Approximate Inference: Sampling Methods (3)

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Probabilistic Machine Learning (CS772A)

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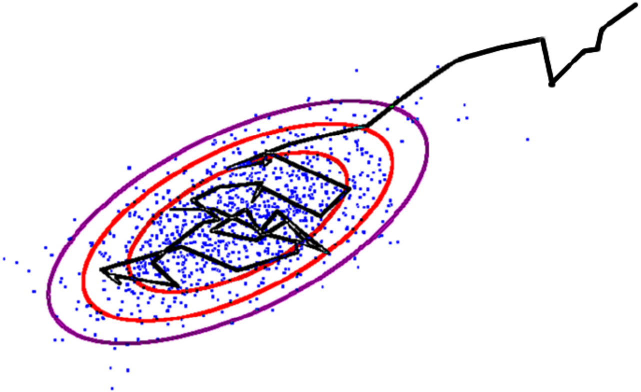
Recap

Markov Chain Monte Carlo (MCMC)

Generates samples from a target distribution by following a first-order Markov chain

$$z^{(1)} \rightarrow z^{(2)} \rightarrow \ldots \rightarrow z^{(L)}$$



Markov Chain

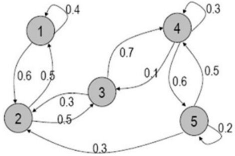
- Consider a sequence of random variables $\boldsymbol{z}^{(1)}, \ldots, \boldsymbol{z}^{(L)}$
- A first-order Markov Chain assumes

$$p(\boldsymbol{z}^{(\ell+1)}|\boldsymbol{z}^{(1)}, \ldots, \boldsymbol{z}^{(\ell)}) = p(\boldsymbol{z}^{(\ell+1)}|\boldsymbol{z}^{(\ell)}) \qquad \forall \ell$$

- A first order Markov chain can be defined by the following
  - An initial state distribution $p(\boldsymbol{z}^{(0)})$
  - Transition probabilities $T_\ell(\boldsymbol{z}^{(\ell)}, \boldsymbol{z}^{(\ell+1)})$ define our proposal distribution $q(\boldsymbol{z}^{(\ell+1)}|\boldsymbol{z}^{(\ell)})$

Transition probabilities can be defined using a *K*x*K* table if **z** is a discrete r.v. with *K* possible values

$$\begin{array}{c c} & \begin{array}{ccccc} 1 & 2 & 3 & 4 & 5 \end{array} \\ \begin{array}{c} 1 \\ 2 \\ 3 \\ 4 \\ 5 \end{array} & \begin{bmatrix} 0.4 & 0.6 & 0.0 & 0.0 & 0.0 \\ 0.5 & 0.0 & 0.5 & 0.0 & 0.0 \\ 0.0 & 0.3 & 0.0 & 0.7 & 0.0 \\ 0.0 & 0.0 & 0.1 & 0.3 & 0.6 \\ 0.0 & 0.3 & 0.0 & 0.5 & 0.2 \end{bmatrix} \end{array}$$



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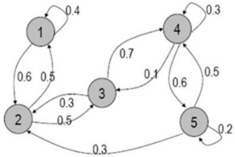

- Homogeneous Markov Chain: Transition probabilities $T_\ell = T$ (same everywhere along the chain)

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    - Else
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- Suppose we wish to sample from a joint distribution $p(\boldsymbol{z})$ where $\boldsymbol{z} = (z_1, z_2, \ldots, z_M)$

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- **Note:** Even <u>w/o local conjugacy</u>, if we can sample from local conditionals, Gibbs sampling applies!

Gibbs Sampling: Sketch of the Algorithm

M: Total number of unknowns to be sampled ($\boldsymbol{z} = [z_1, \ldots, z_M]$), T: number of Gibbs iterations

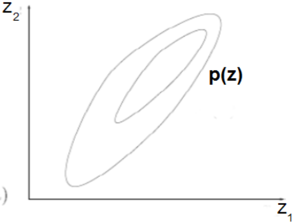
1. Initialize $\{z_i : i = 1, \ldots, M\}$
2. For $\tau = 1, \ldots, T$:
   - Sample $z_1^{(\tau+1)} \sim p(z_1 | z_2^{(\tau)}, z_3^{(\tau)}, \ldots, z_M^{(\tau)})$.
   - Sample $z_2^{(\tau+1)} \sim p(z_2 | z_1^{(\tau+1)}, z_3^{(\tau)}, \ldots, z_M^{(\tau)})$.

     $\vdots$
   - Sample $z_j^{(\tau+1)} \sim p(z_j | z_1^{(\tau+1)}, \ldots, z_{j-1}^{(\tau+1)}, z_{j+1}^{(\tau)}, \ldots, z_M^{(\tau)})$.

     $\vdots$
   - Sample $z_M^{(\tau+1)} \sim p(z_M | z_1^{(\tau+1)}, z_2^{(\tau+1)}, \ldots, z_{M-1}^{(\tau+1)})$.

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)



(a)

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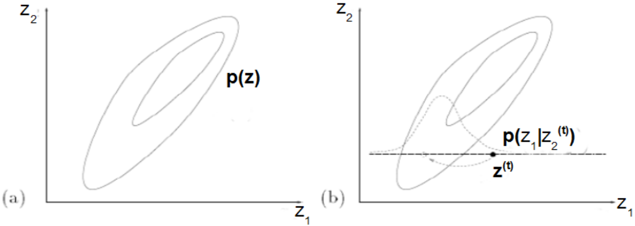

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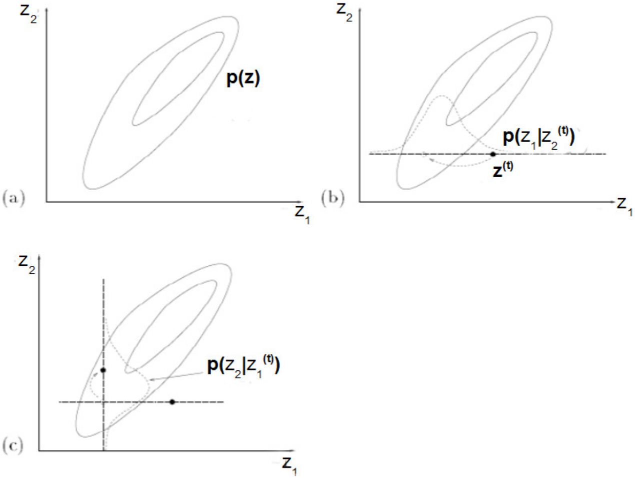

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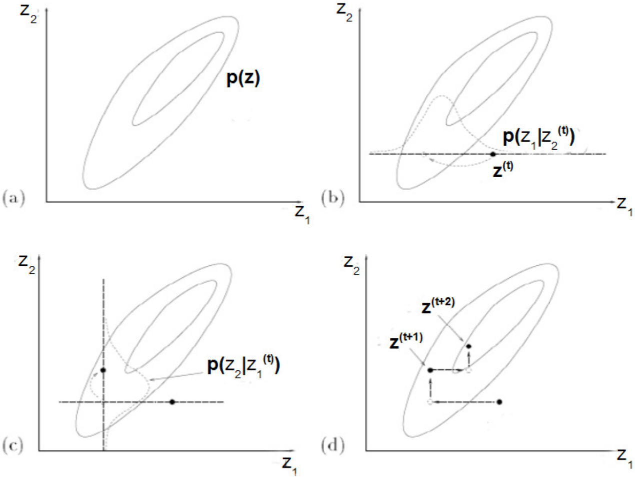
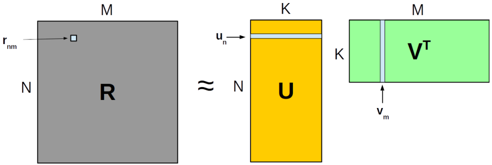


Some Other Examples of Gibbs Sampling

Gibbs Sampling for Probabilistic Matrix Factorization



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$$r_{ij} = \boldsymbol{u}_i^\top \boldsymbol{v}_j + \epsilon_{ij}$$

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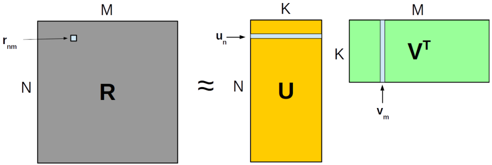

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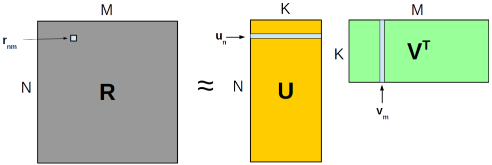

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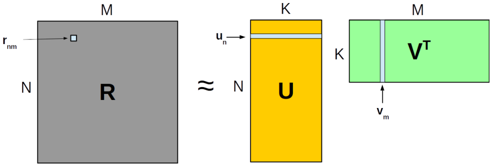

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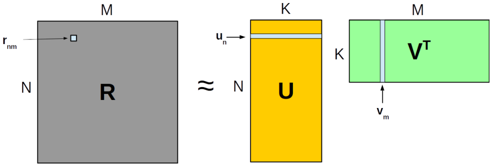

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- Local conditional posteriors for $\boldsymbol{u}_i$ and $\boldsymbol{v}_j$ have closed form (lecture 13). Simple Gibbs sampling!

Gibbs Sampling for Probabilistic Matrix Factorization

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where $\boldsymbol{\Sigma}_{u_i}^{(s)} = (\lambda_u \mathbf{I} + \beta \sum_{j:(i,j)\in\Omega} \boldsymbol{v}_j^{(s-1)} \boldsymbol{v}_j^{(s-1)\top})^{-1}$ and $\boldsymbol{\mu}_{u_i}^{(s)} = \boldsymbol{\Sigma}_{u_i}^{(s)}(\beta \sum_{j:(i,j)\in\Omega} r_{ij} \boldsymbol{v}_j^{(s-1)})$

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Gibbs Sampling for Gaussian Mixture Model

- Recall the GMM, K clusters with parameters $\{\boldsymbol{\mu}_k, \boldsymbol{\Sigma}_k\}_{k=1}^K$ and mixing prop. $\boldsymbol{\pi} = [\pi_1, \ldots, \pi_K]$

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$$
\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)
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- We want to infer the posterior distribution $p(\boldsymbol{z}, \boldsymbol{\mu}, \boldsymbol{\Sigma}, \boldsymbol{\pi}|\boldsymbol{x})$ over the unknowns

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The model has local conjugacy (except for the cluster id z_i, but that isn't a problem)

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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 \overline{\mathbf{x}}_k + \mathbf{V}_0^{-1}\mathbf{m}_0) \\
N_k &\triangleq \sum_{i=1}^{N} \mathbb{I}(z_i = k) \\
\overline{\mathbf{x}}_k &\triangleq \frac{\sum_{i=1}^{N} \mathbb{I}(z_i = k)\mathbf{x}_i}{N_k}
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$$

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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 \\
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Each Gibbs iteration cycles through sampling these variables one-at-a-time (conditioned on the rest)

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  - No. Reason: Mode or label switching

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MCMC and Random Walk

- MCMC methods use a proposal distribution to draw the next sample given the previous sample

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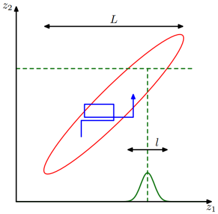

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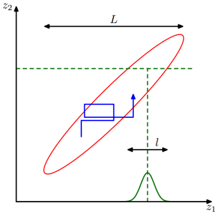

- Can be especially critical when the components of θ are highly correlated

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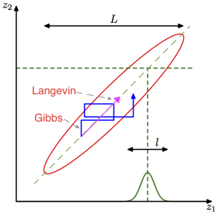

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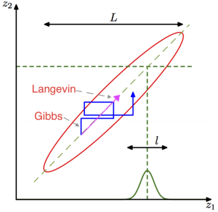

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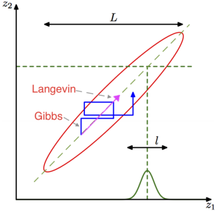

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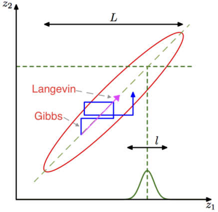

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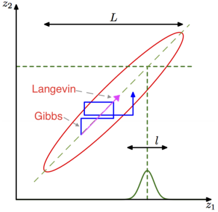

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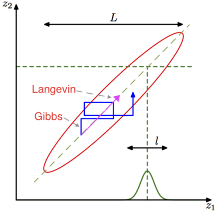

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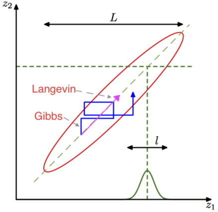

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- This method is called Langevin dynamics (Neal, 2010). Has its origins in statistical Physics.

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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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.. where W_m is the weight assigned to worker m (for more details, see "Bayes and Big Data: The Consensus Monte Carlo Algorithm" by Scott et al (2016)).

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- MCMC is a very general technique for generating samples from a distribution
- Looked at some MCMC algorithms, such as MH and Gibbs sampling
  - MH is very general. Gibbs is very easy to derive is local conditionals can be found easily
- MCMC is random-walk based method, so converge can be slow
- Using gradient information can make convergence faster (e.g., Langevin methods)
  - Several other alternatives too1 (e.g., Hamiltonian Monte Carlo) which we didn't discuss here
- MCMC can be scaled up to large datasets (online and distributed MCMC methods)
- Some other issues of MCMC
  - Assessing convergence can be hard (there exist methods but beyond the scope of this class)
  - Representation of the distribution requires storing all the samples (also, making predictions can be slow since it requires empirically averaging the predictions computed using each MCMC sample)