Inference via Sampling (Contd), and Gradient-based and Online MCMC

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Topics in Probabilistic Modeling and Inference (CS698X)

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Recap: Markov Chain Monte Carlo (MCMC)

- MCMC generates a sequence of "samples" $\boldsymbol{z}^{(1)}, \boldsymbol{z}^{(2)}, \ldots, \boldsymbol{z}^{(L)}$ based on a first-order Markov Chain

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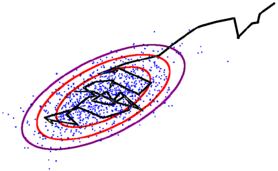

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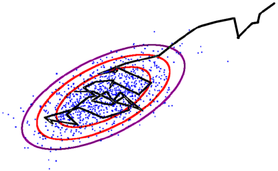

- The generated samples give a sample based approximation of $p(\boldsymbol{z})$

Recap: The MH Sampling Algorithm

Goal: Generate samples from a probability distribution $p(\boldsymbol{z}) = \frac{\tilde{p}(\boldsymbol{z})}{Z_p}$

The MH Sampling Algorithm

Initialize $\boldsymbol{z}^{(0)}$ randomly

For $\ell = 0, \ldots, L-1$

- Sample $\boldsymbol{z}^* \sim q(\boldsymbol{z}|\boldsymbol{z}^{(\ell)})$ and $u \sim \text{Unif}(0,1)$
- Compute the acceptance probability $A(\boldsymbol{z}^*, \boldsymbol{z}^{(\ell)}) = \min\left(1, \frac{\tilde{p}(\boldsymbol{z}^*)q(\boldsymbol{z}^{(\ell)}|\boldsymbol{z}^*)}{\tilde{p}(\boldsymbol{z}^{(\ell)})q(\boldsymbol{z}^*|\boldsymbol{z}^{(\ell)})}\right)$
- If $u < A(\boldsymbol{z}^*, \boldsymbol{z}^{(\ell)})$ then set $\boldsymbol{z}^{(\ell+1)} = \boldsymbol{z}^*$ else $\boldsymbol{z}^{(\ell+1)} = \boldsymbol{z}^{(\ell)}$

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Note: Computing acceptance prob. can be expensive in general, e.g., for posterior inference in which case $\tilde{p}(\boldsymbol{z})$ represents an unnormalized posterior $p(\mathbf{X}|\mathbf{Z})p(\mathbf{Z})$, which is product of likelihood and prior

Recap: Gibbs Sampling

- An instance of MH sampling where the acceptance probability $= 1$
- Based on sampling $\boldsymbol{z}$ one "component" at a time with proposal $=$ conditional distribution

Gibbs Sampling

Initialize $\boldsymbol{z}^{(0)} = [z_1^{(0)}, z_2^{(0)}, \ldots, z_M^{(0)}]$ randomly

For $\ell = 1, \ldots, L$

- Sample $\boldsymbol{z}^{(\ell)}$ by sampling one component at a time (usually cyclic manner)

$$
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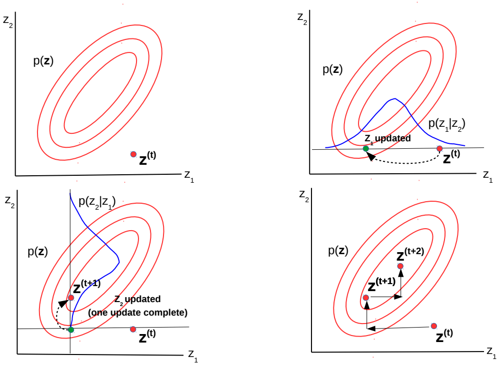
- Very easy to derive if the conditional distributions are easy to obtain

Gibbs Sampling: A Simple Example

Can sample from a 2-D Gaussian using 1-D Gaussians (recall that if the joint distribution is a 2-D Gaussian, conditionals will simply be 1-D Gaussians)



Note that Gibbs updates are like co-ordinate ascent

Deriving A Gibbs Sampler: The General Recipe

- Suppose our target distribution is a posterior distribution $p(\mathbf{Z}|\mathbf{X})$ where $\mathbf{Z} = [\boldsymbol{z}_1, \boldsymbol{z}_2, \ldots, \boldsymbol{z}_M]$

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An Aside: Markov Blanket

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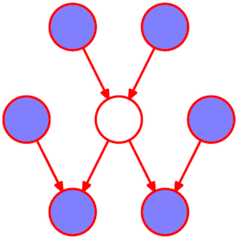
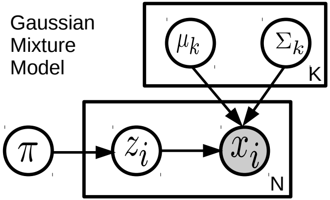


- Very helpful in quickly seeing what to condition on when deriving CPs in complex models

Gibbs Sampling: A Not-So-Simple Example

Gaussian Mixture Model



$$
\begin{aligned}
p(\mathbf{x}, \mathbf{z}, \boldsymbol{\mu}, \boldsymbol{\Sigma}, \boldsymbol{\pi}) &= p(\mathbf{x}|\mathbf{z}, \boldsymbol{\mu}, \boldsymbol{\Sigma}) p(\mathbf{z}|\boldsymbol{\pi}) p(\boldsymbol{\pi}) \prod_{k=1}^{K} p(\boldsymbol{\mu}_k) p(\boldsymbol{\Sigma}_k) \\
&= \left(\prod_{i=1}^{N} \prod_{k=1}^{K} (\pi_k \mathcal{N}(\mathbf{x}_i|\boldsymbol{\mu}_k, \boldsymbol{\Sigma}_k))^{\mathbb{I}(z_i=k)} \right) \times \\
&\quad \mathrm{Dir}(\boldsymbol{\pi}|\boldsymbol{\alpha}) \prod_{k=1}^{K} \mathcal{N}(\boldsymbol{\mu}_k|\mathbf{m}_0, \mathbf{V}_0) \mathrm{IW}(\boldsymbol{\Sigma}_k|\mathbf{S}_0, \nu_0)
\end{aligned}
$$

$$
p(z_i = k|\mathbf{x}_i, \boldsymbol{\mu}, \boldsymbol{\Sigma}, \boldsymbol{\pi}) \quad \propto \quad \pi_k \mathcal{N}(\mathbf{x}_i|\boldsymbol{\mu}_k, \boldsymbol{\Sigma}_k)
$$

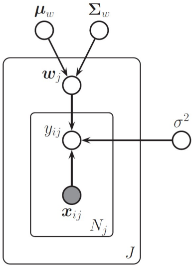
$$
p(\boldsymbol{\pi}|\mathbf{z}) \quad = \quad \mathrm{Dir}(\{\alpha_k + \sum_{i=1}^{N} \mathbb{I}(z_i = k)\}_{k=1}^{K})
$$

$$
\begin{aligned}
p(\boldsymbol{\mu}_k|\boldsymbol{\Sigma}_k, \mathbf{z}, \mathbf{x}) &= \mathcal{N}(\boldsymbol{\mu}_k|\mathbf{m}_k, \mathbf{V}_k) \\
\mathbf{V}_k^{-1} &= \mathbf{V}_0^{-1} + N_k \boldsymbol{\Sigma}_k^{-1} \\
\mathbf{m}_k &= \mathbf{V}_k(\boldsymbol{\Sigma}_k^{-1} N_k \bar{\mathbf{x}}_k + \mathbf{V}_0^{-1} \mathbf{m}_0) \\
N_k &\triangleq \sum_{i=1}^{N} \mathbb{I}(z_i = k) \\
\bar{\mathbf{x}}_k &\triangleq \frac{\sum_{i=1}^{N} \mathbb{I}(z_i = k) \mathbf{x}_i}{N_k}
\end{aligned}
$$

$$
\begin{aligned}
p(\boldsymbol{\Sigma}_k|\boldsymbol{\mu}_k, \mathbf{z}, \mathbf{x}) &= \mathrm{IW}(\boldsymbol{\Sigma}_k|\mathbf{S}_k, \nu_k) \\
\mathbf{S}_k &= \mathbf{S}_0 + \sum_{i=1}^{N} \mathbb{I}(z_i = k)(\mathbf{x}_i - \boldsymbol{\mu}_k)(\mathbf{x}_i - \boldsymbol{\mu}_k)^T \\
\nu_k &= \nu_0 + N_k
\end{aligned}
$$

Gibbs Sampling: Another Not-So-Simple Example

J schools Regression Problem



$$y_{ij} = \mathbf{x}_{ij}^T \mathbf{w}_j + \epsilon_{ij}$$

$$\mathbf{w}_j \sim \mathcal{N}(\boldsymbol{\mu}_w, \boldsymbol{\Sigma}_w)$$

$$\begin{aligned} \boldsymbol{\mu}_w &\sim \mathcal{N}(\boldsymbol{\mu}_0, \mathbf{V}_0) \\ \boldsymbol{\Sigma}_w &\sim \mathrm{IW}(\eta_0, \mathbf{S}_0^{-1}) \\ \sigma^2 &\sim \mathrm{IG}(\nu_0/2, \nu_0\sigma_0^2/2) \end{aligned}$$

$$\begin{aligned} p(\mathbf{w}_j|\mathcal{D}_j, \boldsymbol{\theta}) &= \mathcal{N}(\mathbf{w}_j|\boldsymbol{\mu}_j, \boldsymbol{\Sigma}_j) \\ \boldsymbol{\Sigma}_j^{-1} &= \boldsymbol{\Sigma}^{-1} + \mathbf{X}_j^T\mathbf{X}_j/\sigma^2 \\ \boldsymbol{\mu}_j &= \boldsymbol{\Sigma}_j(\boldsymbol{\Sigma}^{-1}\boldsymbol{\mu} + \mathbf{X}_j^T\mathbf{y}_j/\sigma^2) \end{aligned}$$

$$\begin{aligned} p(\boldsymbol{\mu}_w|\mathbf{w}_{1:J}, \boldsymbol{\Sigma}_w) &= \mathcal{N}(\boldsymbol{\mu}|\boldsymbol{\mu}_N, \boldsymbol{\Sigma}_N) \\ \boldsymbol{\Sigma}_N^{-1} &= \mathbf{V}_0^{-1} + J\boldsymbol{\Sigma}^{-1} \\ \boldsymbol{\mu}_N &= \boldsymbol{\Sigma}_N(\mathbf{V}_0^{-1}\boldsymbol{\mu}_0 + J\boldsymbol{\Sigma}^{-1}\overline{\mathbf{w}}) \\ \overline{\mathbf{w}} &= \frac{1}{J}\sum_j \mathbf{w}_j \end{aligned}$$

$$\begin{aligned} p(\boldsymbol{\Sigma}_w|\boldsymbol{\mu}_w, \mathbf{w}_{1:J}) &= \mathrm{IW}((\mathbf{S}_0 + \mathbf{S}_\mu)^{-1}, \eta_0 + J) \\ \mathbf{S}_\mu &= \sum_j (\mathbf{w}_j - \boldsymbol{\mu}_w)(\mathbf{w}_j - \boldsymbol{\mu}_w)^T \end{aligned}$$

$$\begin{aligned} p(\sigma^2|\mathcal{D}, \mathbf{w}_{1:J}) &= \mathrm{IG}([\nu_0 + N]/2, [\nu_0\sigma_0^2 + \mathrm{SSR}(\mathbf{w}_{1:J})]/2) \\ \mathrm{SSR}(\mathbf{w}_{1:J}) &= \sum_{j=1}^{J}\sum_{i=1}^{N_j}(y_{ij} - \mathbf{w}_j^T\mathbf{x}_{ij})^2 \end{aligned}$$

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  - Called the "Iterative Conditional Mode" (ICM) algorithm (doesn't give the posterior though)

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- Quantities not affected by permutations of latent variables can be safely averaged

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- Multiple Chains: Run multiple chains, take union of generated samples (ignoring burn-in samples)

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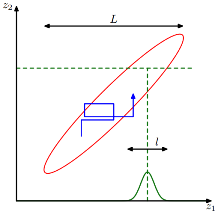

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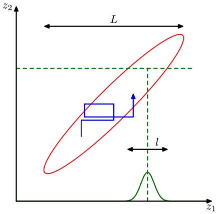

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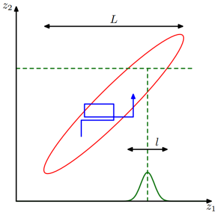

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- Using gradient info of the posterior can be helpful in avoiding the random walk (more in next class)

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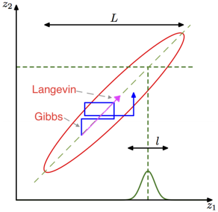
- This method is called Langevin dynamics (Neal, 2010). Has its origins in statistical Physics. (Move proposal's mean towards posterior's mode)



Langevin Dynamics (Contd)

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- Note that the procedure is almost as fast as MAP estimation!

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- Recent flurry of work on this topic (see "Bayesian Learning via Stochastic Gradient Langevin Dynamics" by Welling and Teh (2011) and follow-up works)

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