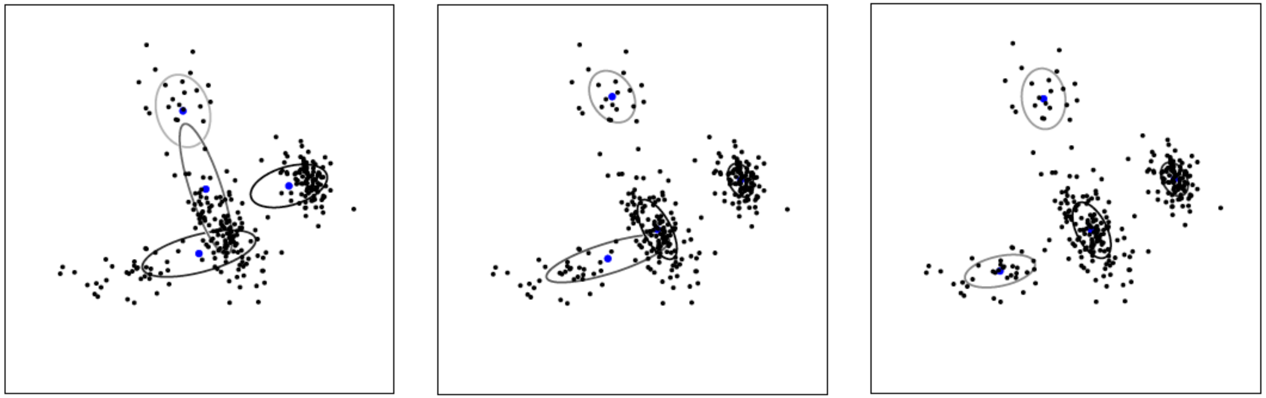
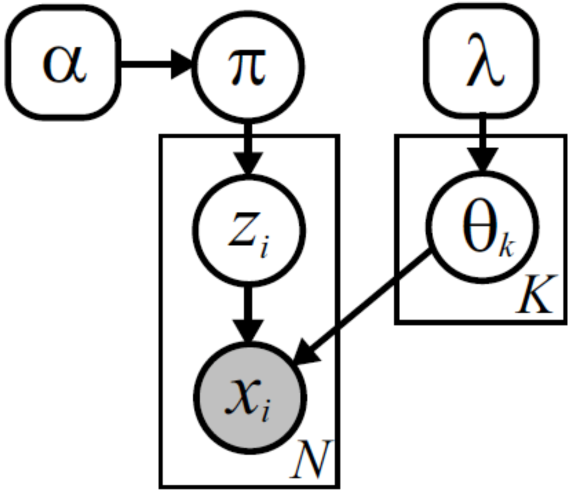
November 6, 2014

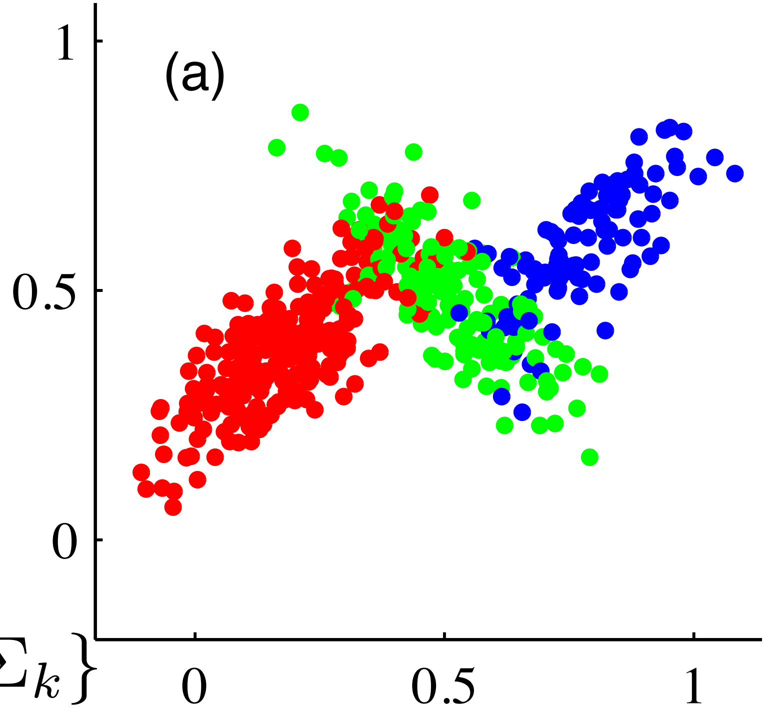
Rao-Blackwellized Estimators & Collapsed Samplers



$\log p(x \mid \pi, \theta) = -539.17$ $\log p(x \mid \pi, \theta) = -404.18$ $\log p(x \mid \pi, \theta) = -397.40$

Probabilistic Mixture Models





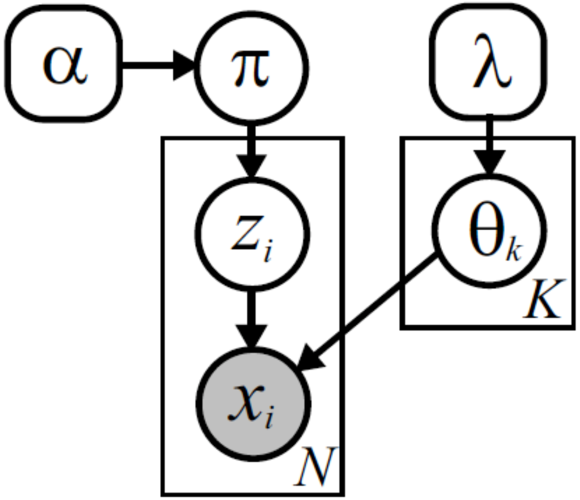
Cluster weights: $\pi \sim \mathrm{Dir}(\alpha)$

Cluster params: $\theta_k \sim H(\lambda) \quad \theta_k = \{\mu_k, \Sigma_k\}$

Cluster assign: $p(z_i \mid \pi) = \mathrm{Cat}(z_i \mid \pi) \qquad z_i \in \{1, \ldots, K\}$

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

A Standard Gibbs Sampler



- Given fixed mixture weights and mixture parameters, the cluster assignments are conditionally independent:

$$p(z \mid x, \pi, \theta) = \prod_{i=1}^{N} p(z_i \mid x_i, \pi, \theta)$$

$$p(z_i = k \mid x_i, \pi, \theta) \propto \pi_k f(x_i \mid \theta_k)$$

Sample from these categorical distributions, once per variable, in arbitrary order.

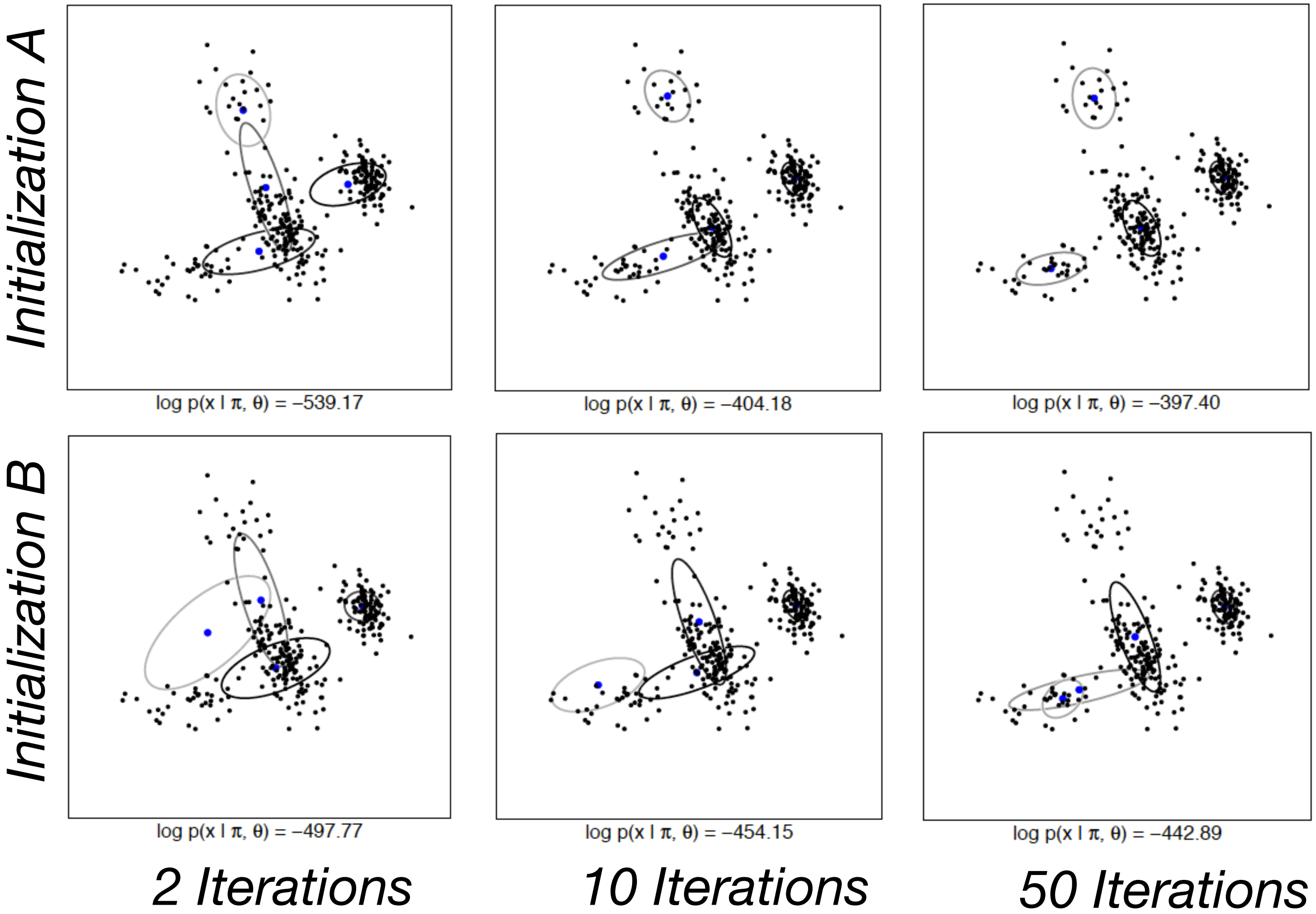
- Given fixed cluster assignments z, all parameters are conditionally independent:

$$p(\pi \mid x, z, \theta) = p(\pi \mid z) = \mathrm{Dir}(\pi \mid N_1 + \alpha, \ldots, N_K + \alpha) \qquad N_k = \sum_{i=1}^{N} \delta(z_i, k)$$

$$p(\theta \mid x, z, \pi) = \prod_{k=1}^{K} p(\theta_k \mid x, z) = \prod_{k=1}^{K} p(\theta_k \mid X_k) \qquad X_k = \{x_i \mid z_i = k\}$$

- Compared to the EM algorithm for finite mixture models:
  - *Form same assignment distributions as in E-step, but then draw a single sample from each*
  - *Sample, rather than taking mode, of parameter distributions from M-step*

Snapshots of Mixture Gibbs Sampler



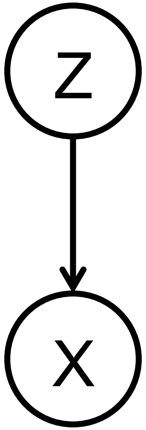
Rao-Blackwellized Estimation

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

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

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

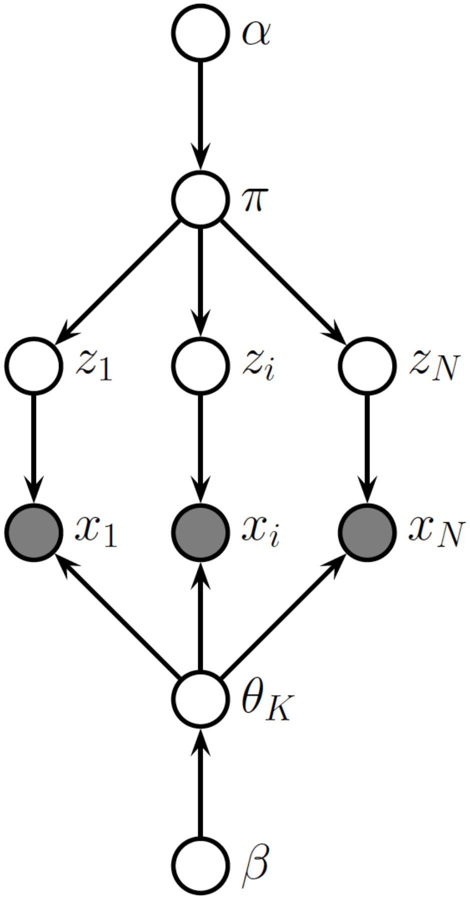
- But suppose that the conditional distribution $p(x \mid z)$ is tractable:



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

- This estimator is guaranteed to have lower variance!

A Collapsed Sampling Algorithm

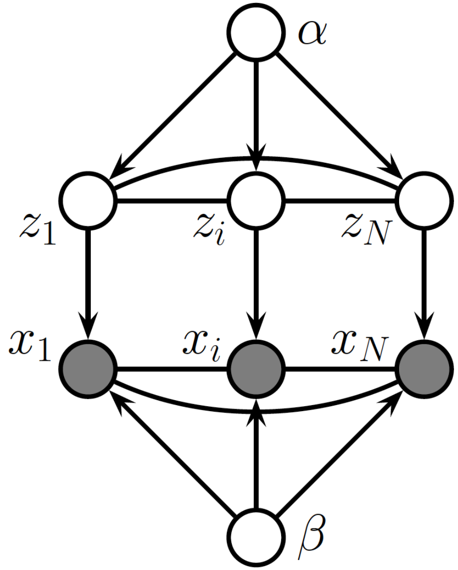


$$\pi \sim \mathrm{Dir}(\alpha)$$

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

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

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



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

Bayesian Learning of Probabilities

Posterior Predictive Distribution: For the next observation,

$$p(z_{N+1} = k \mid z_1, \ldots, z_N) = \int \mu_k p(\mu \mid z_1, \ldots, z_N) \, d\mu$$

$$= \frac{N_k + \alpha_k}{N + \alpha_0} = \mathbb{E}[\mu_k \mid z_1, \ldots, z_N]$$

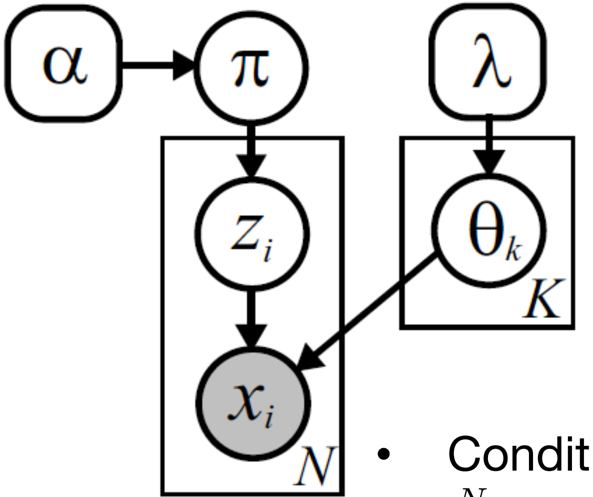
Dirichlet Prior Distribution:

$$p(\mu) = \mathrm{Dir}(\mu \mid \alpha) \propto \prod_{k=1}^{K} \mu_k^{\alpha_k - 1}$$

Dirichlet Posterior Distribution (Conjugate):

$$p(\mu \mid x) \propto \prod_{k=1}^{K} \mu_k^{N_k + \alpha_k - 1} \propto \mathrm{Dir}(\mu \mid N_1 + \alpha_1, \ldots, N_K + \alpha_K)$$

A Collapsed Gibbs Sampler



- Collapsed mixture model representation:

$$p(z \mid x) \propto p(z)p(x \mid z)$$
$$\propto \int_{\Pi} p(z \mid \pi)p(\pi \mid \alpha)\, d\pi \int_{\Theta} p(x \mid z, \theta)p(\theta \mid \lambda)\, d\theta$$

- Apply standard Gibbs sampling updates:

$$p(z_i \mid z_{\setminus i}, x) \propto p(z_i \mid z_{\setminus i})p(x \mid z_i, z_{\setminus i})$$

- Conditional prior:

$$N_k^{\setminus i} = \sum_{j=1, j \neq i}^{N} \delta(z_j, k) \qquad p(z_i = k \mid z_{\setminus i}) = \frac{N_k^{\setminus i} + \alpha/K}{N - 1 + \alpha}$$

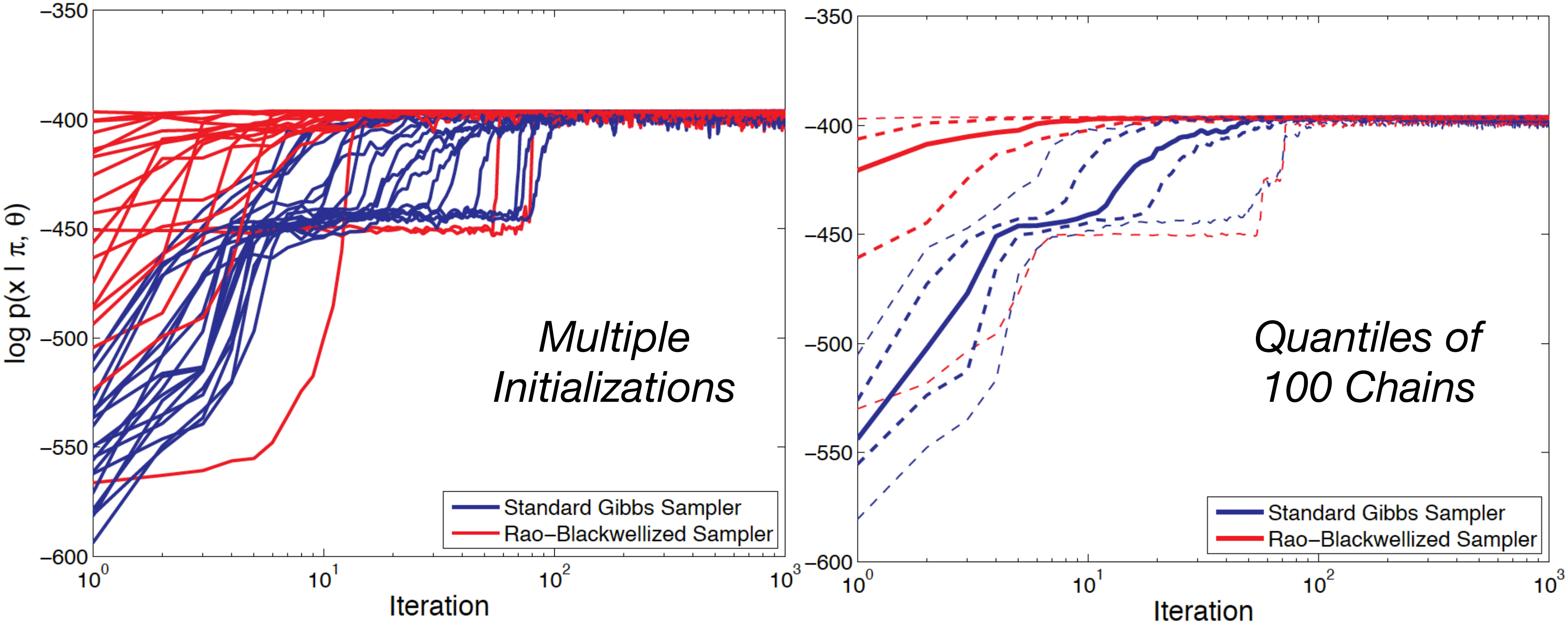
- Conditional likelihood:

$$X_k^{\setminus i} \triangleq \{x_j \mid z_j = k, j \neq i\} \qquad p(x \mid z) \propto p(x_i \mid z, x_{\setminus i})$$
$$p(x_i \mid z_i = k, z_{\setminus i}, x_{\setminus i}) = \int_{\Theta_k} p(x_i \mid \theta_k)p(\theta_k \mid X_k^{\setminus i})\, d\theta_k$$

Conjugate analysis given "other" data assigned to this cluster

Gibbs: Representation & Mixing

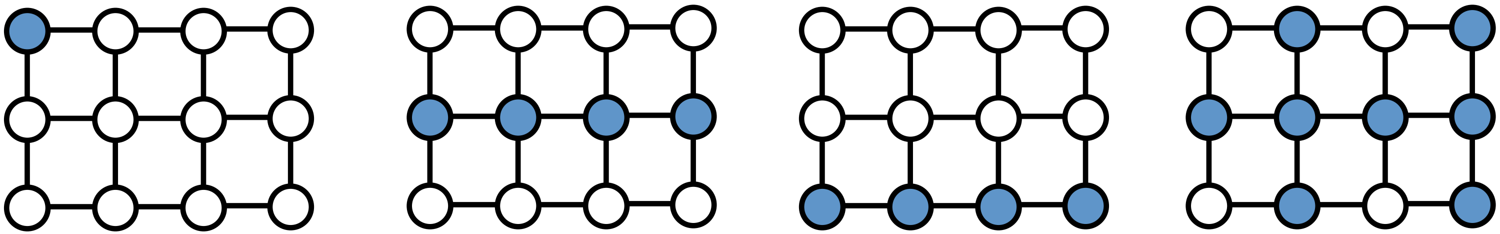
Multiple Trials on 2D Mixture Data from Earlier Slide



Standard Gibbs: Alternatively sample assignments, parameters

Collapsed Gibbs: Marginalize parameters, sample assignments

Blocked Gibbs Samplers



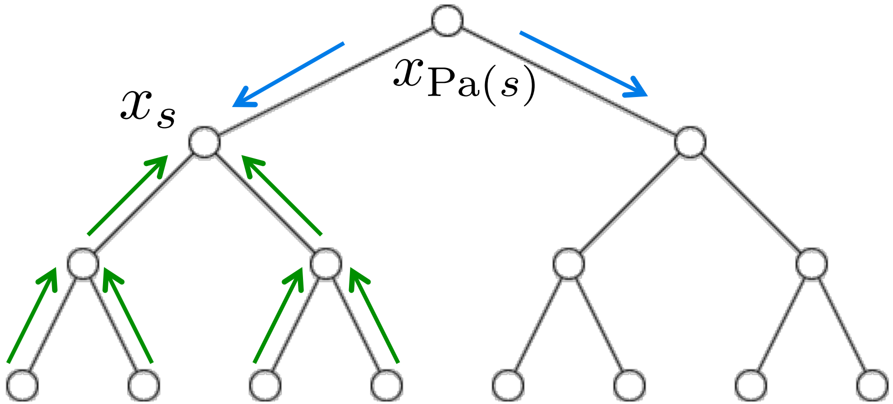
Sum-Product for Blocked Tree Sampling

Global Directed Factorization:

- Choose some node as the root of the tree, order other nodes by depth
- Directed factorization from root to leaves:

$$p(x) = p(x_{\text{Root}}) \prod_s p(x_s \mid x_{\text{Pa}(s)})$$

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



Bottom-Up Message Passing:

- Pass messages from leaves to root
- Compute marginal of root node:

$$m_{ts}(x_s) \propto \sum_{x_t} \psi_{st}(x_s, x_t)\psi_t(x_t) \prod_{u\in\Gamma(t)\setminus s} m_{ut}(x_t)$$

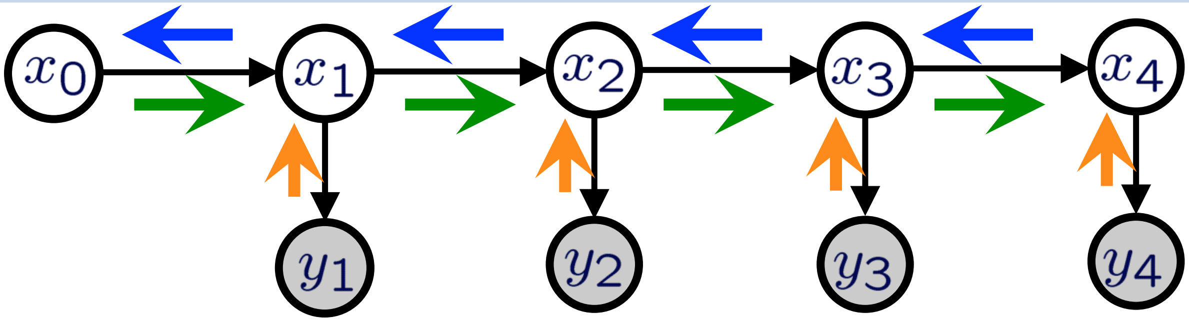
$$q_t(x_t) \propto \psi_t(x_t) \prod_{u\in\Gamma(t)} m_{ut}(x_t)$$

Top-Down Recursive Sampling:

- Sample root from marginal, then sample by depth given parent:

$$p(x_s \mid X_t = \hat{x}_t, t = \text{Pa}(s)) \propto \psi_{ts}(\hat{x}_t, x_s)\psi_s(x_s) \prod_{u\in\Gamma(s)\setminus t} m_{us}(x_s)$$

Example: Hidden Markov Model



- Can efficiently draw joint samples from posterior marginals:
  - Forward Message Passing: $p(x_t \mid y_1, \ldots, y_t)$
  - Backwards Sampling:

$$x_T^{(\ell)} \sim p(x_T \mid y)$$
$$x_{T-1}^{(\ell)} \sim p(x_{T-1} \mid x_T^{(\ell)}, y)$$
$$x_{T-2}^{(\ell)} \sim p(x_{T-2} \mid x_{T-1}^{(\ell)}, y)$$

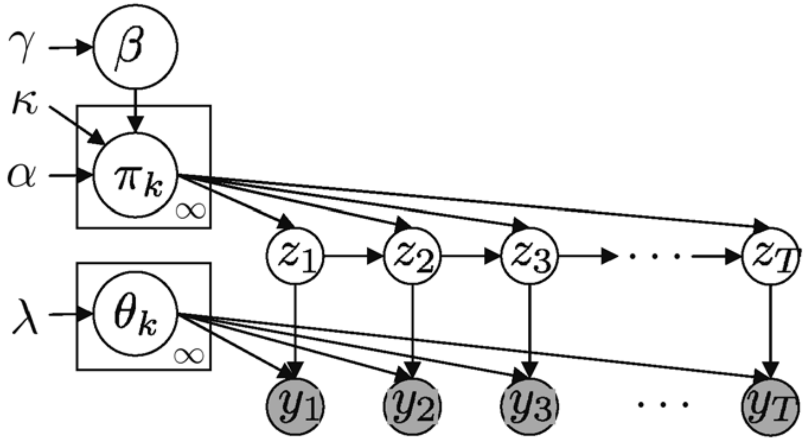
$$(x_1^{(\ell)}, x_2^{(\ell)}, \ldots, x_T^{(\ell)}) \sim p(x \mid y)$$

- Justification from Markov properties of HMM:

$$p(x_t \mid x_{t+1}, y) = p(x_t \mid x_{t+1}, y_1, \ldots, y_t) \propto p(x_t \mid y_1, \ldots, y_t) p(x_{t+1} \mid x_t)$$

Gibbs Sampling for Learning HMMs

- Given a fixed state sequence *z*, the *state transition and state emission* parameters are conditionally independent
  - ➢ Compute posterior given states, as in the M-step of the EM algorithm for HMMs
  - ➢ Sample from posterior (often easy)



- *Standard Gibbs:* Sample state variables z_t one at at time, given parameters and other states:

$$p(z_t \mid z_{\setminus t}, \theta, \pi, y) \propto p(z_t \mid z_{t-1}, \pi) p(z_{t+1} \mid z_t, \pi) p(y_t \mid z_t, \theta)$$

- *Blocked Gibbs:* Sample entire state sequence, given parameters and entire observation sequence, use sum-product dynamic programming

$$p(z \mid \theta, \pi, y) \propto p(z \mid \pi) p(y \mid z, \theta)$$

  - ➢ Similar to use of sum-product to compute marginals in E-step of EM algorithm

Gibbs Sampling for Learning HMMs

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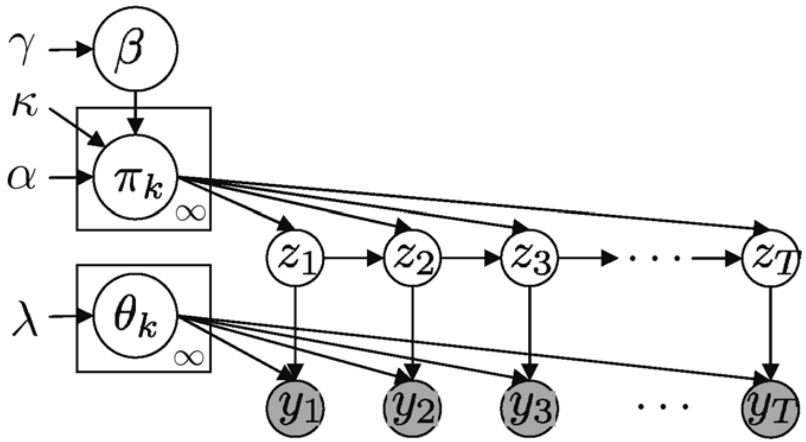
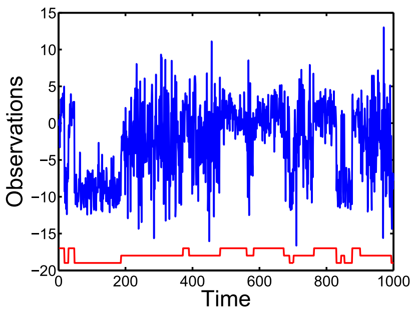
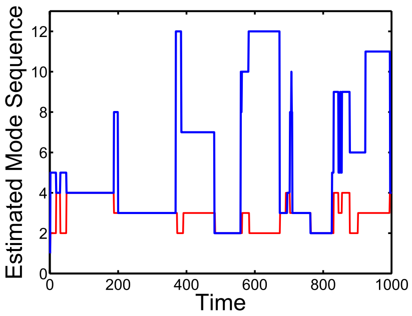
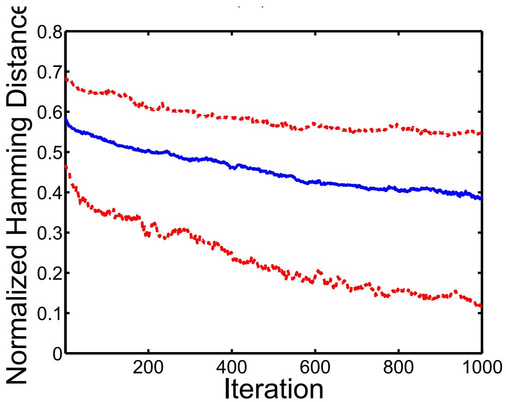


Experiment with Synthetic Data

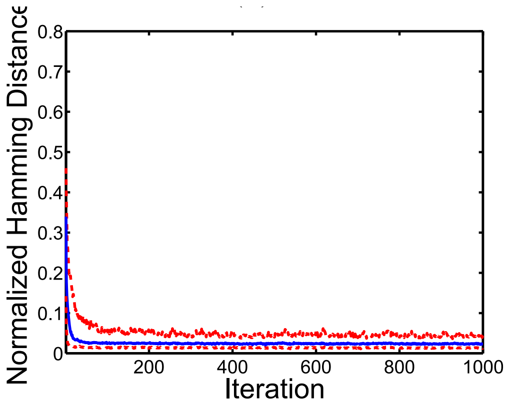




Standard Gibbs

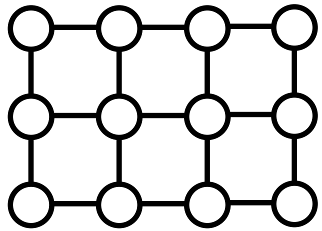


Blocked Gibbs

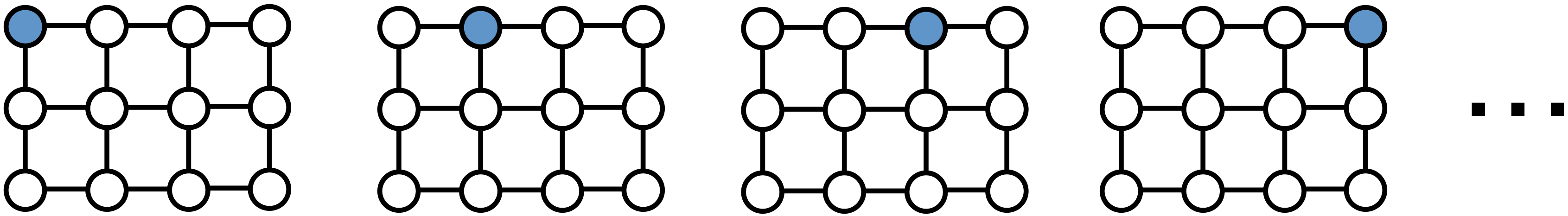


Blocked Gibbs for Markov Random Fields

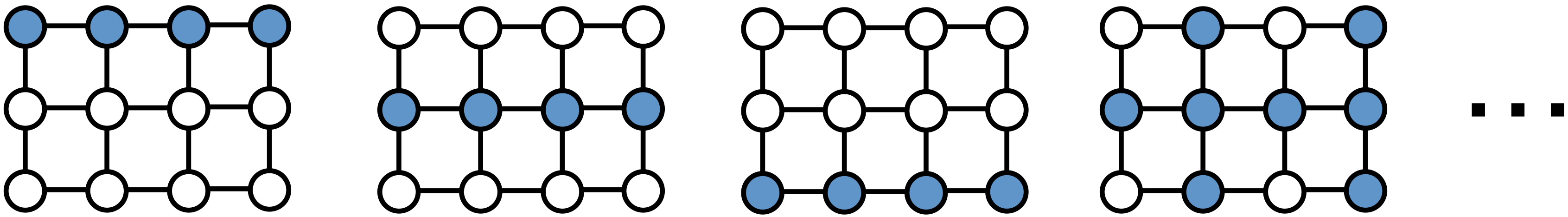
- For general graphs with cycles, cannot use sum-product BP to draw exact samples



- A *standard Gibbs sampler* iteratively resamples the values of single variables, in some order:



- A *blocked Gibbs sampler* iteratively resamples subsets of the original variables that are tractable (form a sub-graph without cycles):



- Draw *exact samples* by applying blocked sampler to junction tree. *Intractable?*