Markov Chain Monte Carlo

Shinichi Nakajima

Technische Universität Berlin

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Shinichi Nakajima

Technische Universität Berlin

Bayesian Learning (easy cases)

Gaussian

F

Posterior:
$$p(\boldsymbol{w}|\mathcal{D}) \propto p(\boldsymbol{w},\mathcal{D}) \propto \underbrace{\exp\left(-\frac{\mu^{\top}C^{-1}\mu}{2}\right)}_{\text{prior}} \underbrace{\prod_{i=1}^{n} \exp\left(-\frac{(\mu-\boldsymbol{x}^{(i)})^{\top}\boldsymbol{\Sigma}^{-1}(\mu-\boldsymbol{x}^{(i)})}{2}\right)}_{\text{likelihood}}$$

Complete the square! $\propto \exp\left(-\frac{(\mu-\boldsymbol{m}_{\mu})^{\top}\boldsymbol{S}_{\mu}^{-1}(\mu-\boldsymbol{m}_{\mu})}{2}\right)$
 $\therefore \quad p(\boldsymbol{w}|\mathcal{D}) = \mathcal{N}(\mu; \boldsymbol{m}_{u}, \boldsymbol{S}_{u})$

Multinomial

Posterior:
$$p(\boldsymbol{w}|\mathcal{D}) \propto p(\boldsymbol{w},\mathcal{D}) \propto \underbrace{\prod_{k=1}^{K} \theta_k^{\phi_k-1}}_{\text{prior}} \underbrace{\prod_{k=1}^{K} \theta_k^{x_k}}_{\text{likelihood}}$$

Add exponents! $\propto \prod_{k=1}^{K} \theta_k^{x_k+\phi_k-1}$
 $\therefore p(\boldsymbol{w}|\mathcal{D}) = \text{Dir}\left(\theta; \{x_k + \phi_k\}_{k=1}^K\right)$

These two patterns cover most of the cases, including approximate learning! Bayesian learning is computationally hard, but Bayesian do easy work. All what you need are square completion, addition, and Wikipedia (to consult on moments)!

Shinichi Nakajima

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If Wikipedia does not know, ...

moments (expectation of some function f(w)) are approximated by

 $\int f(\boldsymbol{w}) \cdot p(\boldsymbol{w}|\mathcal{D}) d\boldsymbol{w} \approx \frac{1}{J} \sum_{j=1}^{J} f(\boldsymbol{w}^{(j)}), \quad \text{where} \quad \boldsymbol{w}^{(j)} \sim p(\boldsymbol{w}|\mathcal{D}).$

MCMC Sampling (Metropolis-Hastings, Gibbs Sampling)

or

$$\int f(\boldsymbol{w}) \cdot p(\boldsymbol{w}|\mathcal{D}) d\boldsymbol{w} \approx \int f(\boldsymbol{w}) \cdot q(\boldsymbol{w}) d\boldsymbol{w} \quad \text{where} \quad q(\boldsymbol{w}) \approx p(\boldsymbol{w}|\mathcal{D}).$$

Deterministic Approximation (Laplace Approximation, Variational Bayes, Expectation Propagation)

q(w) must be in a known form.

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We need samples such that



Metropolis-Hastings (MH) (a general method):

In the *j*-th iteration,

1

Draw a sample
$$w^* \sim r(w|w^{(j-1)})$$
,

$$\boldsymbol{w}^{(j)} = \begin{cases} \boldsymbol{w}^* & \text{with probability} \quad T, \\ \boldsymbol{w}^{(j-1)} & \text{with probability} \quad 1-T, \end{cases}$$

6

with acceptance probability (which satisfies detailed balance property appendix)

$$T = \min\left(1, \frac{p(\boldsymbol{w}^*, \mathcal{D}) r\left(\boldsymbol{w}^{(j-1)} | \boldsymbol{w}^*\right)}{p\left(\boldsymbol{w}^{(j-1)}, \mathcal{D}\right) r\left(\boldsymbol{w}^* | \boldsymbol{w}^{(j-1)}\right)}\right)$$



$$\textbf{e.g., } r(\boldsymbol{w}|\boldsymbol{w}^{(j-1)}) \propto \exp\left(-\frac{\|\boldsymbol{w}-\boldsymbol{w}^{(j-1)}\|^2}{2\gamma^2}\right).$$

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We need samples such that

$$\boldsymbol{w} \sim \underbrace{p(\boldsymbol{w}|\mathcal{D})}_{\text{unknown}} \propto \underbrace{p(\boldsymbol{w},\mathcal{D})}_{\text{known!}}.$$

If $p(w_m | w_{\setminus m}, \mathcal{D})$ is in a known form (sampler available),



We need samples such that





If $p(w_m | w_{\setminus m}, \mathcal{D})$ is in a known form (sampler available),

Gibbs Sampling (GS) (a special case of MH) is efficient:

In the *j*-th iteration,

Draw a sample *element*
$$w_m^* \sim p(w_m | w_{\backslash m}^{(j-1)}, \mathcal{D})$$
, and set $w_{\backslash m}^* = w_{\backslash m}^{(j-1)}$

2 Set
$$w_m^{(j)} = w^*$$
 (with probability 1).

The reason why the acceptance probability is one is

$$T = \min\left(1, \frac{p(\boldsymbol{w}^*, \mathcal{D})r\left(\boldsymbol{w}^{(j-1)} | \boldsymbol{w}^*\right)}{p\left(\boldsymbol{w}^{(j-1)}, \mathcal{D}\right)r\left(\boldsymbol{w}^* | \boldsymbol{w}^{(j-1)}\right)}\right)$$

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Latent Dirichlet Allocation

The William Randolph Hearst Foundation will give \$125 million to Lincoln Center, Metropolitan Opera Co., New York Philharmonic and Juilliard School. "Our board felt that we had a real opportunity to make a mark on the future of the performing arts with these grants an act every bit as important as our traditional areas of support in health, medical research, education and the social services." Hearst Foundation President Randolph A. Hearst said Monday in announcing the grants. Lincoln Center's share will be \$200,000 for its new building, which will house young artists and provide new public facilities. The Metropolitan Opera Co, and the performing arts are taught, will get \$200,000. The Hearst Foundation, a leading supporter of the Lincoln Center Consolidated Corporate Fund, will make its usual annual \$100,000 donation, too.

Likelihood and Prior

$$p(\boldsymbol{w}^{(n,m)}|\boldsymbol{\Theta},\boldsymbol{B}) = \prod_{l=1}^{L} \left((\boldsymbol{B}\boldsymbol{\Theta}^{\top})_{l,m} \right)^{\boldsymbol{w}_{l}^{(n,m)}},$$
$$p(\boldsymbol{\Theta}) \propto \prod_{m=1}^{M} \prod_{h=1}^{H} (\boldsymbol{\Theta}_{m,h})^{\alpha-1},$$
$$p(\boldsymbol{B}) \propto \prod_{h=1}^{H} \prod_{l=1}^{L} (\boldsymbol{B}_{l,h})^{\eta-1}.$$

Word distribution is a mixture of multinomial *topic* distribution.



 $\boldsymbol{\theta} \in [0, 1]^{M \times H}$:Document parameter $\boldsymbol{B} \in [0, 1]^{L \times H}$:Topic parameter

 $\begin{array}{l} M: \# \mbox{ of documents} \\ L: \mbox{vocabulary size} \\ H: \# \mbox{ of topics } (\leq \min(M,L)) \\ N^{(m)}: \# \mbox{ of words in } m \mbox{-th document} \\ \alpha, \beta: \mbox{Hyperparameters} \end{array}$

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Likelihood and Prior

$$p(\boldsymbol{w}^{(n,m)}|\boldsymbol{\Theta},\boldsymbol{B}) = \prod_{l=1}^{L} \left(\sum_{h=1}^{H} B_{l,h} \boldsymbol{\Theta}_{m,h} \right)^{w_l^{(n,m)}},$$
$$p(\boldsymbol{\Theta}) \propto \prod_{m=1}^{M} \prod_{h=1}^{H} (\boldsymbol{\Theta}_{m,h})^{\alpha-1},$$
$$p(\boldsymbol{B}) \propto \prod_{h=1}^{H} \prod_{l=1}^{L} (B_{l,h})^{\eta-1}.$$

Sum in the probability (mixture) is intractable.



 $\boldsymbol{\Theta} \in [0, 1]^{M \times H}$:Document parameter $\boldsymbol{B} \in [0, 1]^{L \times H}$:Topic parameter

$$\label{eq:model} \begin{split} M:& \text{# of documents} \\ L: \text{vocabulary size} \\ H:& \text{# of topics } (\leq \min(M,L)) \\ N^{(m)}:& \text{# of words in m-th document} \end{split}$$

 α, β :Hyperparameters

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Complete Likelihood and Prior

$$p(\boldsymbol{w}^{(n,m)}, \boldsymbol{z}^{(n,m)} | \boldsymbol{\Theta}, \boldsymbol{B}) = \prod_{l=1}^{L} \left(\prod_{h=1}^{H} \left(B_{l,h} \Theta_{m,h} \right)^{\boldsymbol{z}_{h}^{(n,m)}} \right)^{\boldsymbol{w}_{l}^{(n,m)}},$$
$$p(\boldsymbol{\Theta}) \propto \prod_{m=1}^{M} \prod_{h=1}^{H} (\Theta_{m,h})^{\alpha-1},$$
$$p(\boldsymbol{B}) \propto \prod_{h=1}^{H} \prod_{l=1}^{L} (B_{l,h})^{\eta-1}.$$

Latent variable $z^{(n,m)}$ changes the sum to the product,

$$\begin{split} \boldsymbol{\theta} &\in [0,1]^{M \times H} : \text{Document parameter} \\ \boldsymbol{B} &\in [0,1]^{L \times H} : \text{Topic parameter} \\ \boldsymbol{z}^{(n,m)} &\in [0,1]^{H} : \text{Topic assignment for each word} \\ &\boldsymbol{M} : \# \text{ of documents} \\ &\boldsymbol{L} : \text{vocabulary size} \\ &\boldsymbol{H} : \# \text{ of topics }(\leq \min(M,L)) \\ &\boldsymbol{N}^{(m)} : \# \text{ of words in } m\text{-th document} \\ &\boldsymbol{a}, \boldsymbol{\beta} : \text{Hoorparameters} \end{split}$$

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Complete Likelihood and Prior

$$p(\boldsymbol{w}^{(n,m)}, \boldsymbol{z}^{(n,m)} | \boldsymbol{\Theta}, \boldsymbol{B}) = \prod_{h=1}^{H} (\boldsymbol{\Theta}_{m,h})^{z_{h}^{(n,m)}} \prod_{l=1}^{L} (\boldsymbol{B}_{l,h})^{w_{l}^{(n,m)} z_{h}^{(n,m)}},$$

$$p(\boldsymbol{\Theta}) \propto \prod_{m=1}^{M} \prod_{h=1}^{H} (\boldsymbol{\Theta}_{m,h})^{\alpha-1},$$

$$p(\boldsymbol{B}) \propto \prod_{h=1}^{H} \prod_{l=1}^{L} (\boldsymbol{B}_{l,h})^{\eta-1}.$$

Latent variable $z^{(n,m)}$ changes the sum to the product, and makes likelihood separable.

$$\begin{split} \boldsymbol{\theta} &\in [0,1]^{M \times H} : \texttt{Document parameter} \\ \boldsymbol{B} &\in [0,1]^{L \times H} : \texttt{Topic parameter} \\ \boldsymbol{z}^{(n,m)} &\in [0,1]^{H} : \texttt{Topic assignment for each word} \\ & \boldsymbol{M} : \texttt{\# of documents} \\ & \boldsymbol{L} : \texttt{vocabulary size} \\ & \boldsymbol{H} : \texttt{\# of topics} (\leq \min(M,L)) \\ & \boldsymbol{N}^{(m)} : \texttt{\# of words in } m \text{-th document} \end{split}$$

 α, β : Hyperparameters

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Joint is NOT in known form, but ...

 $\text{Posterior: } p\left(\{\boldsymbol{z}^{(n,m)}\}, \boldsymbol{\Theta}, \boldsymbol{B} | \{\boldsymbol{w}^{(n,m)}\}\right) \propto p(\{\boldsymbol{z}^{(n,m)}\}, \boldsymbol{\Theta}, \boldsymbol{B}, \{\boldsymbol{w}^{(n,m)}\}), \text{ where }$

$$p(\{z^{(n,m)}\}, \Theta, B, \{w^{(n,m)}\}) = p(\{w^{(n,m)}\}, \{z^{(n,m)}\}|\Theta, B)p(\Theta)p(B)$$

$$\propto \prod_{m=1}^{M} \prod_{n=1}^{N(m)} \prod_{h=1}^{H} (\Theta_{m,h})^{z_{h}^{(n,m)} + (\alpha-1)/N^{(m)}} \prod_{l=1}^{L} (B_{l,h})^{w_{l}^{(n,m)} z_{h}^{(n,m)} + (\eta-1)/(MN^{(m)})}.$$

Joint distribution (on $\{z^{(n,m)}\}, \Theta, B$) is not in a known form, but *conditionals*

$$p(\{z^{(n,m)}\}|\boldsymbol{\Theta}, \boldsymbol{B}, \{w^{(n,m)}\}) \propto \prod_{m=1}^{M} \prod_{n=1}^{N^{(m)}} \prod_{h=1}^{H} \left(\boldsymbol{\Theta}_{m,h} \prod_{l=1}^{L} (B_{l,h})^{w_{l}^{(n,m)}}\right)^{z_{h}^{(n,m)}} \qquad \text{Multinomial}$$

$$p(\boldsymbol{\Theta}|\{z^{(n,m)}\}, \{w^{(n,m)}\}) \propto \prod_{m=1}^{M} \prod_{n=1}^{N^{(m)}} \prod_{h=1}^{H} (\boldsymbol{\Theta}_{m,h})^{z_{h}^{(n,m)} + (\alpha-1)/N^{(m)}} \qquad \text{Dirichlet}$$

$$p(\boldsymbol{B}|\{z^{(n,m)}\}, \{w^{(n,m)}\}) \propto \prod_{m=1}^{M} \prod_{n=1}^{N^{(m)}} \prod_{h=1}^{H} \prod_{l=1}^{L} (B_{l,h})^{w_{l}^{(n,m)}} z_{h}^{(n,m)} + (\eta-1)/(MN^{(m)}) \qquad \text{Dirichlet}$$

are in known forms. \rightarrow Gibbs sampling!

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(Naive) Gibbs Sampling:

In *j*-th step,

- 1 For each (n,m) independently, draw $z^{(j,n,m)} \sim p(z^{(n,m)}|\Theta^{(j-1)}, B^{(j-1)}, \{w^{(n,m)}\})$,
- 2 For each *m* independently, draw $\widetilde{\theta}_m^{(j)} \sim p(\widetilde{\theta}_m | \{z^{(j,n,m)}\}, \{w^{(n,m)}\})$,
- 3 For each *h* independently, draw $\beta_h^{(j)} \sim p(\beta_h | \{z^{(j,n,m)}\}, \{w^{(n,m)}\})$.

$$p(\{z^{(n,m)}\}|\boldsymbol{\Theta}, \boldsymbol{B}, \{w^{(n,m)}\}) \propto \prod_{m=1}^{M} \prod_{n=1}^{N^{(m)}} \prod_{h=1}^{H} \left(\boldsymbol{\Theta}_{m,h} \prod_{l=1}^{L} (B_{l,h})^{w_{l}^{(n,m)}} \tilde{\boldsymbol{\zeta}}_{h}^{(m,m)}\right)^{\tilde{\boldsymbol{\zeta}}_{h}^{(m,m)}} \qquad \text{Multinomial}$$

$$p(\boldsymbol{\Theta}|\{z^{(n,m)}\}, \{w^{(n,m)}\}) \propto \prod_{m=1}^{M} \prod_{n=1}^{N^{(m)}} \prod_{h=1}^{H} (\boldsymbol{\Theta}_{m,h})^{\tilde{\boldsymbol{\zeta}}_{h}^{(n,m)} + (\alpha-1)/N^{(m)}} \qquad \text{Dirichlet}$$

$$p(\boldsymbol{B}|\{z^{(n,m)}\}, \{w^{(n,m)}\}) \propto \prod_{m=1}^{M} \prod_{n=1}^{N^{(m)}} \prod_{h=1}^{H} \prod_{l=1}^{L} (B_{l,h})^{w_{l}^{(n,m)}} \tilde{\boldsymbol{\zeta}}_{h}^{(n,m)} + (\eta-1)/(MN^{(m)}) \qquad \text{Dirichlet}$$

Conditionally independent! (\rightarrow easily parallelized) But we can do better.

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Bayesian Learning 0000 Markov Chain Monte Carlo (MCMC) Sampling Approximate Bayesian Learning

Gibbs Sampling

Since joint is in (independent) Dirichlet forms of Θ and **B**, given $\{z^{(n,m)}\}$, we can marginalize:

$$p(\{z^{(n,m)}\}, \{w^{(n,m)}\}) = \int p(\{z^{(n,m)}\}, \Theta, B, \{w^{(n,m)}\}) d\Theta dB$$
$$\propto \prod_{h=1}^{H} \left\{ \left(\prod_{m=1}^{M} \Gamma\left(\alpha + \sum_{n=1}^{N^{(m)}} z_{h}^{(n,m)}\right) \right) \left(\frac{\prod_{l=1}^{L} \Gamma\left(\eta + \sum_{m=1}^{M} \sum_{n=1}^{N^{(m)}} w_{l}^{(n,m)} z_{n}^{(n,m)}\right)}{\Gamma\left(L\eta + \sum_{m=1}^{M} \sum_{n=1}^{N^{(m)}} z_{m}^{(n,m)}\right)} \right) \right\}.$$

Now $\{z^{(n,m)}\}$ are mutually dependent, and

$$p(\boldsymbol{z}^{(n,m)}|\{\boldsymbol{z}^{(n',m')}\}_{(n',m')\neq(n,m)},\{\boldsymbol{w}^{(n,m)}\}) = \frac{p(\{\boldsymbol{z}^{(n,m)}\},\{\boldsymbol{w}^{(n,m)}\})}{p(\{\boldsymbol{z}^{(n',m')}\}_{n'\neq n,m'\neq m},\{\boldsymbol{w}^{(n,m)}\})} \\ \propto \prod_{h=1}^{H} \left\{ \frac{\left(\alpha + \sum_{n'\neq n} z_{h}^{(n',m')}\right)\left(\eta + \sum_{(n',m')\neq(n,m)} w_{l(\boldsymbol{w}^{(n,m)})}^{(n',m')} \sum_{l} z_{h}^{(n,m)}}{\left(L\eta + \sum_{(n',m')\neq(n,m)} z_{h}^{(n',m')}\right)} \right\}^{\boldsymbol{z}_{h}^{(n,m)}}$$

For derivation, see Wikipedia for Dirichlet moments, and use $\Gamma(\tau + 1) = \tau \Gamma(\tau)$.

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Collapsed Gibbs Sampling:

In *j*-th step,

For a pair
$$(n, m)$$
 chosen,
draw a sample $z^{(j,n,m)} \sim p(z^{(n,m)}|\{z^{(j-1,n',m')}\}_{(n',m')\neq(n,m)}, \{w^{(n,m)}\})$,
and set $z^{(j,n',m')} = z^{(j-1,n',m')}$ for $(n',m') \neq (n,m)$.

Usually, (n, m) is chosen sequentially, and pick a sample every after all $\{z^{(n,m)}\}$ are updated.

$$p(\boldsymbol{z}^{(n,m)}|\{\boldsymbol{z}^{(n',m')}\}_{(n',m')\neq(n,m)},\{\boldsymbol{w}^{(n,m)}\}) = \frac{p(\{\boldsymbol{z}^{(n,m)}\},\{\boldsymbol{w}^{(n,m)}\})}{p(\{\boldsymbol{z}^{(n',m')}\}_{n'\neq n,m'\neq m},\{\boldsymbol{w}^{(n,m)}\})} \\ \propto \prod_{h=1}^{H} \left\{ \frac{\left(\alpha + \sum_{n'\neq n} z_{h}^{(n',m)}\right) \left(\eta + \sum_{(n',m')\neq(n,m)} w_{l(\boldsymbol{w}^{(n,m)})}^{(n',m')} z_{h}^{(n',m')}\right)}{\left(L\eta + \sum_{(n',m')\neq(n,m)} z_{h}^{(n',m')}\right)} \right\}^{z_{h}^{(n,m)}}.$$

Shinichi Nakajima

Technische Universität Berlin

Collapsed Gibbs Sampling:

In j-th step,

For a pair
$$(n, m)$$
 chosen,
draw a sample $z^{(j,n,m)} \sim p(z^{(n,m)}|\{z^{(j-1,n',m')}\}_{(n',m')\neq(n,m)}, \{w^{(n,m)}\})$,
and set $z^{(j,n',m')} = z^{(j-1,n',m')}$ for $(n', m') \neq (n, m)$.

Usually, (n, m) is chosen sequentially, and pick a sample every after all $\{z^{(n,m)}\}$ are updated.

* The energy in the right figure is a collapsed likelihood

$$p(\{z^{(n,m)}\}, \{w^{(n,m)}\}) = \int p(\{z^{(n,m)}\}, \Theta, B, \{w^{(n,m)}\}) d\Theta dB,$$

which is proportional to the posterior $p(\{\widehat{z}^{(n,m)}\}|\{w^{(n,m)}\}\})$.



Collapsed Gibbs Sampling:

In j-th step,

For a pair
$$(n, m)$$
 chosen,
draw a sample $z^{(j,n,m)} \sim p(z^{(n,m)}|\{z^{(j-1,n',m')}\}_{(n',m')\neq(n,m)}, \{w^{(n,m)}\})$,
and set $z^{(j,n',m')} = z^{(j-1,n',m')}$ for $(n',m') \neq (n,m)$.

Usually, (n, m) is chosen sequentially, and pick a sample every after all $\{z^{(n,m)}\}$ are updated.

With the estimator $\widehat{z}^{(n,m)} = \frac{1}{J - J_{\text{burn-in}}} \sum_{j=J_{\text{burn-in}}+1}^{J} z^{(j,n,m)}$,



Collapsed Gibbs Sampling:

In *j*-th step,

1 For a pair (n, m) chosen, draw a sample $z^{(j,n,m)} \sim p(z^{(n,m)}|\{z^{(j-1,n',m')}\}_{(n',m')\neq(n,m)}, \{w^{(n,m)}\})$, and set $z^{(j,n',m')} = z^{(j-1,n',m')}$ for $(n',m')\neq(n,m)$.

Usually, (n, m) is chosen sequentially, and pick a sample every after all $\{z^{(n,m)}\}$ are updated.

With the estimator $\widehat{z}^{(n,m)} = \frac{1}{J - J_{\text{burn-in}}} \sum_{j=J_{\text{burn-in}}+1}^{J} z^{(j,n,m)}$,

$$\begin{split} p(\widetilde{\theta}_{m}|\{\widehat{z}^{(n,m)}\},\{w^{(n,m)}\}) &\propto \prod_{h=1}^{H} (\theta_{m,h})^{\alpha-1+\sum_{n=1}^{M(m)} \widehat{z}_{h}^{(n,m)}} \\ p(\beta_{h}|\{\widehat{z}^{(n,m)}\},\{w^{(n,m)}\}) &\propto \prod_{l=1}^{L} (B_{l,h})^{\eta-1+\sum_{m=1}^{M} \sum_{n=1}^{M(m)} w_{l}^{(n,m)} \widehat{z}_{h}^{(n,m)}} \end{split}$$



Shinichi Nakajima

Technische Universität Berlin

Collapsed Gibbs Sampling:

In j-th step,

For a pair (n, m) chosen, draw a sample $z^{(j,n,m)} \sim p(z^{(n,m)}|\{z^{(j-1,n',m')}\}_{(n',m')\neq(n,m)}, \{w^{(n,m)}\})$, and set $z^{(j,n',m')} = z^{(j-1,n',m')}$ for $(n',m') \neq (n,m)$.

Usually, (n, m) is chosen sequentially, and pick a sample every after all $\{z^{(n,m)}\}$ are updated.

With the estimator
$$\hat{z}^{(n,m)} = \frac{1}{J - J_{\text{burn-in}}} \sum_{j=J_{\text{burn-in}}+1}^{J} z^{(j,n,m)}$$
,

$$\begin{split} p(\widetilde{\boldsymbol{\theta}}_{m}|\{\widehat{\boldsymbol{z}}^{(n,m)}\}, \{\boldsymbol{w}^{(n,m)}\}) &= \mathrm{Dir}\left(\{\alpha + \sum_{n=1}^{N^{(m)}} \widehat{\boldsymbol{z}}_{h}^{(n,m)}\}_{h=1}^{H}\right) \\ p(\boldsymbol{\beta}_{h}|\{\widehat{\boldsymbol{z}}^{(n,m)}\}, \{\boldsymbol{w}^{(n,m)}\}) &= \mathrm{Dir}\left(\{\eta + \sum_{m=1}^{M} \sum_{n=1}^{N^{(m)}} w_{l}^{(n,m)} \widehat{\boldsymbol{z}}_{h}^{(n,m)}\}_{l=1}^{L}\right) \end{split}$$



More efficient! But lost independence... ($\{z^{(n,m)}\}\$ are mutually dependent).

Shinichi Nakajima

Collapsed Gibbs Sampling:

In *j*-th step,

1 For a pair (n,m) chosen, estimate $\widehat{\Theta}_{\backslash (n,m)} = \langle \Theta \rangle_{p(\Theta|\{z^{(j-1,n',m')}\}_{\backslash (n,m)}, \{w^{(n,m)}\})}, \quad \widehat{B}_{\backslash (n,m)} = \langle B \rangle_{p(B|\{z^{(j-1,n',m')}\}_{\backslash (n,m)}, \{w^{(n,m)}\})}.$ 2 Draw a sample $z^{(j,n,m)} \sim p(z^{(n,m)})\widehat{\Theta}_{\backslash (n,m)}, \widehat{B}_{\backslash (n,m)}, \{w^{(n,m)}\}),$ and set $z^{(j,n',m')} = z^{(j-1,n',m')}$ for $(n',m') \neq (n,m).$

Usually, (n, m) is chosen sequentially, and pick a sample every after all $\{z^{(n,m)}\}$ are updated.

With the estimator $\overline{z}^{(n,m)} = \frac{1}{J - J_{\text{burn-in}}} \sum_{j=J_{\text{burn-in}}+1}^{J} z^{(j,n,m)}$,

$$\begin{split} p(\widetilde{\boldsymbol{\theta}}_{m}|\{\widehat{\boldsymbol{z}}^{(n,m)}\},\{\boldsymbol{w}^{(n,m)}\}) &= \operatorname{Dir}\left(\{\alpha + \sum_{n=1}^{N^{(m)}}\widehat{\boldsymbol{z}}_{h}^{(n,m)}\}_{h=1}^{H}\right)\\ p(\boldsymbol{\beta}_{h}|\{\widehat{\boldsymbol{z}}^{(n,m)}\},\{\boldsymbol{w}^{(n,m)}\}) &= \operatorname{Dir}\left(\{\eta + \sum_{m=1}^{M}\sum_{n=1}^{N^{(m)}}w_{l}^{(n,m)}\widehat{\boldsymbol{z}}_{h}^{(n,m)}\}_{l=1}^{L}\right) \end{split}$$



Amounts to global parameter update after each element sampling.

Shinichi Nakajima

Approximate Collapsed Gibbs Sampling

In j-th step,

- For chosen pairs (n, m), independently draw $z^{(j,n,m)} \sim p(z^{(n,m)}|\widehat{\boldsymbol{\Theta}}^{(j-1)}, \widehat{\boldsymbol{B}}^{(j-1)}, \{w^{(n,m)}\})$,
- 2 Estimate $\widehat{\Theta}^{(j)} = \langle \Theta \rangle_{p(\Theta|\{z^{(j,n,m)}\}, \{w^{(n,m)}\})},$
- 3 Estimate $\widehat{\boldsymbol{B}}^{(j)} = \langle \boldsymbol{B} \rangle_{p(\boldsymbol{B}|[\boldsymbol{z}^{(j,n,m)}], \{\boldsymbol{w}^{(n,m)}\})}$.

With the estimator
$$\hat{z}^{(n,m)} = \frac{1}{J - J_{\text{burn-in}}} \sum_{j=J_{\text{burn-in}}+1}^{J} z^{(j,n,m)}$$
,

$$\begin{split} p(\widetilde{\boldsymbol{\theta}}_{m}|\{\widehat{\boldsymbol{z}}^{(n,m)}\}, \{\boldsymbol{w}^{(n,m)}\}) &= \operatorname{Dir}\left(\{\alpha + \sum_{n=1}^{N^{(m)}} \widehat{\boldsymbol{z}}_{h}^{(n,m)}\}_{h=1}^{H}\right) \\ p(\boldsymbol{\beta}_{h}|\{\widehat{\boldsymbol{z}}^{(n,m)}\}, \{\boldsymbol{w}^{(n,m)}\}) &= \operatorname{Dir}\left(\{\eta + \sum_{m=1}^{M} \sum_{n=1}^{N^{(m)}} w_{l}^{(n,m)} \widehat{\boldsymbol{z}}_{h}^{(n,m)}\}_{l=1}^{L}\right) \end{split}$$



This should work.

Shinichi Nakajima

Markov Chain Monte Carlo

Technische Universität Berlin

Variational Bayesian Learning

Variational Bayesian Approximation:

In j-th step,

- 1 For chosen pairs (n,m), estimate $\widehat{z}^{(j,n,m)} = \langle z^{(n,m)} \rangle_{p(z^{(n,m)})\widehat{\theta}^{(j-1)}, \widehat{B}^{(j-1)}, \{w^{(n,m)}\})}$
- 2 Estimate $\widehat{\Theta}^{(j)} = \langle \Theta \rangle_{p(\Theta|\{z^{(j,n,m)}\}, \{w^{(n,m)}\})},$
- 3 Estimate $\widehat{B}^{(j)} = \langle B \rangle_{p(B|\{z^{(j,n,m)}\}, \{w^{(n,m)}\})}$.

Variational Bayes is similar.

Shinichi Nakajima

Variational Bayesian Learning

Variational Bayesian Approximation:

In j-th step,

- **1** For chosen pairs (n, m), estimate $\widehat{z}^{(j,n,m)} = \langle z^{(n,m)} \rangle_{p(\overline{z}^{(n,m)}) \widehat{\Theta}^{(j-1)}, \widehat{B}^{(j-1)}, [w^{(n,m)}]}$
- 2 Estimate $\widehat{\Theta}^{(j)} = \langle \Theta \rangle_{p(\Theta|\{z^{(j,n,m)}\}, \{w^{(n,m)}\})},$
- 3 Estimate $\widehat{\boldsymbol{B}}^{(j)} = \langle \boldsymbol{B} \rangle_{p(\boldsymbol{B}|\{\boldsymbol{z}^{(j,n,m)}\},\{\boldsymbol{w}^{(n,m)}\})}$.

For each k (a part of unknowns) in turn,

Gibbs sampling draws a sample from conditional $w_k \sim p(w_k | w_{\setminus k}, \mathcal{D})$.

- Slow (each iteration gives one sample from the distribution).
- Accurate (correlation between $\{w_k\}$ is taken into account).

Variational Bayes estimates the mean of conditional $\widehat{w}_k = \langle w_k \rangle_{p(w_k | \widehat{w}_{\setminus k}, \mathcal{D})}$.

- Fast (each iteration estimates whole distribution).
- Inaccurate (correlation between $\{w_k\}$ is neglected).

Variational Bayes is similar.

Shinichi Nakajima

Properties of MCMC methods

- Converges to the Bayesian posterior.
- Generally) slower than deterministic methods.
- To get independent samples, we have to subsample from the MCMC sequence.
- Efficient methods are being developed (Hamiltonian Monte Carlo, distributed computation, stochastic gradient).

Appendix: Detailed Balance Property

Transition probability is (all probability below is conditional on \mathcal{D})

$$p(\mathbf{w}^{(j)}|\mathbf{w}^{(j-1)}) = T(\mathbf{w}^{(j)}|\mathbf{w}^{(j-1)}) \cdot r(\mathbf{w}^{(j)}|\mathbf{w}^{(j-1)})$$

= min $\left(r(\mathbf{w}^{(j)}|\mathbf{w}^{(j-1)}), \frac{p(\mathbf{w}^{(j)})r(\mathbf{w}^{(j-1)}|\mathbf{w}^{(j)})}{p(\mathbf{w}^{(j-1)})}\right).$

Therefore,

$$p\left(\mathbf{w}^{(j)}|\mathbf{w}^{(j-1)}\right) p\left(\mathbf{w}^{(j-1)}\right) = \min\left(p\left(\mathbf{w}^{(j-1)}\right) r\left(\mathbf{w}^{(j)}|\mathbf{w}^{(j-1)}\right), p\left(\mathbf{w}^{(j)}\right) r\left(\mathbf{w}^{(j-1)}|\mathbf{w}^{(j)}\right)\right)$$

$$= \min\left(p\left(\mathbf{w}^{(j)}\right) r\left(\mathbf{w}^{(j-1)}|\mathbf{w}^{(j)}\right), p\left(\mathbf{w}^{(j-1)}\right) r\left(\mathbf{w}^{(j)}|\mathbf{w}^{(j-1)}\right)\right)$$

$$= T\left(\mathbf{w}^{(j-1)}|\mathbf{w}^{(j)}\right) r\left(\mathbf{w}^{(j-1)}|\mathbf{w}^{(j)}\right) p\left(\mathbf{w}^{(j)}\right)$$

$$= p\left(\mathbf{w}^{(j-1)}|\mathbf{w}^{(j)}\right) p\left(\mathbf{w}^{(j)}\right) \text{ Detailed Balance Property}$$

$$p\left(\mathbf{w}^{(j)}|\mathbf{w}^{(j-1)}\right) p\left(\mathbf{w}^{(j-1)}\right) d\mathbf{w}^{(j-1)} = \int p\left(\mathbf{w}^{(j-1)}|\mathbf{w}^{(j)}\right) p\left(\mathbf{w}^{(j)}\right) d\mathbf{w}^{(j-1)} = p\left(\mathbf{w}^{(j)}\right)$$

Detailed balance $\Rightarrow p(w^{(j)})$ is stationary of Markov process. back

Shinichi Nakajima

Technische Universität Berlin