Variational inference

Partly based on material developed together with Helge Langseth

Andrés Masegosa and Thomas Dyhre Nielsen

Variational inference – Part II

Plan for this week

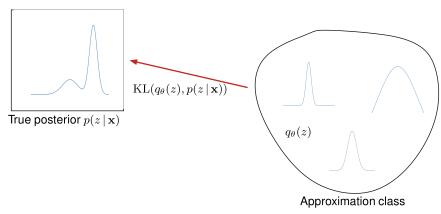
- Day 1: Probabilistic programming
 - Introduction to probabilistic programming
 - Probabilistic programming in Pyro
- Day 2: Variational inference
 - Recap of variational inference (variational inference as optimization)
 - Derivation and implementation of selected examples
 - Bayesian linear regression
 - Factor analysis
 - . .
- Day 3: Variational inference cont'd
 - Black box variational inference
 - Variational inference in Pyro
 - Variational auto-encoders

Variational inference – Part II

Introduction

What is variational inference?

We will approximate the true posterior distribution $p(z \mid \mathbf{x})$ with a variational distribution belonging to a tractable family of distributions.



Task: Fit the variational parameters θ so that the 'distance' $\mathrm{KL}(q_{\theta}(z), p(z \,|\, \mathbf{x}))$ is minimized:

$$\hat{q}(z) = \arg\min_{\theta} \mathrm{KL}(q_{\theta}(z), p(z \mid \mathbf{x})) = \arg\min_{\theta} \int_{\mathbf{z}} q(z) \, \log\left(\frac{q(z)}{p(z \mid \mathbf{x})}\right) \mathrm{d}z$$

Variational inference – Part II Introduction

ELBO: Evidence Lower-BOund

We can rearrange the KL divergence as follows:

$$\begin{aligned} \operatorname{KL}\left(q(\mathbf{z})||p(\mathbf{z}\,|\,\mathbf{x})\right) &= & \mathbb{E}_q \left[\log \frac{q(\mathbf{z})}{p(\mathbf{z}\,|\,\mathbf{x})} \right] \\ &= & \mathbb{E}_q \left[\log \frac{q(\mathbf{z}) \cdot p(\mathbf{x})}{p(\mathbf{z}\,|\,\mathbf{x}) \cdot p(\mathbf{x})} \right] \\ &= & \log p(\mathbf{x}) - \mathbb{E}_q \left[\log \frac{q(\mathbf{z})}{p(\mathbf{z},\mathbf{x})} \right] = \log p(\mathbf{x}) - \mathcal{L}\left(q\right) \end{aligned}$$

where
$$\mathcal{L}\left(q\right) = -\mathbb{E}_q\left[\log \frac{q(\mathbf{z})}{p(\mathbf{z},\mathbf{x})}\right]$$
 is the so-called Evidence Lower Bound (ELBO)

Variational inference - Part II

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VI focuses on the ELBO:

$$\log p(\mathbf{x}) = \mathcal{L}(q) + \mathrm{KL}(q(\mathbf{z})||p(\mathbf{z} | \mathbf{x}))$$

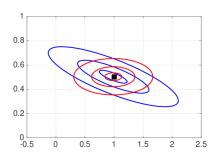
Since $\log p(\mathbf{x})$ is constant wrt. q and $\mathrm{KL}\left(q(\mathbf{z})||p(\mathbf{z}\,|\,\mathbf{x})\right) \geq 0$ it follows:

- We can minimize $\frac{\mathrm{KL}(q(\mathbf{z})||p(\mathbf{z}|\mathbf{x}))}{\mathrm{KL}(q(\mathbf{z})||p(\mathbf{z}|\mathbf{x}))}$ by maximizing $\mathcal{L}(q)$
- This is **computationally simpler** because it uses $p(\mathbf{z}, \mathbf{x})$ instead of $p(\mathbf{z} \mid \mathbf{x})$.
- ullet $\mathcal{L}\left(q
 ight)$ is a *lower bound* of the marginal data log likelihood $\log p(\mathbf{x})$.
- \rightsquigarrow During inference, we will look for $\hat{q}(\mathbf{z}) = \arg \max_{q \in \mathcal{Q}} \mathcal{L}(q)$.

The mean field assumption

We will often use the mean field assumption, which states that $\mathcal Q$ consists of all distributions that *factorizes* according to the equation

$$q(\mathbf{z}) = \prod_{i} q_i \left(z_i \right)$$



Note! This may seem like a very restricted set. However, we can choose any $q(\mathbf{z}) \in \mathcal{Q}$, and this is how the magic (\sim "absorbing information from \mathbf{x} ") happens.

Wrapping it all up: The VB algorithm under MF

Algorithm:

- We have observed X = x, and have access to the full joint p(z, x).
- We posit a *variational family* of distributions $q_j(\cdot | \lambda_j)$, i.e., we choose the distributional form, while wanting to optimize the parameterization λ_j .
- The posterior approximation is assumed to factorize according to the mean-field assumption, and we use the $\mathrm{KL}\left(q(\mathbf{z})||p(\mathbf{z}\,|\,\mathbf{x})\right)$ as our objective.

Algorithm:

Repeat until negligible improvement in terms of $\mathcal{L}\left(q\right)$:

- For each *j*:
 - Somehow choose λ_j to maximize $\mathcal{L}(q)$, typically based on $\{\lambda_i\}_{i\neq j}$.
- Calculate the new $\mathcal{L}(q)$.

Solving the VB optimization

We will maximize $\mathcal{L}\left(q\right) = \mathbb{E}_q\left[\log\frac{p(\mathbf{z},\mathbf{x})}{q(\mathbf{z})}\right]$ under the assumption that $q(\cdot)$ factorizes. Let us pick one j, utilize that $q(\mathbf{z}) = q_j(z_j) \cdot q_{\neg j}(\mathbf{z}_{\neg j})$, and assume $q_{\neg j}(\cdot)$ is kept fixed.

$$\begin{split} \mathcal{L}\left(q\right) &= & \mathbb{E}_{q}\left[\log p(\mathbf{z}, \mathbf{x})\right] - \mathbb{E}_{q}\left[\log q(\mathbf{z})\right] \\ &= & \mathbb{E}_{q_{j}}\mathbb{E}_{q_{\neg j}}\left[\log p(\mathbf{z}, \mathbf{x})\right] - \mathbb{E}_{q_{j}}\mathbb{E}_{q_{\neg j}}\left[\log q(\mathbf{z})\right] \end{split}$$

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For the term $\mathbb{E}_{q_{\neg j}}\left[\log p(\mathbf{z},\mathbf{x})\right]$ we simply define $f_j(z_j)$ so that

$$\log f_j(z_j) = \mathbb{E}_{q_{\neg j}} \left[\log p(\mathbf{z}, \mathbf{x}) \right]$$

We will maximize $\mathcal{L}\left(q\right) = \mathbb{E}_q\left[\log\frac{p(\mathbf{z},\mathbf{x})}{q(\mathbf{z})}\right]$ under the assumption that $q(\cdot)$ factorizes. Let us pick one j, utilize that $q(\mathbf{z}) = q_j(z_j) \cdot q_{\neg j}(\mathbf{z}_{\neg j})$, and assume $q_{\neg j}(\cdot)$ is kept fixed.

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For the other term, notice that $\log q(\mathbf{z}) = \log q_j(z_j) + \log q_{\neg j}(\mathbf{z}_{\neg j})$ Therefore

$$\begin{split} \mathbb{E}_{q_j} \mathbb{E}_{q_{\neg j}} \left[\log q(\mathbf{z}) \right] &= \mathbb{E}_{q_j} \mathbb{E}_{q_{\neg j}} \left[\log q_j(z_j) + \log q_{\neg j}(\mathbf{z}_{\neg j}) \right] \\ &= \mathbb{E}_{q_j} \left[\log q_j(z_j) \right] + \mathbb{E}_{q_{\neg j}} \left[\log q_{\neg j}(\mathbf{z}_{\neg j}) \right] \\ &= \mathbb{E}_{q_j} \left[\log q_j(z_j) \right] + c, \end{split}$$

because $\mathbb{E}_{q_{\neg j}}\left[\log q_{\neg j}(\mathbf{z}_{\neg j})\right]$ is constant wrt. $q_{j}(\cdot)$.

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We get the following result:

The ELBO is maximized wrt. q_i by choosing

$$q_j(z_j) = \frac{1}{Z} \exp \left(\mathbb{E}_{q_{\neg j}} \left[\log p(\mathbf{z}, \mathbf{x}) \right] \right)$$

... and made the following assumptions to get there:

- Mean field: $q(\mathbf{z}) = \prod_i q_i(z_i)$, and specifically $q(\mathbf{z}) = q_j(z_j) \cdot q_{\neg j}(\mathbf{z}_{\neg j})$.
- We optimize wrt. $q_j(\cdot)$, while keeping $q_{\neg j}(\cdot)$ fixed i.e., we do coordinate ascent in probability distribution space.

Variational inference – Part II Solving the VB optimization

VB w/ MF: algorithm

Setup

- We have observed X = x, and can calculate the full joint p(z, x).
- The posterior approximation is assumed to factorize according to the mean-field assumption, and we use the $\mathrm{KL}\left(q(\mathbf{z})||p(\mathbf{z}\,|\,\mathbf{x})\right)$ as our objective.
- We posit a *variational family* of distributions $q_j(z_j | \lambda_j)$, i.e., we choose the distributional form, while wanting to optimize the parameterization λ_j .
- The optimal λ_j will depend on x in fact λ_j encodes all the information about the other variables in the domain that Z_j is "aware of".

VB w/ MF: algorithm

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Algorithm

Repeat until negligible improvement in terms of $\mathcal{L}(q)$:

- For each j:
 - Calculate $\mathbb{E}_{q_{\neg j}}\left[\log p(\mathbf{z}, \mathbf{x})\right]$ using current estimates for $q_i(\cdot \mid \boldsymbol{\lambda}_i), i \neq j$.
 - Choose λ_j so that $q_j(z_j | \lambda_j) \propto \exp(\mathbb{E}_{q_{\neg j}}[\log p(\mathbf{z}, \mathbf{x})])$.
- Calculate the new $\mathcal{L}(q)$.

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Calculating $q_j(z_j\,|\, oldsymbol{\lambda}_j)$ - an observation

The update-rule can equivalently be expressed as

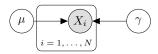
$$\begin{split} \log q_j(z_j \mid \boldsymbol{\lambda}_j) &= \mathbb{E}_{q_{\neg j}} \left[\ln p(\mathbf{z}, \mathbf{x}) \right] + c. \\ &= \sum_{x \in \mathrm{mb}(z_j)} \mathbb{E}_{q_{\neg j}} \log p(x \mid \mathrm{pa}(x)) + \sum_{z \in \mathrm{mb}(z_j)} \mathbb{E}_{q_{\neg j}} \log p(z \mid \mathrm{pa}(z)) + c'. \end{split}$$

Note!

- We only need to consider terms that share a factor with z_j all other terms get absorbed into the constant c.
- \leadsto need only reason about variables in the Markov blanket of Z_j just as for Gibbs sampling!

A simple Gaussian model

A Gaussian model with unknown mean and precision

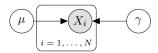


- $X_i \mid \{\mu, \gamma\} \sim \mathcal{N}(\mu, 1/\gamma)$
- $\mu \sim \mathcal{N}(0, \tau^{-1})$
- $\quad \bullet \ \, \gamma \sim \mathsf{Gamma}(\alpha,\beta)$

The probability model

$$p(\mathbf{x}, \mu, \gamma | \tau, \alpha, \beta) = \prod_{i=1}^{N} p(x_i | \mu, \gamma^{-1}) p(\mu | 0, \tau^{-1}) p(\gamma | \alpha, \beta)$$

A Gaussian model with unknown mean and precision



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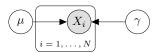
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... after taking the log

$$\log p(\mathbf{x}, \mu, \gamma | \tau, \alpha, \beta) = \sum_{i=1}^{N} \log p(x_i | \mu, \gamma^{-1}) + \log p(\mu | 0, \tau^{-1}) + \log p(\gamma | \alpha, \beta)$$

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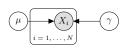
The variational model (full mean field)

$$q(\mu, \gamma) = q(\mu)q(\gamma),$$

where

- $q(\mu) = \mathcal{N}(\nu_p, \tau_p^{-1})$
- $q(\gamma) = \text{Gamma}(\alpha_p, \beta_p)$

$$\log q(\mu) = \mathop{\mathbb{E}}_{\gamma} \log p(\mathbf{x}, \mu, \gamma | \tau, \alpha, \beta) + c =$$



We choose the variational distribution so that

$$\begin{array}{c|c}
\mu & X_i \\
\hline
i = 1, \dots, N
\end{array}$$

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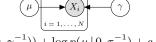
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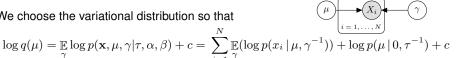
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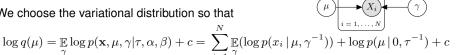
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$$\log p(x_i \mid \mu, \gamma^{-1}) = \mathcal{N}(\mu, \gamma^{-1}) = -\frac{1}{2}\log(2\pi) + \frac{1}{2}\log(\gamma) - \frac{\gamma}{2}(x_i - \mu)^2$$
$$\log p(\mu \mid 0, \tau^{-1}) = \mathcal{N}(0, \tau^{-1}) = -\frac{1}{2}\log(2\pi) + \frac{1}{2}\log(\tau) - \frac{\tau}{2}(\mu)^2$$

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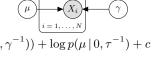
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$$\mu, \gamma^{-1}) + \log p(\mu \mid 0, \tau^{-1}) + c$$

$$\log q(\mu) = \underset{\gamma}{\mathbb{E}} \log p(\mathbf{x}, \mu, \gamma | \tau, \alpha, \beta) + c = \sum_{i=1}^{N} \underset{\gamma}{\mathbb{E}} (\log p(x_i | \mu, \gamma^{-1})) + \log p(\mu | 0, \tau^{-1}) + c$$

$$= \sum_{i=1}^{N} \underset{\gamma}{\mathbb{E}} \left(-\frac{\gamma}{2} (x_i - \mu)^2 \right) - \frac{\tau}{2} (\mu)^2 + c$$

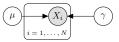
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$$= -\frac{1}{2} \mathbb{E} (\gamma) \left(\sum_{i=1}^{N} x_i^2 + N \cdot \mu^2 - 2\mu \sum_{i=1}^{N} x_i \right) - \frac{\tau}{2} (\mu)^2 + c$$

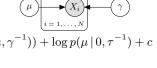


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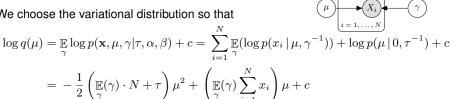
$$= -\frac{1}{2} \left(\underset{\gamma}{\mathbb{E}} (\gamma) \cdot N + \tau \right) \mu^2 + \left(\underset{\gamma}{\mathbb{E}} (\gamma) \sum_{i=1}^{N} x_i \right) \mu + c$$



$$\log q(\mu) = \underset{\gamma}{\mathbb{E}} \log p(\mathbf{x}, \mu, \gamma | \tau, \alpha, \beta) + c = \sum_{i=1}^{N} \underset{\gamma}{\mathbb{E}} (\log p(x_i | \mu, \gamma^{-1})) + \log p(\mu | 0, \tau^{-1}) + c$$

$$= -\frac{1}{2} \left(\underset{\gamma}{\mathbb{E}} (\gamma) \cdot N + \tau \right) \mu^2 + \left(\underset{\gamma}{\mathbb{E}} (\gamma) \sum_{i=1}^{N} x_i \right) \mu + c$$

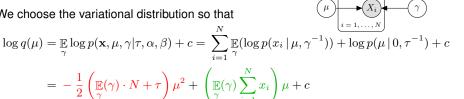
We choose the variational distribution so that



Recall the normal distribution

$$\begin{aligned} \log q(\mu \mid \nu_p, \tau_p^{-1}) &= -\frac{1}{2} \log(2\pi) + \frac{1}{2} \log(\tau_p) - \frac{\tau_p}{2} (\mu - \nu_p)^2 \\ &= -\frac{1}{2} \log(2\pi) + \frac{1}{2} \log(\tau_p) - \tau_p \nu_p^2 - \frac{1}{2} \tau_p \mu^2 + \tau_p \nu_p \mu \end{aligned}$$

We choose the variational distribution so that



Recall the normal distribution

$$\begin{split} \log q(\mu \,|\, \nu_p, \tau_p^{-1}) &= -\frac{1}{2} \log(2\pi) + \frac{1}{2} \log(\tau_p) - \frac{\tau_p}{2} (\mu - \nu_p)^2 \\ &= -\frac{1}{2} \log(2\pi) + \frac{1}{2} \log(\tau_p) - \tau_p \nu_p^2 - \frac{1}{2} \tau_p \mu^2 + \tau_p \nu_p \mu \end{split}$$

We choose the variational distribution so that

We choose the variational distribution so that
$$\log q(\mu) = \mathop{\mathbb{E}}_{\gamma} \log p(\mathbf{x}, \mu, \gamma | \tau, \alpha, \beta) + c = \sum_{i=1}^{N} \mathop{\mathbb{E}}_{\gamma} (\log p(x_i \mid \mu, \gamma^{-1})) + \log p(\mu \mid 0, \tau^{-1}) + c$$

$$= -\frac{1}{2} \left(\mathbb{E}(\gamma) \cdot N + \tau \right) \mu^2 + \left(\mathbb{E}(\gamma) \sum_{i=1}^{N} x_i \right) \mu + c$$

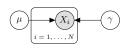
Thus, we see that $q(\mu)$ is normally distributed with

- precision $\tau_p \leftarrow \mathbb{E}_{\gamma}(\gamma) \cdot N + \tau$
- mean $\nu_p \leftarrow \tau_p^{-1} \left(\mathbb{E}_{\gamma}(\gamma) \sum_{i=1}^N x_i \right)$

Recall the normal distribution

$$\log q(\mu \mid \nu_p, \tau_p^{-1}) = -\frac{1}{2}\log(2\pi) + \frac{1}{2}\log(\tau_p) - \frac{\tau_p}{2}(\mu - \nu_p)^2$$
$$= -\frac{1}{2}\log(2\pi) + \frac{1}{2}\log(\tau_p) - \tau_p\nu_p^2 - \frac{1}{2}\tau_p\mu^2 + \tau_p\nu_p\mu$$

$$\log q(\gamma) = \mathop{\mathbb{E}}_{\mu} \log p(\mathbf{x}, \mu, \gamma | \tau, \alpha, \beta) + c =$$



We choose the variational distribution so that

$$\begin{array}{c|c}
\mu & & \\
\hline
 & X_i \\
\hline
 & i = 1, \dots, N
\end{array}$$

$$\log q(\gamma) = \mathop{\mathbb{E}}_{\mu} \log p(\mathbf{x}, \mu, \gamma | \tau, \alpha, \beta) + c =$$

$$\log p(\mathbf{x}, \mu, \gamma | \tau, \alpha, \beta) = \sum_{i=1}^{N} \log p(x_i | \mu, \gamma^{-1}) + \log p(\mu | 0, \tau^{-1}) + \log p(\gamma | \alpha, \beta)$$

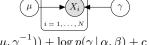
We choose the variational distribution so that

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\hline
 & X_i \\
\hline
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\end{array}$$

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$$\log p(\mathbf{x}, \mu, \gamma | \tau, \alpha, \beta) = \sum_{i=1}^{N} \log p(x_i | \mu, \gamma^{-1}) + \log p(\mu | 0, \tau^{-1}) + \log p(\gamma | \alpha, \beta)$$

We choose the variational distribution so that



$$\log q(\gamma) = \mathbb{E} \log p(\mathbf{x}, \mu, \gamma | \tau, \alpha, \beta) + c = \sum_{i=1}^{N} \mathbb{E} (\log p(x_i | \mu, \gamma^{-1})) + \log p(\gamma | \alpha, \beta) + c$$

$$\log p(\mathbf{x}, \mu, \gamma | \tau, \alpha, \beta) = \sum_{i=1}^{N} \log p(x_i | \mu, \gamma^{-1}) + \log p(\mu | 0, \tau^{-1}) + \log p(\gamma | \alpha, \beta)$$

We choose the variational distribution so that

$$(\mu) \underbrace{X_i}_{i=1,\ldots,N} (\gamma)$$

$$(\lambda, \gamma^{-1}) + \log p(\gamma \mid \alpha, \beta) + c$$

$$\log q(\gamma) = \mathbb{E} \log p(\mathbf{x}, \mu, \gamma | \tau, \alpha, \beta) + c = \sum_{i=1}^{N} \mathbb{E} (\log p(x_i | \mu, \gamma^{-1})) + \log p(\gamma | \alpha, \beta) + c$$

$$\log p(x_i \mid \mu, \gamma^{-1}) = \mathcal{N}(\mu, \gamma^{-1}) = -\frac{1}{2}\log(2\pi) + \frac{1}{2}\log(\gamma) - \frac{\gamma}{2}(x_i - \mu)^2$$
$$\log p(\gamma \mid \alpha, \beta) = \mathsf{Gamma}(\alpha, \beta) = \alpha \cdot \log(\beta) + (\alpha - 1)\log(\gamma) - \beta \cdot \gamma - \log(\Gamma(\alpha))$$

We choose the variational distribution so that

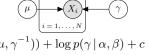
$$\begin{array}{c|c}
\mu & X_i & \gamma \\
\downarrow i=1,\dots,N & \gamma
\end{array}$$

$$\mu_i \gamma^{-1}) + \log p(\gamma \mid \alpha, \beta) + c$$

$$\log q(\gamma) = \mathbb{E} \log p(\mathbf{x}, \mu, \gamma | \tau, \alpha, \beta) + c = \sum_{i=1}^{N} \mathbb{E} (\log p(x_i | \mu, \gamma^{-1})) + \log p(\gamma | \alpha, \beta) + c$$

$$\log p(x_i \mid \mu, \gamma^{-1}) = \mathcal{N}(\mu, \gamma^{-1}) = -\frac{1}{2}\log(2\pi) + \frac{1}{2}\log(\gamma) - \frac{\gamma}{2}(x_i - \mu)^2$$
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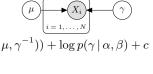
We choose the variational distribution so that



$$\log q(\gamma) = \mathbb{E} \log p(\mathbf{x}, \mu, \gamma | \tau, \alpha, \beta) + c = \sum_{i=1}^{N} \mathbb{E} (\log p(x_i | \mu, \gamma^{-1})) + \log p(\gamma | \alpha, \beta) + c$$
$$= \frac{N}{2} \log(\gamma) - \frac{\gamma}{2} \sum_{i=1}^{N} \mathbb{E} (x_i - \mu)^2 + (\alpha - 1) \log(\gamma) - \beta \cdot \gamma + c$$

$$\log p(x_i \mid \mu, \gamma^{-1}) = \mathcal{N}(\mu, \gamma^{-1}) = -\frac{1}{2}\log(2\pi) + \frac{1}{2}\log(\gamma) - \frac{\gamma}{2}(x_i - \mu)^2$$
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We choose the variational distribution so that

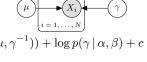


$$\log q(\gamma) = \mathbb{E} \log p(\mathbf{x}, \mu, \gamma | \tau, \alpha, \beta) + c = \sum_{i=1}^{N} \mathbb{E} (\log p(x_i | \mu, \gamma^{-1})) + \log p(\gamma | \alpha, \beta) + c$$

$$= \frac{N}{2} \log(\gamma) - \frac{\gamma}{2} \sum_{i=1}^{N} \mathbb{E} (x_i - \mu)^2 + (\alpha - 1) \log(\gamma) - \beta \cdot \gamma + c$$

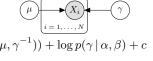
$$= \left(\frac{N}{2} + \alpha - 1\right) \log(\gamma) - \left(\frac{1}{2} \sum_{i=1}^{N} \mathbb{E} (x_i - \mu)^2 + \beta\right) \cdot \gamma + c$$

We choose the variational distribution so that



$$\log q(\gamma) = \mathbb{E} \log p(\mathbf{x}, \mu, \gamma | \tau, \alpha, \beta) + c = \sum_{i=1}^{N} \mathbb{E} (\log p(x_i | \mu, \gamma^{-1})) + \log p(\gamma | \alpha, \beta) + c$$
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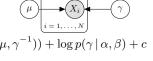
We choose the variational distribution so that



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$$\log q(\gamma \mid \alpha_p, \beta_p) = \alpha_p \cdot \log(\beta_p) + (\alpha_p - 1) \log(\gamma) - \beta \cdot \gamma - \log(\Gamma(\alpha_p))$$

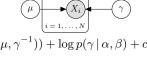
We choose the variational distribution so that



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$$\log q(\gamma \mid \alpha_p, \beta_p) = \alpha_p \cdot \log(\beta_p) + (\alpha_p - 1) \log(\gamma) - \beta \cdot \gamma - \log(\Gamma(\alpha_p))$$

We choose the variational distribution so that



$$\log q(\gamma) = \mathbb{E} \log p(\mathbf{x}, \mu, \gamma | \tau, \alpha, \beta) + c = \sum_{i=1}^{N} \mathbb{E} (\log p(x_i | \mu, \gamma^{-1})) + \log p(\gamma | \alpha, \beta) + c$$
$$= \left(\frac{N}{2} + \alpha - 1\right) \log(\gamma) - \left(\frac{1}{2} \sum_{i=1}^{N} \mathbb{E} (x_i - \mu)^2 + \beta\right) \cdot \gamma + c$$

Thus, we see that $q(\gamma)$ is normally distributed with

•
$$\alpha_p \leftarrow \frac{N}{2} + \alpha$$

•
$$\beta_p \leftarrow \beta + \frac{1}{2} \sum_{i=1}^N \mathbb{E}_q (x_i - \mu)^2$$

Note that:

$$\bullet \mathbb{E}_q(x_i - \mu)^2 = x_i^2 + \mathbb{E}_q(\mu^2) - 2 \cdot x_i \cdot \mathbb{E}_q(\mu)$$

$$\bullet \ \mathbb{E}_q(\mu^2) = \mathsf{Var}(\mu) + \mathbb{E}_q(\mu)^2$$

Monitoring the ELBO

The variational updating rules are guaranteed to never decrease the ELBO $\mathcal{L}(q)$:

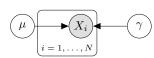
$$\mathcal{L}(q) = \underset{q}{\mathbb{E}} \log p(\mathbf{x}, \mu, \gamma \mid \tau, \alpha, \beta) - \underset{q}{\mathbb{E}} \log q(\mu, \gamma)$$

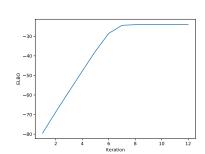
$$= \sum_{i=1}^{N} \underset{q}{\mathbb{E}} \log p(x_i \mid \mu, \gamma) + \underset{q}{\mathbb{E}} \log p(\mu \mid 0, \tau) + \underset{q}{\mathbb{E}} \log p(\gamma \mid \alpha, \beta) - \underset{q}{\mathbb{E}} \log q(\mu) - \underset{q}{\mathbb{E}} \log q(\gamma)$$

at any updating step. With some pencil pushing we arrive at a somewhat complicated but closed form expression (not show here).

Monitoring the ELBO can be useful for

- Assessing convergence
- Doing debugging
- ...





Code-task: VB for a simple Gaussian model

Code Task: VB for a simple Gaussian model



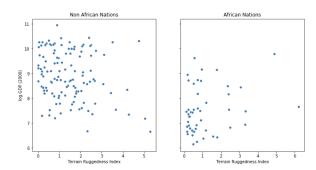
- $X_i \mid \{\mu, \gamma\} \sim \mathcal{N}(\mu, 1/\gamma)$
- $\mu \sim \mathcal{N}(0, \tau)$
- $\gamma \sim \text{Gamma}(\alpha, \beta)$

In this task you need to use mean-field, and look for $q(\mu, \gamma) = q(\mu) \cdot q(\gamma)$ that best approximates $p(\mu, \tau \mid x_1, \dots, x_N)$ wrt. the VB measure $\mathrm{KL}\,(q \mid p)$.

Go though the notebook

- Implement the update rules for $q(\mu)$ and $q(\gamma)$ (from the slides) in the notebook.
- Experiment with the model and the data set; try changing the prior and the data generating process.

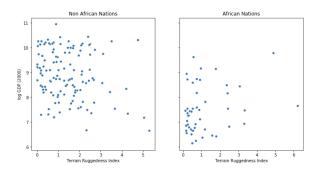
Bayesian linear regression



Relationship between topographic heterogeneity and GDP per capita

 Terrain ruggedness or bad geography is related to poorer economic performance outside of Africa.

Variational inference – Part II Bayesian linear regression

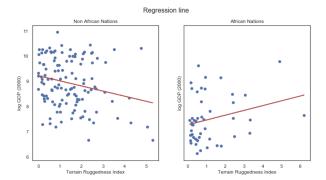


Relationship between topographic heterogeneity and GDP per capita

- Terrain ruggedness or bad geography is related to poorer economic performance outside of Africa.
- Rugged terrains have had a reverse effect on income for African nations.

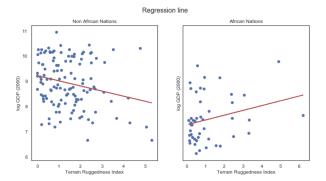
Day2/students_bayesian_regression_VI.ipynb

Variational inference – Part II Bayesian linear regression



Linear Regression Model

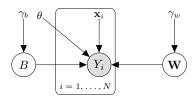
- Negative slope for Non African Nations.
- Positive slope for African Nations.



Bayesian Linear Regression Model

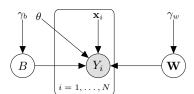
- Modeling data noise (aleatoric uncertainty). To be addressed tomorrow.
- Modeling uncertainty about the linear coefficients (epistemic uncertainty).

The Bayesian linear regression model



- Num. of data dim: M
- Num. of data inst: N
- $Y_i | \{\mathbf{w}, \mathbf{x}_i, b, \theta\} \sim \mathcal{N}(\mathbf{w}^\mathsf{T} \mathbf{x}_i + b, 1/\theta)$
- $\mathbf{W} \sim \mathcal{N}(\mathbf{0}, \gamma_w^{-1} \mathbf{I}_{M \times M})$
- $B \sim \mathcal{N}(0, \gamma_b^{-1})$

The Bayesian linear regression model



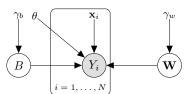
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- $\mathbf{W} \sim \mathcal{N}(\mathbf{0}, \gamma_w^{-1} \mathbf{I}_{M \times M})$
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The probability model

$$p(\cdot \mid \mathbf{x}, \theta, \gamma_w, \gamma_b) = \prod_{i=1}^{N} p(y_i \mid \mathbf{x}_i, \mathbf{w}, b, \theta) p(\mathbf{w} \mid \gamma_w) p(b \mid \gamma_b)$$

VB for Bayesian linear regression

The Bayesian linear regression model



- Num. of data dim: M
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The probability model

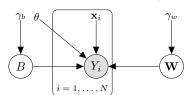
$$p(\cdot \mid \mathbf{x}, \theta, \gamma_w, \gamma_b) = \prod_{i=1}^{N} p(y_i \mid \mathbf{x}_i, \mathbf{w}, b, \theta) p(\mathbf{w} \mid \gamma_w) p(b \mid \gamma_b)$$

... after taking the log

$$\log p(\cdot \mid \mathbf{x}, \theta, \gamma_w, \gamma_b) = \sum_{i=1}^{N} \log p(y_i \mid \mathbf{x}_i, \mathbf{w}, b, \theta) + \log p(\mathbf{w} \mid \gamma_w) + \log p(b \mid \gamma_b)$$

VB for Bayesian linear regression

The Bayesian linear regression model



- Num. of data dim: M
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- $Y_i | \{\mathbf{w}, \mathbf{x}_i, b, \theta\} \sim \mathcal{N}(\mathbf{w}^\mathsf{T} \mathbf{x}_i + b, 1/\theta)$
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The probability model

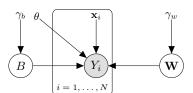
$$p(\cdot \mid \mathbf{x}, \theta, \gamma_w, \gamma_b) = \prod_{i=1}^{N} p(y_i \mid \mathbf{x}_i, \mathbf{w}, b, \theta) p(\mathbf{w} \mid \gamma_w) p(b \mid \gamma_b)$$

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$$= \sum_{i=1}^{N} \log p(y_i \mid \mathbf{x}_i, \mathbf{w}, b, \theta) + \sum_{j=1}^{M} \log p(w_j \mid \gamma_w) + \log p(b \mid \gamma_b)$$

VB for Bayesian linear regression

The Bayesian linear regression model



- Num. of data dim: M
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- $Y_i \mid \{\mathbf{w}, \mathbf{x}_i, b, \theta\} \sim \mathcal{N}(\mathbf{w}^\mathsf{T} \mathbf{x}_i + b, 1/\theta)$
- $\mathbf{W} \sim \mathcal{N}(\mathbf{0}, \gamma_w^{-1} \mathbf{I}_{M \times M})$
- $B \sim \mathcal{N}(0, \gamma_b^{-1})$

The probability model

$$p(\cdot \mid \mathbf{x}, \theta, \gamma_w, \gamma_b) = \prod_{i=1}^{N} p(y_i \mid \mathbf{x}_i, \mathbf{w}, b, \theta) p(\mathbf{w} \mid \gamma_w) p(b \mid \gamma_b)$$

The variational model (full mean field)

$$q(\cdot) = q(b \mid \cdot) \prod_{i=1}^{M} q(w_i \mid \cdot)$$

We choose the variational distribution so that

$$\log q(w_j) = \mathop{\mathbb{E}}_{q \neg w_j} \log p(\cdot \mid \mathbf{x}, \theta, \gamma_w, \gamma_b) + c$$

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$$\log p(\cdot \mid \mathbf{x}, \theta, \gamma_w, \gamma_b) = \sum_{i=1}^{N} \log p(y_i \mid \mathbf{x}_i, \mathbf{w}, b, \theta) + \sum_{i=1}^{M} \log p(w_j \mid \gamma_w) + \log p(b \mid \gamma_b)$$

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The normal distribution

$$\log p(y_i \mid \mathbf{x}_i, \mathbf{w}, b, \theta) = -\frac{1}{2} \log(2\pi) + \frac{1}{2} \log(\theta) - \frac{\theta}{2} (y_i - (\mathbf{w}^\mathsf{T} \mathbf{x}_i + b))^2$$
$$\log p(w_j \mid \gamma_w) = \log \mathcal{N}(w_j \mid 0, \gamma_w^{-1}) = -\frac{1}{2} \log(2\pi) + \frac{1}{2} \log(\gamma_w) - \frac{\gamma_w}{2} w_j^2$$

We choose the variational distribution so that

$$\log q(w_j) = \underset{q \neg w_j}{\mathbb{E}} \log p(\cdot \mid \mathbf{x}, \theta, \gamma_w, \gamma_b) + c = \sum_{i=1}^{N} \mathbb{E} \log p(y_i \mid \mathbf{x}_i, \mathbf{W}, B, \theta) + \log p(w_j \mid \gamma_w) + c$$

The normal distribution

$$\log p(y_i | \mathbf{x}_i, \mathbf{w}, b, \theta) = -\frac{1}{2} \log(2\pi) + \frac{1}{2} \log(\theta) - \frac{\theta}{2} (y_i - (\mathbf{w}^\mathsf{T} \mathbf{x}_i + b))^2$$
$$\log p(w_j | \gamma_w) = \log \mathcal{N}(w_j | 0, \gamma_w^{-1}) = -\frac{1}{2} \log(2\pi) + \frac{1}{2} \log(\gamma_w) - \frac{\gamma_w}{2} w_j^2$$

We choose the variational distribution so that

$$\log q(w_j) = \underset{q \neg w_j}{\mathbb{E}} \log p(\cdot \mid \mathbf{x}, \theta, \gamma_w, \gamma_b) + c = \sum_{i=1}^{N} \mathbb{E} \log p(y_i \mid \mathbf{x}_i, \mathbf{W}, B, \theta) + \log p(w_j \mid \gamma_w) + c$$
$$= -\frac{\gamma_w}{2} w_j^2 - \frac{\theta}{2} \sum_{i=1}^{N} \mathbb{E}((y_i - (\mathbf{W}^\mathsf{T} \mathbf{x}_i + B))^2) + c$$

The normal distribution

$$\log p(y_i \mid \mathbf{x}_i, \mathbf{w}, b, \theta) = -\frac{1}{2} \log(2\pi) + \frac{1}{2} \log(\theta) - \frac{\theta}{2} (y_i - (\mathbf{w}^\mathsf{T} \mathbf{x}_i + b))^2$$
$$\log p(w_j \mid \gamma_w) = \log \mathcal{N}(w_j \mid 0, \gamma_w^{-1}) = -\frac{1}{2} \log(2\pi) + \frac{1}{2} \log(\gamma_w) - \frac{\gamma_w}{2} w_j^2$$

We choose the variational distribution so that

$$\log q(w_j) = \underset{q \to w_j}{\mathbb{E}} \log p(\cdot \mid \mathbf{x}, \theta, \gamma_w, \gamma_b) + c = \sum_{i=1}^{N} \mathbb{E} \log p(y_i \mid \mathbf{x}_i, \mathbf{W}, B, \theta) + \log p(w_j \mid \gamma_w) + c$$
$$= -\frac{\gamma_w}{2} w_j^2 - \frac{\theta}{2} \sum_{i=1}^{N} \mathbb{E}((y_i - (\mathbf{W}^{\mathsf{T}} \mathbf{x}_i + B))^2) + c$$

Expanding the square

$$(y - (\mathbf{w}^{\mathsf{T}}\mathbf{x} + b))^{2} = y^{2} + \mathbf{x}^{\mathsf{T}}\mathbf{w}\mathbf{w}^{\mathsf{T}}\mathbf{x} + b^{2} + 2\mathbf{w}^{\mathsf{T}}\mathbf{x}b - 2y\mathbf{w}^{\mathsf{T}}\mathbf{x} - 2yb$$
$$\mathbf{x}^{\mathsf{T}}\mathbf{w}\mathbf{w}^{\mathsf{T}}\mathbf{x} = x_{j}^{2}w_{j}^{2} + \sum_{h,k\neq j} x_{k}x_{h}w_{k}w_{h} + 2x_{j}w_{j}\sum_{k\neq j} x_{k}w_{k}$$

We choose the variational distribution so that

$$\log q(w_j) = \underset{q \to w_j}{\mathbb{E}} \log p(\cdot \mid \mathbf{x}, \theta, \gamma_w, \gamma_b) + c = \sum_{i=1}^{N} \mathbb{E} \log p(y_i \mid \mathbf{x}_i, \mathbf{W}, B, \theta) + \log p(w_j \mid \gamma_w) + c$$
$$= -\frac{\gamma_w}{2} w_j^2 - \frac{\theta}{2} \sum_{i=1}^{N} \mathbb{E}((y_i - (\mathbf{W}^{\mathsf{T}} \mathbf{x}_i + B))^2) + c$$

Expanding the square

$$(y - (\mathbf{w}^{\mathsf{T}}\mathbf{x} + b))^{2} = y^{2} + \mathbf{x}^{\mathsf{T}}\mathbf{w}\mathbf{w}^{\mathsf{T}}\mathbf{x} + b^{2} + 2\mathbf{w}^{\mathsf{T}}\mathbf{x}b - 2y\mathbf{w}^{\mathsf{T}}\mathbf{x} - 2yb$$
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We choose the variational distribution so that

$$\log q(w_j) = \underset{q \neg w_j}{\mathbb{E}} \log p(\cdot \mid \mathbf{x}, \theta, \gamma_w, \gamma_b) + c = \sum_{i=1}^{N} \mathbb{E} \log p(y_i \mid \mathbf{x}_i, \mathbf{W}, B, \theta) + \log p(w_j \mid \gamma_w) + c$$

$$= -\frac{\gamma_w}{2} w_j^2 - \frac{\theta}{2} \sum_{i=1}^{N} \mathbb{E}((y_i - (\mathbf{W}^\mathsf{T} \mathbf{x}_i + B))^2) + c$$

$$= -\frac{\gamma_w}{2} w_j^2 - \theta \sum_{i=1}^{N} (\frac{1}{2} x_{ij}^2 w_j^2 + w_j (\sum_{i \neq j} x_{ij} x_{ik} \mathbb{E}(W_k) + x_{ij} \mathbb{E}(B) - y x_{ij}) + c$$

Expanding the square

$$(y - (\mathbf{w}^{\mathsf{T}}\mathbf{x} + b))^{2} = y^{2} + \mathbf{x}^{\mathsf{T}}\mathbf{w}\mathbf{w}^{\mathsf{T}}\mathbf{x} + b^{2} + 2\mathbf{w}^{\mathsf{T}}\mathbf{x}b - 2y\mathbf{w}^{\mathsf{T}}\mathbf{x} - 2yb$$
$$\mathbf{x}^{\mathsf{T}}\mathbf{w}\mathbf{w}^{\mathsf{T}}\mathbf{x} = x_{j}^{2}w_{j}^{2} + \sum_{h,k\neq j} x_{k}x_{h}w_{k}w_{h} + 2x_{j}w_{j}\sum_{k\neq j} x_{k}w_{k}$$

We choose the variational distribution so that

$$\log q(w_{j}) = \underset{q \to w_{j}}{\mathbb{E}} \log p(\cdot \mid \mathbf{x}, \theta, \gamma_{w}, \gamma_{b}) + c = \sum_{i=1}^{N} \mathbb{E} \log p(y_{i} \mid \mathbf{x}_{i}, \mathbf{W}, B, \theta) + \log p(w_{j} \mid \gamma_{w}) + c$$

$$= -\frac{\gamma_{w}}{2} w_{j}^{2} - \frac{\theta}{2} \sum_{i=1}^{N} \mathbb{E}((y_{i} - (\mathbf{W}^{\mathsf{T}} \mathbf{x}_{i} + B))^{2}) + c$$

$$= -\frac{\gamma_{w}}{2} w_{j}^{2} - \theta \sum_{i=1}^{N} (\frac{1}{2} x_{ij}^{2} w_{j}^{2} + w_{j} (\sum_{k \neq j} x_{ij} x_{ik} \mathbb{E}(W_{k}) + x_{ij} \mathbb{E}(B) - y x_{ij}) + c$$

$$= -\frac{1}{2} (\gamma_{w} + \theta \sum_{i=1}^{N} (x_{ij}^{2}) w_{j}^{2} + w_{j} \theta \sum_{i=1}^{N} x_{ij} (y_{i} - (\sum_{k \neq i} x_{ik} \mathbb{E}(W_{k}) + \mathbb{E}(B))) + c$$

We choose the variational distribution so that

$$\log q(w_j) = \underset{q \to w_j}{\mathbb{E}} \log p(\cdot \mid \mathbf{x}, \theta, \gamma_w, \gamma_b) + c = \sum_{i=1}^{N} \mathbb{E} \log p(y_i \mid \mathbf{x}_i, \mathbf{W}, B, \theta) + \log p(w_j \mid \gamma_w) + c$$

$$= -\frac{1}{2} (\gamma_w + \theta \sum_{i=1}^{N} (x_{ij}^2) w_j^2 + w_j \theta \sum_{i=1}^{N} x_{ij} (y_i - (\sum_{k \neq i} x_{ik} \mathbb{E}(W_k) + \mathbb{E}(B))) + c$$

We choose the variational distribution so that

$$\log q(w_j) = \underset{q \to w_j}{\mathbb{E}} \log p(\cdot \mid \mathbf{x}, \theta, \gamma_w, \gamma_b) + c = \sum_{i=1}^{N} \mathbb{E} \log p(y_i \mid \mathbf{x}_i, \mathbf{W}, B, \theta) + \log p(w_j \mid \gamma_w) + c$$

$$= -\frac{1}{2} (\gamma_w + \theta \sum_{i=1}^{N} (x_{ij}^2) w_j^2 + w_j \theta \sum_{i=1}^{N} x_{ij} (y_i - (\sum_{k \neq i} x_{ik} \mathbb{E}(W_k) + \mathbb{E}(B))) + c$$

Recall the normal distribution

$$\log p(w \mid \mu, \tau) = \log \mathcal{N}(w \mid \mu, \tau^{-1}) = -\frac{1}{2} \log(2\pi) + \frac{1}{2} \log(\tau) - \frac{\tau}{2} (w - \mu)^{2}$$
$$= -\frac{1}{2} \log(2\pi) + \frac{1}{2} \log(\tau) - \frac{1}{2} \tau w^{2} - \frac{\tau}{2} \mu^{2} + w\tau \mu$$

VB for Bayesian linear regression: updating $q(w_j)$

We choose the variational distribution so that

$$\log q(w_j) = \underset{q \to w_j}{\mathbb{E}} \log p(\cdot \mid \mathbf{x}, \theta, \gamma_w, \gamma_b) + c = \sum_{i=1}^{N} \mathbb{E} \log p(y_i \mid \mathbf{x}_i, \mathbf{W}, B, \theta) + \log p(w_j \mid \gamma_w) + c$$

$$= -\frac{1}{2} (\gamma_w + \theta \sum_{i=1}^{N} (x_{ij}^2) w_j^2 + w_j \theta \sum_{i=1}^{N} x_{ij} (y_i - (\sum_{k \neq j} x_{ik} \mathbb{E}(W_k) + \mathbb{E}(B))) + c$$

Recall the normal distribution

$$\log p(w \mid \mu, \tau) = \log \mathcal{N}(w \mid \mu, \tau^{-1}) = -\frac{1}{2} \log(2\pi) + \frac{1}{2} \log(\tau) - \frac{\tau}{2} (w - \mu)^{2}$$
$$= -\frac{1}{2} \log(2\pi) + \frac{1}{2} \log(\tau) - \frac{1}{2} \tau w^{2} - \frac{\tau}{2} \mu^{2} + w\tau\mu$$

VB for Bayesian linear regression: updating $q(w_j)$

We choose the variational distribution so that

$$\log q(w_j) = \underset{q \to w_j}{\mathbb{E}} \log p(\cdot \mid \mathbf{x}, \theta, \gamma_w, \gamma_b) + c = \sum_{i=1}^{N} \mathbb{E} \log p(y_i \mid \mathbf{x}_i, \mathbf{W}, B, \theta) + \log p(w_j \mid \gamma_w) + c$$

$$= -\frac{1}{2} (\gamma_w + \theta \sum_{i=1}^{N} (x_{ij}^2) w_j^2 + w_j \theta \sum_{i=1}^{N} x_{ij} (y_i - (\sum_{k \neq j} x_{ik} \mathbb{E}(W_k) + \mathbb{E}(B))) + c$$

Thus, we see that $q(w_j)$ is normally distributed with

- precision $\tau \leftarrow (\gamma_w + \theta \sum_{i=1}^N (x_{ij}^2))$
- mean $\mu \leftarrow au^{-1} \theta \sum_{i=1}^N x_{ij} (y_i (\sum_{k \neq j} x_{ik} \mathop{\mathbb{E}}(W_k) + \mathop{\mathbb{E}}(B)))$

Recall the normal distribution

$$\begin{split} \log p(w \mid \mu, \tau) &= \log \mathcal{N}(w \mid \mu, \tau^{-1}) = -\frac{1}{2} \log(2\pi) + \frac{1}{2} \log(\tau) - \frac{\tau}{2} (w - \mu)^2 \\ &= -\frac{1}{2} \log(2\pi) + \frac{1}{2} \log(\tau) - \frac{1}{2} \tau w^2 - \frac{\tau}{2} \mu^2 + w \tau \mu \end{split}$$

Exercise: Derive the updating rule for q(b)

Now it is your turn!

- Derive the updating rule for q(b).
- Implement the updating rule in the notebook

It may be useful to recall the definition:

• Gauss: $\log p(x \mid \mu, 1/\gamma) = -\frac{1}{2} \log(2\pi) + \frac{1}{2} \log(\gamma) - \frac{\gamma}{2} (x - \mu)^2$.

VB for Bayesian linear regression: updating q(b)

We choose the variational distribution so that

$$\log q(b) = \underset{q \to w_j}{\mathbb{E}} \log p(\cdot \mid \mathbf{W}, B, \theta, \gamma) + c = \sum_{i=1}^{N} \mathbb{E} \log p(y_i \mid \mathbf{x}_i, \mathbf{W}, \theta) + \log p(b \mid \gamma_b) + c$$

$$= \dots$$

$$= -\frac{1}{2} (\gamma_b + \theta N) b^2 + b \left(\theta \sum_{i=1}^{N} (y_i - \mathbb{E}(\mathbf{W}^{\mathsf{T}}) \mathbf{x}_i) \right) + c$$

VB for Bayesian linear regression: updating q(b)

We choose the variational distribution so that

$$\log q(b) = \underset{q \neg w_j}{\mathbb{E}} \log p(\cdot \mid \mathbf{W}, B, \theta, \gamma) + c = \sum_{i=1}^{N} \mathbb{E} \log p(y_i \mid \mathbf{x}_i, \mathbf{W}, \theta) + \log p(b \mid \gamma_b) + c$$

$$= \dots$$

$$= -\frac{1}{2} (\gamma_b + \theta N) b^2 + b \left(\theta \sum_{i=1}^{N} (y_i - \mathbb{E}(\mathbf{W}^{\mathsf{T}}) \mathbf{x}_i) \right) + c$$

Recall the normal distribution

$$\log p(b \mid \mu, \tau) = \log \mathcal{N}(b \mid \mu, \tau^{-1}) = -\frac{1}{2} \log(2\pi) + \frac{1}{2} \log(\tau) - \frac{\tau}{2} (b - \mu)^{2}$$
$$= -\frac{1}{2} \log(2\pi) + \frac{1}{2} \log(\tau) - \frac{1}{2} \tau b^{2} - \frac{\tau}{2} \mu^{2} + b\tau \mu$$

VB for Bayesian linear regression: updating q(b)

We choose the variational distribution so that

$$\log q(b) = \underset{q \to w_j}{\mathbb{E}} \log p(\cdot \mid \mathbf{W}, B, \theta, \gamma) + c = \sum_{i=1}^{N} \mathbb{E} \log p(y_i \mid \mathbf{x}_i, \mathbf{W}, \theta) + \log p(b \mid \gamma_b) + c$$

$$= \dots$$

$$= -\frac{1}{2} (\gamma_b + \theta N) b^2 + b \left(\theta \sum_{i=1}^{N} (y_i - \mathbb{E}(\mathbf{W}^\mathsf{T}) \mathbf{x}_i) \right) + c$$

Thus, we get that q(b) is normally distributed with

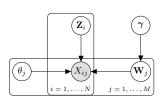
- precision $\tau \leftarrow (\gamma_b + \theta N)$
- mean $\mu \leftarrow au^{-1} heta \sum_{i=1}^N (y_i \mathbb{E}(\mathbf{W}^{\mathsf{T}}) \mathbf{x}_i)$

Recall the normal distribution

$$\log p(b \mid \mu, \tau) = \log \mathcal{N}(b \mid \mu, \tau^{-1}) = -\frac{1}{2} \log(2\pi) + \frac{1}{2} \log(\tau) - \frac{\tau}{2} (b - \mu)^{2}$$
$$= -\frac{1}{2} \log(2\pi) + \frac{1}{2} \log(\tau) - \frac{1}{2} \tau b^{2} - \frac{\tau}{2} \mu^{2} + b\tau \mu$$

Factor analysis

The factor analysis model

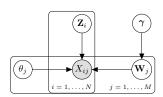


•
$$X_{ij} | \{ \mathbf{w}_j, \mathbf{z}_i, \theta_j \} \sim \mathcal{N}(\mathbf{w}_j^{\mathsf{T}} \mathbf{z}_i, 1/\theta_j)$$

- $\mathbf{Z}_i \sim \mathcal{N}(\mathbf{0}, \mathbf{I}_{D \times D})$
- $\mathbf{W}_j \sim \mathcal{N}(\mathbf{0}, \gamma^{-1} \mathbf{I}_{D \times D})$
- $\theta_j \sim \mathsf{Gamma}(\alpha_\theta, \beta_\theta)$
- $\gamma \sim \mathsf{Gamma}(\alpha_{\gamma}, \beta_{\gamma})$

- Num. of latent dim: D
- Num. of data dim: M
- Num. of data inst: N

The factor analysis model



- $X_{ij} | \{ \mathbf{w}_j, \mathbf{z}_i, \theta_j \} \sim \mathcal{N}(\mathbf{w}_j^{\mathsf{T}} \mathbf{z}_i, 1/\theta_j)$
- $\bullet \ \mathbf{Z}_i \sim \mathcal{N}(\mathbf{0}, \mathbf{I}_{D \times D})$
- $\mathbf{W}_j \sim \mathcal{N}(\mathbf{0}, \gamma^{-1} \mathbf{I}_{D \times D})$
- $\theta_j \sim \mathsf{Gamma}(\alpha_\theta, \beta_\theta)$
- $\quad \bullet \ \, \gamma \sim \mathsf{Gamma}(\alpha_\gamma,\beta_\gamma)$

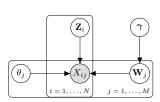
- Num. of latent dim: D
- Num. of data dim: M
- Num. of data inst: N

The probability model

$$p(\cdot) = p(\gamma) \left[\prod_{i=1}^{N} p(\mathbf{z}_i) \right] \left[\prod_{j=1}^{M} p(\mathbf{w}_j \mid \gamma) p(\theta_j) \right] \left[\prod_{i=1}^{N} \prod_{j=1}^{M} p(x_{ij} \mid \mathbf{w}_j, \mathbf{z}_i, \theta_j) \right]$$

VB for the factor analysis model

The factor analysis model



•
$$X_{ij} | \{ \mathbf{w}_j, \mathbf{z}_i, \theta_j \} \sim \mathcal{N}(\mathbf{w}_j^{\mathsf{T}} \mathbf{z}_i, 1/\theta_j)$$

- $\mathbf{Z}_i \sim \mathcal{N}(\mathbf{0}, \mathbf{I}_{D \times D})$
- $\mathbf{W}_j \sim \mathcal{N}(\mathbf{0}, \gamma^{-1} \mathbf{I}_{D \times D})$
- $\theta_j \sim \mathsf{Gamma}(\alpha_\theta, \beta_\theta)$
- $\quad \bullet \ \, \gamma \sim \mathsf{Gamma}(\alpha_\gamma,\beta_\gamma)$

- Num. of latent dim: D
- Num. of data dim: M
- Num. of data inst: N

The probability model

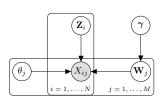
$$p(\cdot) = p(\gamma) \left[\prod_{i=1}^{N} p(\mathbf{z}_i) \right] \left[\prod_{j=1}^{M} p(\mathbf{w}_j \mid \gamma) p(\theta_j) \right] \left[\prod_{i=1}^{N} \prod_{j=1}^{M} p(x_{ij} \mid \mathbf{w}_j, \mathbf{z}_i, \theta_j) \right]$$

... after taking the log

$$\log p(\cdot) = \log p(\gamma) + \sum_{i=1}^{N} \log p(\mathbf{z}_i) + \sum_{i=1}^{M} [\log p(\mathbf{w}_i \mid \gamma) + \log p(\theta_i)] + \sum_{i=1}^{N} \sum_{i=1}^{M} \log p(x_{ij} \mid \mathbf{w}_j, \mathbf{z}_i, \theta_j)$$

VB for the factor analysis model

The factor analysis model



- $X_{ij} | \{ \mathbf{w}_j, \mathbf{z}_i, \theta_j \} \sim \mathcal{N}(\mathbf{w}_j^{\mathsf{T}} \mathbf{z}_i, 1/\theta_j)$
- $\mathbf{Z}_i \sim \mathcal{N}(\mathbf{0}, \mathbf{I}_{D \times D})$
- $\mathbf{W}_j \sim \mathcal{N}(\mathbf{0}, \gamma^{-1} \mathbf{I}_{D \times D})$
- $\theta_j \sim \mathsf{Gamma}(\alpha_\theta, \beta_\theta)$
- $\quad \bullet \ \, \gamma \sim \mathsf{Gamma}(\alpha_\gamma,\beta_\gamma)$

- ullet Num. of latent dim: D
- Num. of data dim: M
- Num. of data inst: N

The probability model

$$p(\cdot) = p(\gamma) \left[\prod_{i=1}^{N} p(\mathbf{z}_i) \right] \left[\prod_{j=1}^{M} p(\mathbf{w}_j \mid \gamma) p(\theta_j) \right] \left[\prod_{i=1}^{N} \prod_{j=1}^{M} p(x_{ij} \mid \mathbf{w}_j, \mathbf{z}_i, \theta_j) \right]$$

The variational model

$$q(\cdot) = q(\gamma) \prod_{i=1}^{N} q(\mathbf{z}_i \mid \cdot) \prod_{j=1}^{M} q(\mathbf{w}_j \mid \cdot) q(\theta_j \mid \cdot)$$

We choose the variational distribution so that

$$\log q(\gamma \mid \cdot) = \mathbb{E}_{q \to \gamma} \left[\log p(\cdot) \right] + c$$

We choose the variational distribution so that

$$\log q(\gamma \mid \cdot) = \mathbb{E}_{q_{\neg \gamma}} \left[\log p(\cdot) \right] + c$$

$$\log p(\cdot)$$

$$= \log p(\gamma) + \sum_{i=1}^{N} \log p(\mathbf{z}_{i}) + \sum_{j=1}^{M} [\log p(\mathbf{w}_{j} | \gamma) + \log p(\theta_{j})] + \sum_{i=1}^{N} \sum_{j=1}^{M} \log p(x_{ij} | \mathbf{w}_{j}, \mathbf{z}_{i}, \theta_{j})$$

We choose the variational distribution so that

$$\log q(\gamma \mid \cdot) = \mathbb{E}_{q_{\neg \gamma}} \left[\log p(\cdot) \right] + c$$

$$\log p(\cdot)$$

$$= \log p(\gamma) + \sum_{i=1}^{N} \log p(\mathbf{z}_{i}) + \sum_{j=1}^{M} [\log p(\mathbf{w}_{j} | \gamma) + \log p(\theta_{j})] + \sum_{i=1}^{N} \sum_{j=1}^{M} \log p(x_{ij} | \mathbf{w}_{j}, \mathbf{z}_{i}, \theta_{j})$$

We choose the variational distribution so that

$$\log q(\gamma \mid \cdot) = \mathbb{E}_{q \rightarrow \gamma} \left[\log p(\cdot) \right] + c = \log p(\gamma) + \sum_{j=1}^{M} \mathbb{E}_{q \rightarrow \gamma} \log p(\mathbf{W}_j \mid \gamma) + c$$

$$\log p(\cdot)$$

$$= \log p(\gamma) + \sum_{i=1}^{N} \log p(\mathbf{z}_i) + \sum_{j=1}^{M} [\log p(\mathbf{w}_j \mid \gamma) + \log p(\theta_j)] + \sum_{i=1}^{N} \sum_{j=1}^{M} \log p(x_{ij} \mid \mathbf{w}_j, \mathbf{z}_i, \theta_j)$$

We choose the variational distribution so that

$$\log q(\gamma \mid \cdot) = \mathbb{E}_{q \to \gamma} \left[\log p(\cdot) \right] + c = \log p(\gamma) + \sum_{i=1}^{M} \mathbb{E}_{q \to \gamma} \log p(\mathbf{W}_j \mid \gamma) + c$$

The gamma and multivariate normal

$$\log p(\gamma \mid \alpha_{\gamma}, \beta_{\gamma}) = \alpha_{\gamma} \log(\beta_{\gamma}) + (\alpha_{\gamma} - 1) \log(\gamma) - \beta_{\gamma} \cdot \gamma - \log(\Gamma(\alpha_{\gamma}))$$
$$\log p(\mathbf{w}_{j} \mid \gamma) = \log \mathcal{N}(\mathbf{w}_{j} \mid \mathbf{0}, \gamma^{-1}\mathbf{I}) = -\frac{D}{2} \log(2\pi) + \frac{D}{2} \log(\gamma) - \frac{\gamma}{2} \mathbf{w}_{j}^{T} \mathbf{w}_{j}$$

We choose the variational distribution so that

$$\log q(\gamma \mid \cdot) = \mathbb{E}_{q \to \gamma} \left[\log p(\cdot) \right] + c = \log p(\gamma) + \sum_{i=1}^{M} \mathbb{E}_{q \to \gamma} \log p(\mathbf{W}_j \mid \gamma) + c$$

The gamma and multivariate normal

$$\log p(\gamma \mid \alpha_{\gamma}, \beta_{\gamma}) = \alpha_{\gamma} \log(\beta_{\gamma}) + (\alpha_{\gamma} - 1) \log(\gamma) - \beta_{\gamma} \cdot \gamma - \log(\Gamma(\alpha_{\gamma}))$$
$$\log p(\mathbf{w}_{j} \mid \gamma) = \log \mathcal{N}(\mathbf{w}_{j} \mid \mathbf{0}, \gamma^{-1}\mathbf{I}) = -\frac{D}{2} \log(2\pi) + \frac{D}{2} \log(\gamma) - \frac{\gamma}{2} \mathbf{w}_{j}^{T} \mathbf{w}_{j}$$

We choose the variational distribution so that

$$\log q(\gamma \mid \cdot) = \mathbb{E}_{q \to \gamma} \left[\log p(\cdot) \right] + c = \log p(\gamma) + \sum_{j=1}^{M} \mathbb{E}_{q \to \gamma} \log p(\mathbf{W}_j \mid \gamma) + c$$
$$= (\alpha_{\gamma} - 1) \log(\gamma) - \beta_{\gamma} \cdot \gamma + \frac{D \cdot M}{2} \log(\gamma) - \frac{\gamma}{2} \sum_{j=1}^{M} \mathbb{E}(\mathbf{W}_j^T \mathbf{W}_j) + c$$

The gamma and multivariate normal

$$\log p(\gamma \mid \alpha_{\gamma}, \beta_{\gamma}) = \alpha_{\gamma} \log(\beta_{\gamma}) + (\alpha_{\gamma} - 1) \log(\gamma) - \beta_{\gamma} \cdot \gamma - \log(\Gamma(\alpha_{\gamma}))$$
$$\log p(\mathbf{w}_{j} \mid \gamma) = \log \mathcal{N}(\mathbf{w}_{j} \mid \mathbf{0}, \gamma^{-1}\mathbf{I}) = -\frac{D}{2} \log(2\pi) + \frac{D}{2} \log(\gamma) - \frac{\gamma}{2} \mathbf{w}_{j}^{T} \mathbf{w}_{j}$$

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We choose the variational distribution so that

$$\log q(\gamma \mid \cdot) = \mathbb{E}_{q \sim \gamma} \left[\log p(\cdot) \right] + c = \log p(\gamma) + \sum_{j=1}^{M} \mathbb{E}_{q \sim \gamma} \log p(\mathbf{W}_j \mid \gamma) + c$$

$$= (\alpha_{\gamma} - 1) \log(\gamma) - \beta_{\gamma} \cdot \gamma + \frac{D \cdot M}{2} \log(\gamma) - \frac{\gamma}{2} \sum_{j=1}^{M} \mathbb{E}(\mathbf{W}_j^T \mathbf{W}_j) + c$$

$$= \left[\alpha_{\gamma} - 1 + \frac{D \cdot M}{2} \right] \log(\gamma) - \left[\beta_{\gamma} + \frac{1}{2} \sum_{j=1}^{M} \mathbb{E}(\mathbf{W}_j^T \mathbf{W}_j) \right] \cdot \gamma + c$$

We choose the variational distribution so that

$$\log q(\gamma \mid \cdot) = \mathbb{E}_{q \to \gamma} \left[\log p(\cdot) \right] + c = \log p(\gamma) + \sum_{j=1}^{M} \mathbb{E}_{q \to \gamma} \log p(\mathbf{W}_j \mid \gamma) + c$$

$$= (\alpha_{\gamma} - 1) \log(\gamma) - \beta_{\gamma} \cdot \gamma + \frac{D \cdot M}{2} \log(\gamma) - \frac{\gamma}{2} \sum_{j=1}^{M} \mathbb{E}(\mathbf{W}_j^T \mathbf{W}_j) + c$$

$$= \left[\alpha_{\gamma} - 1 + \frac{D \cdot M}{2} \right] \log(\gamma) - \left[\beta_{\gamma} + \frac{1}{2} \sum_{j=1}^{M} \mathbb{E}(\mathbf{W}_j^T \mathbf{W}_j) \right] \cdot \gamma + c$$

Recall the (generic) gamma distribution

$$\log p(x \mid \alpha, \beta) = \alpha \log(\beta) + (\alpha - 1) \log(x) - \beta \cdot x - \log(\Gamma(\alpha))$$

Variational inference – Part II Factor analysis

We choose the variational distribution so that

$$\log q(\gamma \mid \cdot) = \mathbb{E}_{q \to \gamma} \left[\log p(\cdot) \right] + c = \log p(\gamma) + \sum_{j=1}^{M} \mathbb{E}_{q \to \gamma} \log p(\mathbf{W}_j \mid \gamma) + c$$

$$= (\alpha_{\gamma} - 1) \log(\gamma) - \beta_{\gamma} \cdot \gamma + \frac{D \cdot M}{2} \log(\gamma) - \frac{\gamma}{2} \sum_{j=1}^{M} \mathbb{E}(\mathbf{W}_j^T \mathbf{W}_j) + c$$

$$= \left[\alpha_{\gamma} - 1 + \frac{D \cdot M}{2} \right] \log(\gamma) - \left[\beta_{\gamma} + \frac{1}{2} \sum_{j=1}^{M} \mathbb{E}(\mathbf{W}_j^T \mathbf{W}_j) \right] \cdot \gamma + c$$

Recall the (generic) gamma distribution

$$\log p(x \mid \alpha, \beta) = \alpha \log(\beta) + (\alpha - 1) \log(x) - \beta \cdot x - \log(\Gamma(\alpha))$$

We choose the variational distribution so that

$$\log q(\gamma \mid \cdot) = \mathbb{E}_{q \to \gamma} \left[\log p(\cdot) \right] + c = \log p(\gamma) + \sum_{j=1}^{M} \mathbb{E}_{q \to \gamma} \log p(\mathbf{W}_{j} \mid \gamma) + c$$

$$= (\alpha_{\gamma} - 1) \log(\gamma) - \beta_{\gamma} \cdot \gamma + \frac{D \cdot M}{2} \log(\gamma) - \frac{\gamma}{2} \sum_{j=1}^{M} \mathbb{E}(\mathbf{W}_{j}^{T} \mathbf{W}_{j}) + c$$

$$= \left[\alpha_{\gamma} - 1 + \frac{D \cdot M}{2} \right] \log(\gamma) - \left[\beta_{\gamma} + \frac{1}{2} \sum_{j=1}^{M} \mathbb{E}(\mathbf{W}_{j}^{T} \mathbf{W}_{j}) \right] \cdot \gamma + c$$

Thus we see that $q(\gamma \mid \cdot)$ is gamma distributed with

- shape parameter: $\alpha \leftarrow \alpha_{\gamma} + \frac{DM}{2}$
- rate parameter: $\beta \leftarrow \beta_{\gamma} + \frac{1}{2} \sum_{j=1}^{M} \mathbb{E}_{q(\mathbf{w}_{j})} \left[\mathbf{W}_{j}^{T} \mathbf{W}_{j} \right]$

Recall the (generic) gamma distribution

$$\log p(x \mid \alpha, \beta) = \alpha \log(\beta) + (\alpha - 1) \log(x) - \beta \cdot x - \log(\Gamma(\alpha))$$

We choose the variational distribution so that

$$\log q(\gamma \mid \cdot) = \mathbb{E}_{q \sim \gamma} \left[\log p(\cdot) \right] + c = \log p(\gamma) + \sum_{j=1}^{M} \mathbb{E}_{q \sim \gamma} \log p(\mathbf{W}_{j} \mid \gamma) + c$$

$$= (\alpha_{\gamma} - 1) \log(\gamma) - \beta_{\gamma} \cdot \gamma + \frac{D \cdot M}{2} \log(\gamma) - \frac{\gamma}{2} \sum_{j=1}^{M} \mathbb{E}(\mathbf{W}_{j}^{T} \mathbf{W}_{j}) + c$$

$$= \left[\alpha_{\gamma} - 1 + \frac{D \cdot M}{2} \right] \log(\gamma) - \left[\beta_{\gamma} + \frac{1}{2} \sum_{j=1}^{M} \mathbb{E}(\mathbf{W}_{j}^{T} \mathbf{W}_{j}) \right] \cdot \gamma + c$$

Thus we see that $q(\gamma \mid \cdot)$ is gamma distributed with

- shape parameter: $\alpha \leftarrow \alpha_{\gamma} + \frac{DM}{2}$
- rate parameter: $eta \leftarrow eta_\gamma + \frac{1}{2} \sum_{j=1}^M \mathbb{E}_{q(\mathbf{w}_j)} \left[\mathbf{W}_j^T \mathbf{W}_j \right]$

Calculation of $\mathbb{E}_{q(\mathbf{w}_j)}\left[\mathbf{W}_j^T\mathbf{W}_j\right]$

$$\mathbb{E}_{q(\mathbf{w}_j)}\left[\mathbf{W}_j^T\mathbf{W}_j\right] = \sum_{d=1}^D \mathsf{Var}_{q(\mathbf{w}_j)}\left[\mathbf{W}_{jd}\right] + \sum_{d=1}^D \left(\mathbb{E}_{q(\mathbf{w}_j)}\left[\mathbf{W}_{j,d}\right]\right)^2$$

We choose the variational distribution so that

$$\log q(\gamma \mid \cdot) = \mathbb{E}_{q \to \gamma} \left[\log p(\cdot) \right] + c = \log p(\gamma) + \sum_{j=1}^{M} \mathbb{E}_{q \to \gamma} \log p(\mathbf{W}_{j} \mid \gamma) + c$$

$$= (\alpha_{\gamma} - 1) \log(\gamma) - \beta_{\gamma} \cdot \gamma + \frac{D \cdot M}{2} \log(\gamma) - \frac{\gamma}{2} \sum_{j=1}^{M} \mathbb{E}(\mathbf{W}_{j}^{T} \mathbf{W}_{j}) + c$$

$$= \left[\alpha_{\gamma} - 1 + \frac{D \cdot M}{2} \right] \log(\gamma) - \left[\beta_{\gamma} + \frac{1}{2} \sum_{j=1}^{M} \mathbb{E}(\mathbf{W}_{j}^{T} \mathbf{W}_{j}) \right] \cdot \gamma + c$$

Thus we see that $q(\gamma | \cdot)$ is gamma distributed with

- shape parameter: $\alpha \leftarrow \alpha_{\gamma} + \frac{DM}{2}$
- rate parameter: $\beta \leftarrow \beta_{\gamma} + \frac{1}{2} \sum_{j=1}^{M} \mathbb{E}_{q(\mathbf{w}_{j})} \left[\mathbf{W}_{j}^{T} \mathbf{W}_{j} \right]$

Compare this to the Gibbs sampler:

- shape parameter: $\alpha \leftarrow \alpha_{\gamma} + \frac{DM}{2}$
- rate parameter: $\beta \leftarrow \beta_{\gamma} + \frac{1}{2} \sum_{i=1}^{M} \mathbf{w}_{i}^{\mathsf{T}} \mathbf{w}_{j}$

VB uses posterior expectations where Gibbs uses samples!

We choose the variational distribution so that

$$\log q(\mathbf{w}_j) = \mathbb{E}_{q \neg \mathbf{w}_j}[\log p(\cdot)] + c$$

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$$\log q(\mathbf{w}_j) = \mathbb{E}_{q \neg \mathbf{w}_j}[\log p(\cdot)] + c$$

Recall

 $\log p(\cdot)$

$$= \log p(\gamma) + \sum_{i=1}^{N} \log p(\mathbf{z}_i) + \sum_{j=1}^{M} [\log p(\mathbf{w}_j | \gamma) + \log p(\theta_j)] + \sum_{i=1}^{N} \sum_{j=1}^{M} \log p(x_{ij} | \mathbf{w}_j, \mathbf{z}_i, \theta_j)$$

We choose the variational distribution so that

$$\log q(\mathbf{w}_j) = \mathbb{E}_{q \neg \mathbf{w}_j}[\log p(\cdot)] + c$$

Recall

 $\log p(\cdot)$

$$= \log p(\gamma) + \sum_{i=1}^{N} \log p(\mathbf{z}_i) + \sum_{j=1}^{M} \left[\log p(\mathbf{w}_j \mid \gamma) + \log p(\theta_j) \right] + \sum_{i=1}^{N} \sum_{j=1}^{M} \log p(x_{ij} \mid \mathbf{w}_j, \mathbf{z}_i, \theta_j)$$

We choose the variational distribution so that

$$\log q(\mathbf{w}_j) = \mathbb{E}_{q \neg \mathbf{w}_j}[\log p(\cdot)] + c = \mathbb{E}\log p(\mathbf{w}_j \mid \gamma) + \sum_{i=1}^{N} \mathbb{E}\log p(x_{ij} \mid \mathbf{w}_j, \mathbf{z}_i, \theta_j) + c$$

$$\log p(\cdot)$$

$$= \log p(\gamma) + \sum_{i=1}^{N} \log p(\mathbf{z}_i) + \sum_{j=1}^{M} \left[\log p(\mathbf{w}_j \mid \gamma) + \log p(\theta_j) \right] + \sum_{i=1}^{N} \sum_{j=1}^{M} \log p(x_{ij} \mid \mathbf{w}_j, \mathbf{z}_i, \theta_j)$$

We choose the variational distribution so that

$$\log q(\mathbf{w}_j) = \mathbb{E}_{q \neg \mathbf{w}_j}[\log p(\cdot)] + c = \mathbb{E}\log p(\mathbf{w}_j \mid \gamma) + \sum_{i=1}^N \mathbb{E}\log p(x_{ij} \mid \mathbf{w}_j, \mathbf{z}_i, \theta_j) + c$$

The (multivariate) normal distribution

$$\log p(\mathbf{w}_j \mid \gamma) = \log \mathcal{N}(\mathbf{0}, \gamma^{-1} \mathbf{I}) = -\frac{D}{2} \log(2\pi) + \frac{D}{2} \log(\gamma) - \frac{\gamma}{2} \mathbf{w}_j^T \mathbf{w}_j$$
$$\log p(x_{ij} \mid \mathbf{w}_j, \mathbf{z}_i, \theta_j) = \log \mathcal{N}(\mathbf{w}_j^\mathsf{T} \mathbf{z}_i, \theta_j) = -\frac{1}{2} \log(2\pi) + \frac{1}{2} \log(\theta_j) - \frac{\theta_j}{2} (x_{ij} - \mathbf{w}_j^T \mathbf{z}_i)^2$$

We choose the variational distribution so that

$$\log q(\mathbf{w}_j) = \mathbb{E}_{q \neg \mathbf{w}_j}[\log p(\cdot)] + c = \mathbb{E}\log p(\mathbf{w}_j \mid \gamma) + \sum_{i=1}^N \mathbb{E}\log p(x_{ij} \mid \mathbf{w}_j, \mathbf{z}_i, \theta_j) + c$$

The (multivariate) normal distribution

$$\log p(\mathbf{w}_j \mid \gamma) = \log \mathcal{N}(\mathbf{0}, \gamma^{-1}\mathbf{I}) = -\frac{D}{2}\log(2\pi) + \frac{D}{2}\log(\gamma) - \frac{\gamma}{2}\mathbf{w}_j^T\mathbf{w}_j$$
$$\log p(x_{ij} \mid \mathbf{w}_j, \mathbf{z}_i, \theta_j) = \log \mathcal{N}(\mathbf{w}_j^T\mathbf{z}_i, \theta_j) = -\frac{1}{2}\log(2\pi) + \frac{1}{2}\log(\theta_j) - \frac{\theta_j}{2}(x_{ij} - \mathbf{w}_j^T\mathbf{z}_i)^2$$

We choose the variational distribution so that

$$\log q(\mathbf{w}_j) = \mathbb{E}_{q \to \mathbf{w}_j}[\log p(\cdot)] + c = \mathbb{E} \log p(\mathbf{w}_j \mid \gamma) + \sum_{i=1}^N \mathbb{E} \log p(x_{ij} \mid \mathbf{w}_j, \mathbf{z}_i, \theta_j) + c$$
$$= -\frac{\mathbb{E}(\gamma)}{2} \mathbf{w}_j^T \mathbf{w}_j - \frac{\mathbb{E}(\theta_j)}{2} \sum_{i=1}^N \mathbb{E}(x_{ij} - \mathbf{w}_j^T \mathbf{Z}_i)^2 + c$$

The (multivariate) normal distribution

$$\log p(\mathbf{w}_j \mid \gamma) = \log \mathcal{N}(\mathbf{0}, \gamma^{-1}\mathbf{I}) = -\frac{D}{2}\log(2\pi) + \frac{D}{2}\log(\gamma) - \frac{\gamma}{2}\mathbf{w}_j^T\mathbf{w}_j$$
$$\log p(x_{ij} \mid \mathbf{w}_j, \mathbf{z}_i, \theta_j) = \log \mathcal{N}(\mathbf{w}_j^\mathsf{T}\mathbf{z}_i, \theta_j) = -\frac{1}{2}\log(2\pi) + \frac{1}{2}\log(\theta_j) - \frac{\theta_j}{2}(x_{ij} - \mathbf{w}_j^T\mathbf{z}_i)^2$$

We choose the variational distribution so that

$$\log q(\mathbf{w}_j) = \mathbb{E}_{q \to \mathbf{w}_j}[\log p(\cdot)] + c = \mathbb{E}\log p(\mathbf{w}_j \mid \gamma) + \sum_{i=1}^N \mathbb{E}\log p(x_{ij} \mid \mathbf{w}_j, \mathbf{z}_i, \theta_j) + c$$
$$= -\frac{\mathbb{E}(\gamma)}{2}\mathbf{w}_j^T \mathbf{w}_j - \frac{\mathbb{E}(\theta_j)}{2}\sum_{i=1}^N \mathbb{E}(x_{ij} - \mathbf{w}_j^T \mathbf{Z}_i)^2 + c$$

Expanding the square

$$(x_{ij} - \mathbf{w}_j^T \mathbf{z}_i)^2 = x_{ij}^2 - 2x_{ij} \mathbf{w}_j^\mathsf{T} \mathbf{z}_i + \mathbf{w}_j^\mathsf{T} \mathbf{z}_i \mathbf{w}_j^\mathsf{T} \mathbf{z}_i$$
$$= x_{ij}^2 - 2x_{ij} \mathbf{w}_j^\mathsf{T} \mathbf{z}_i + \mathbf{w}_j^\mathsf{T} \mathbf{z}_i \mathbf{z}_i^\mathsf{T} \mathbf{w}_j$$

We choose the variational distribution so that

$$\log q(\mathbf{w}_j) = \mathbb{E}_{q \to \mathbf{w}_j}[\log p(\cdot)] + c = \mathbb{E}\log p(\mathbf{w}_j \mid \gamma) + \sum_{i=1}^N \mathbb{E}\log p(x_{ij} \mid \mathbf{w}_j, \mathbf{z}_i, \theta_j) + c$$

$$= -\frac{\mathbb{E}(\gamma)}{2}\mathbf{w}_j^T \mathbf{w}_j - \frac{\mathbb{E}(\theta_j)}{2} \sum_{i=1}^N \mathbb{E}(x_{ij} - \mathbf{w}_j^T \mathbf{Z}_i)^2 + c$$

$$= -\frac{\mathbb{E}(\gamma)}{2}\mathbf{w}_j^T \mathbf{w}_j - \mathbb{E}(\theta_j) \frac{1}{2} \sum_{i=1}^N \left[-2x_{ij}\mathbf{w}_j^T \mathbb{E}(\mathbf{Z}_i) + \mathbf{w}_j^T \mathbb{E}(\mathbf{Z}_i \mathbf{Z}_i^T) \mathbf{w}_j \right] + c$$

Expanding the square

$$(x_{ij} - \mathbf{w}_j^T \mathbf{z}_i)^2 = x_{ij}^2 - 2x_{ij} \mathbf{w}_j^\mathsf{T} \mathbf{z}_i + \mathbf{w}_j^\mathsf{T} \mathbf{z}_i \mathbf{w}_j^\mathsf{T} \mathbf{z}_i$$
$$= x_{ij}^2 - 2x_{ij} \mathbf{w}_j^\mathsf{T} \mathbf{z}_i + \mathbf{w}_j^\mathsf{T} \mathbf{z}_i \mathbf{z}_i^\mathsf{T} \mathbf{w}_j$$

We choose the variational distribution so that

$$\log q(\mathbf{w}_{j}) = \mathbb{E}_{q \to \mathbf{w}_{j}}[\log p(\cdot)] + c = \mathbb{E} \log p(\mathbf{w}_{j} \mid \gamma) + \sum_{i=1}^{N} \mathbb{E} \log p(x_{ij} \mid \mathbf{w}_{j}, \mathbf{z}_{i}, \theta_{j}) + c$$

$$= -\frac{\mathbb{E}(\gamma)}{2} \mathbf{w}_{j}^{T} \mathbf{w}_{j} - \frac{\mathbb{E}(\theta_{j})}{2} \sum_{i=1}^{N} \mathbb{E}(x_{ij} - \mathbf{w}_{j}^{T} \mathbf{Z}_{i})^{2} + c$$

$$= -\frac{\mathbb{E}(\gamma)}{2} \mathbf{w}_{j}^{T} \mathbf{w}_{j} - \mathbb{E}(\theta_{j}) \frac{1}{2} \sum_{i=1}^{N} \left[-2x_{ij} \mathbf{w}_{j}^{T} \mathbb{E}(\mathbf{Z}_{i}) + \mathbf{w}_{j}^{T} \mathbb{E}(\mathbf{Z}_{i} \mathbf{Z}_{i}^{T}) \mathbf{w}_{j} \right] + c$$

$$= -\frac{1}{2} \mathbf{w}_{j}^{T} \left[\mathbb{E}(\gamma) \mathbf{I} + \mathbb{E}(\theta_{j}) \sum_{i=1}^{N} \mathbb{E}(\mathbf{Z}_{i} \mathbf{Z}_{i}^{T}) \right] \mathbf{w}_{j} + \mathbf{w}_{j}^{T} \mathbb{E}(\theta_{j}) \sum_{i=1}^{N} x_{ij} \mathbb{E}(\mathbf{Z}_{i}) + c$$

We choose the variational distribution so that

$$\log q(\mathbf{w}_j) = \mathbb{E}_{q \to \mathbf{w}_j}[\log p(\cdot)] + c = \mathbb{E} \log p(\mathbf{w}_j \mid \gamma) + \sum_{i=1}^N \mathbb{E} \log p(x_{ij} \mid \mathbf{w}_j, \mathbf{z}_i, \theta_j) + c$$

$$= -\frac{1}{2} \mathbf{w}_j^T \left[\mathbb{E}(\gamma) \mathbf{I} + \mathbb{E}(\theta_j) \sum_{i=1}^N \mathbb{E}(\mathbf{Z}_i \mathbf{Z}_i^{\mathsf{T}}) \right] \mathbf{w}_j + \mathbf{w}_j^{\mathsf{T}} \mathbb{E}(\theta_j) \sum_{i=1}^N x_{ij} \mathbb{E}(\mathbf{Z}_i) + c$$

We choose the variational distribution so that

$$\log q(\mathbf{w}_j) = \mathbb{E}_{q \to \mathbf{w}_j}[\log p(\cdot)] + c = \mathbb{E}\log p(\mathbf{w}_j \mid \gamma) + \sum_{i=1}^N \mathbb{E}\log p(x_{ij} \mid \mathbf{w}_j, \mathbf{z}_i, \theta_j) + c$$
$$= -\frac{1}{2}\mathbf{w}_j^T \left[\mathbb{E}(\gamma)\mathbf{I} + \mathbb{E}(\theta_j) \sum_{i=1}^N \mathbb{E}(\mathbf{Z}_i \mathbf{Z}_i^{\mathsf{T}}) \right] \mathbf{w}_j + \mathbf{w}_j^{\mathsf{T}} \mathbb{E}(\theta_j) \sum_{i=1}^N x_{ij} \mathbb{E}(\mathbf{Z}_i) + c$$

Recall the (generic) multivariate normal distribution

$$\begin{split} \log p(\mathbf{y} \,|\, \boldsymbol{\mu}, \mathbf{Q}) &= \log \mathcal{N}(\mathbf{y} \,|\, \boldsymbol{\mu}, \mathbf{Q}^{-1}) = -\frac{D}{2} \log(2\pi) + \frac{1}{2} \log |\mathbf{Q}] - \frac{1}{2} (\mathbf{y} - \boldsymbol{\mu})^\mathsf{T} \mathbf{Q} (\mathbf{y} - \boldsymbol{\mu})^\mathsf{T}) \\ &= -\frac{D}{2} \log(2\pi) + \frac{1}{2} \log |\mathbf{Q}] - \frac{1}{2} \mathbf{y}^\mathsf{T} \mathbf{Q} \mathbf{y} + \mathbf{y}^\mathsf{T} \mathbf{Q} \boldsymbol{\mu} - \frac{1}{2} \boldsymbol{\mu}^\mathsf{T} \mathbf{Q} \boldsymbol{\mu}) \end{split}$$

VB for the factor analysis model: updating $q(\mathbf{w}_j)$

We choose the variational distribution so that

$$\begin{aligned} \log q(\mathbf{w}_j) &= \mathbb{E}_{q \neg \mathbf{w}_j}[\log p(\cdot)] + c = \mathbb{E} \log p(\mathbf{w}_j \mid \gamma) + \sum_{i=1}^N \mathbb{E} \log p(x_{ij} \mid \mathbf{w}_j, \mathbf{z}_i, \theta_j) + c \\ &= -\frac{1}{2} \mathbf{w}_j^T \left[\mathbb{E}(\gamma) \mathbf{I} + \mathbb{E}(\theta_j) \sum_{i=1}^N \mathbb{E}(\mathbf{Z}_i \mathbf{Z}_i^\mathsf{T}) \right] \mathbf{w}_j + \mathbf{w}_j^\mathsf{T} \mathbb{E}(\theta_j) \sum_{i=1}^N x_{ij} \mathbb{E}(\mathbf{Z}_i) + c \end{aligned}$$

Thus we see that $q(\mathbf{w}_j | \cdot)$ is normally distributed with

- precision $\mathbf{Q} \leftarrow \mathbb{E}(\gamma)\mathbf{I} + \mathbb{E}(\theta_j) \sum_{i=1}^N \mathbb{E}(\mathbf{Z}_i \mathbf{Z}_i^{\mathsf{T}})$
- ullet mean $oldsymbol{\mu} \leftarrow \mathbf{Q}^{-1} \left[\mathbb{E}(heta_j) \sum_{i=1}^N x_{ij} \mathbb{E}(\mathbf{Z}_i)
 ight]$

Recall the (generic) multivariate normal distribution

$$\begin{split} \log p(\mathbf{y} \mid \boldsymbol{\mu}, \mathbf{Q}) &= \log \mathcal{N}(\mathbf{y} \mid \boldsymbol{\mu}, \mathbf{Q}^{-1}) = -\frac{D}{2} \log(2\pi) + \frac{1}{2} \log |\mathbf{Q}| - \frac{1}{2} (\mathbf{y} - \boldsymbol{\mu})^{\mathsf{T}} \mathbf{Q} (\mathbf{y} - \boldsymbol{\mu})^{\mathsf{T}}) \\ &= -\frac{D}{2} \log(2\pi) + \frac{1}{2} \log |\mathbf{Q}| - \frac{1}{2} \mathbf{y}^{\mathsf{T}} \mathbf{Q} \mathbf{y} + \mathbf{y}^{\mathsf{T}} \mathbf{Q} \boldsymbol{\mu} - \frac{1}{2} \boldsymbol{\mu}^{\mathsf{T}} \mathbf{Q} \boldsymbol{\mu}) \end{split}$$

VB for the factor analysis model: updating $q(\mathbf{w}_j)$

We choose the variational distribution so that

$$\log q(\mathbf{w}_j) = \mathbb{E}_{q \neg \mathbf{w}_j}[\log p(\cdot)] + c = \mathbb{E} \log p(\mathbf{w}_j \mid \gamma) + \sum_{i=1}^N \mathbb{E} \log p(x_{ij} \mid \mathbf{w}_j, \mathbf{z}_i, \theta_j) + c$$

$$= -\frac{1}{2} \mathbf{w}_j^T \left[\mathbb{E}(\gamma) \mathbf{I} + \mathbb{E}(\theta_j) \sum_{i=1}^N \mathbb{E}(\mathbf{Z}_i \mathbf{Z}_i^\mathsf{T}) \right] \mathbf{w}_j + \mathbf{w}_j^\mathsf{T} \mathbb{E}(\theta_j) \sum_{i=1}^N x_{ij} \mathbb{E}(\mathbf{Z}_i) + c$$

Thus we see that $q(\mathbf{w}_j | \cdot)$ is normally distributed with

- precision $\mathbf{Q} \leftarrow \mathbb{E}(\gamma)\mathbf{I} + \mathbb{E}(\theta_j) \sum_{i=1}^N \mathbb{E}(\mathbf{Z}_i \mathbf{Z}_i^{\mathsf{T}})$
- mean $\mu \leftarrow \mathbf{Q}^{-1}\left[\mathbb{E}(\theta_j)\sum_{i=1}^N x_{ij}\mathbb{E}(\mathbf{Z}_i)\right]$

Calculation of $\mathbb{E}(\mathbf{Z}_i\mathbf{Z}_i^{\mathsf{T}})$

$$\mathbb{E}(\mathbf{Z}_i\mathbf{Z}_i^{\mathsf{T}}) = \mathsf{Cov}(\mathbf{Z}_i) + \mathbb{E}(\mathbf{Z}_i)\mathbb{E}(\mathbf{Z}_i)^{\mathsf{T}}$$

We choose the variational distribution so that

$$\log q(\mathbf{w}_j) = \mathbb{E}_{q \to \mathbf{w}_j}[\log p(\cdot)] + c = \mathbb{E}\log p(\mathbf{w}_j \mid \gamma) + \sum_{i=1}^N \mathbb{E}\log p(x_{ij} \mid \mathbf{w}_j, \mathbf{z}_i, \theta_j) + c$$

$$= -\frac{1}{2}\mathbf{w}_j^T \left[\mathbb{E}(\gamma)\mathbf{I} + \mathbb{E}(\theta_j) \sum_{i=1}^N \mathbb{E}(\mathbf{Z}_i \mathbf{Z}_i^\mathsf{T}) \right] \mathbf{w}_j + \mathbf{w}_j^\mathsf{T} \mathbb{E}(\theta_j) \sum_{i=1}^N x_{ij} \mathbb{E}(\mathbf{Z}_i) + c$$

Thus we see that $q(\mathbf{w}_j | \cdot)$ is normally distributed with

- precision $\mathbf{Q} \leftarrow \mathbb{E}(\gamma)\mathbf{I} + \mathbb{E}(\theta_j)\sum_{i=1}^N \mathbb{E}(\mathbf{Z}_i\mathbf{Z}_i^{\mathsf{T}})$
- ullet mean $oldsymbol{\mu} \leftarrow \mathbf{Q}^{-1} \left[\mathbb{E}(heta_j) \sum_{i=1}^N x_{ij} \mathbb{E}(\mathbf{Z}_i)
 ight]$

Compare this to the Gibbs sampler:

- $\mathbf{Q} \leftarrow \gamma \mathbf{I} + \theta_j \sum_{i=1}^N \mathbf{z}_i \mathbf{z}_i^\mathsf{T}$
- $\bullet \ \mu \leftarrow \mathbf{Q}^{-1} \left[\theta_j \sum_{i=1}^N x_{ij} \mathbf{z}_i \right]$

Once again, the only difference between VB and Gibbs is that where VB uses posterior expectations, Gibbs uses samples.

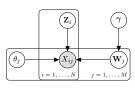
Exercise

Play around with the notebook

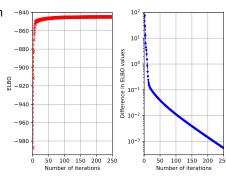
- Compare the implementation to the updating rules on the slides.
- Do you see any structure in the latent space (try with different seed values)
- Try investigating the learned distributions.

100 data points was randomly sampled from a 5-dim multivariate Gaussian distribution.

Global model



Monitoring convergence

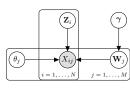


Local model



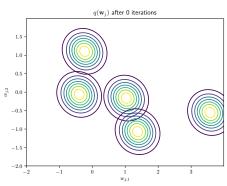
100 data points was randomly sampled from a 5-dim multivariate Gaussian distribution.

Global model



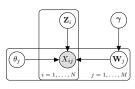
Local model



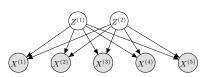


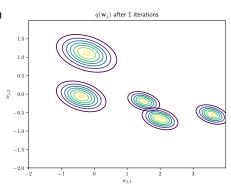
100 data points was randomly sampled from a 5-dim multivariate Gaussian distribution.

Global model



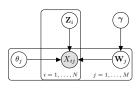
Local model



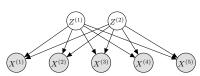


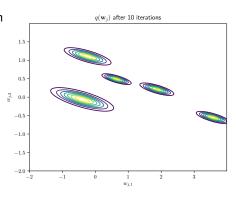
100 data points was randomly sampled from a 5-dim multivariate Gaussian distribution.

Global model



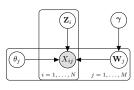
Local model





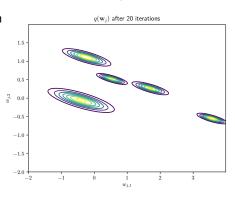
100 data points was randomly sampled from a 5-dim multivariate Gaussian distribution.

Global model



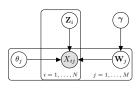
Local model



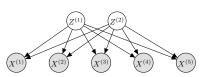


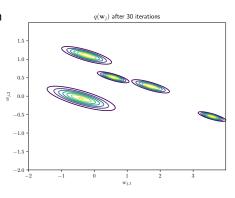
100 data points was randomly sampled from a 5-dim multivariate Gaussian distribution.

Global model



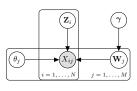
Local model





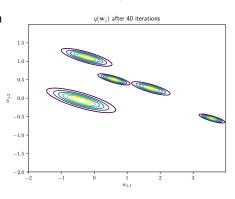
100 data points was randomly sampled from a 5-dim multivariate Gaussian distribution.

Global model



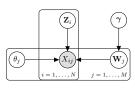
Local model



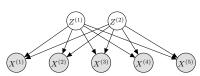


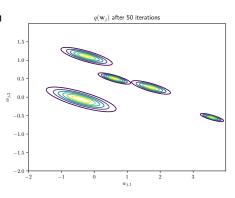
100 data points was randomly sampled from a 5-dim multivariate Gaussian distribution.

Global model



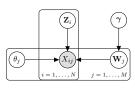
Local model



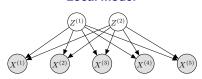


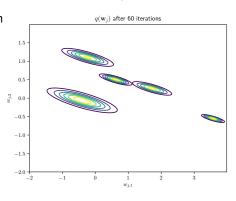
100 data points was randomly sampled from a 5-dim multivariate Gaussian distribution.

Global model



Local model



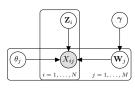


VB for the factor analysis model

Data

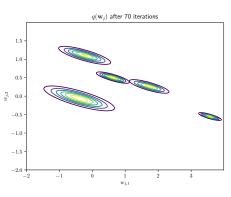
100 data points was randomly sampled from a 5-dim multivariate Gaussian distribution.

Global model



Local model



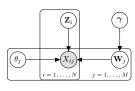


VB for the factor analysis model

Data

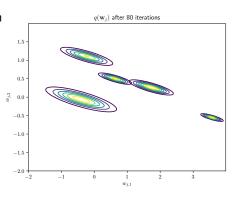
100 data points was randomly sampled from a 5-dim multivariate Gaussian distribution.

Global model



Local model



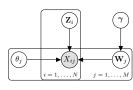


VB for the factor analysis model

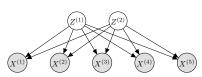
Data

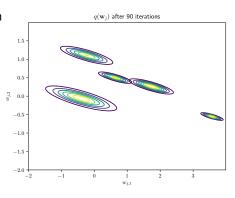
100 data points was randomly sampled from a 5-dim multivariate Gaussian distribution.

Global model



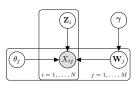
Local model



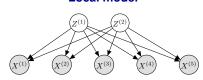


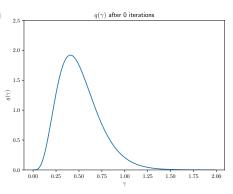
100 data points was randomly sampled from a 5-dim multivariate Gaussian distribution.

Global model



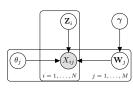
Local model



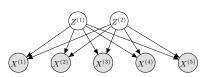


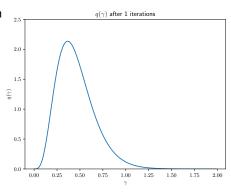
100 data points was randomly sampled from a 5-dim multivariate Gaussian distribution.

Global model



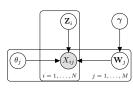
Local model



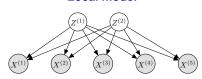


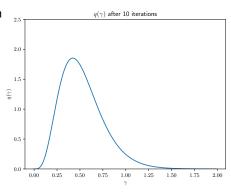
100 data points was randomly sampled from a 5-dim multivariate Gaussian distribution.

Global model



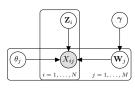
Local model





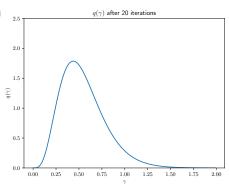
100 data points was randomly sampled from a 5-dim multivariate Gaussian distribution.

Global model



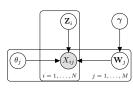
Local model



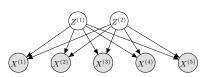


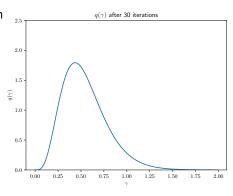
100 data points was randomly sampled from a 5-dim multivariate Gaussian distribution.

Global model



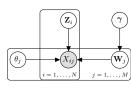
Local model



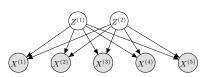


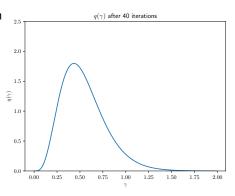
100 data points was randomly sampled from a 5-dim multivariate Gaussian distribution.

Global model



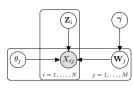
Local model



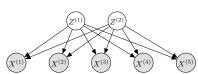


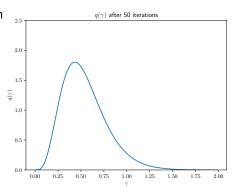
100 data points was randomly sampled from a 5-dim multivariate Gaussian distribution.

Global model



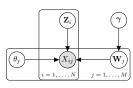
Local model





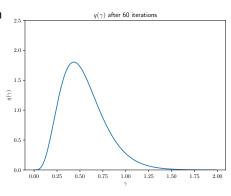
100 data points was randomly sampled from a 5-dim multivariate Gaussian distribution.

Global model



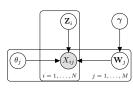
Local model



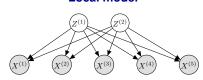


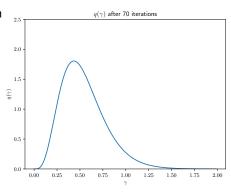
100 data points was randomly sampled from a 5-dim multivariate Gaussian distribution.

Global model



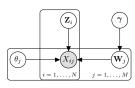
Local model





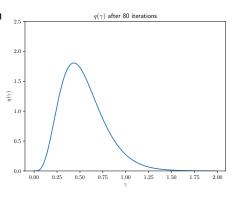
100 data points was randomly sampled from a 5-dim multivariate Gaussian distribution.

Global model



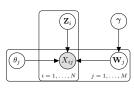
Local model





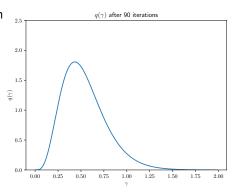
100 data points was randomly sampled from a 5-dim multivariate Gaussian distribution.

Global model



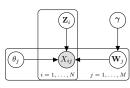
Local model





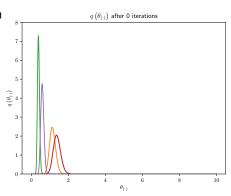
100 data points was randomly sampled from a 5-dim multivariate Gaussian distribution.

Global model



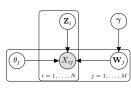
Local model





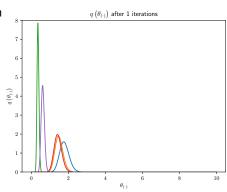
100 data points was randomly sampled from a 5-dim multivariate Gaussian distribution.

Global model



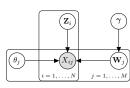
Local model





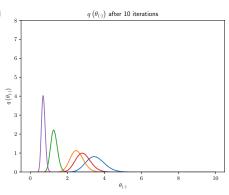
100 data points was randomly sampled from a 5-dim multivariate Gaussian distribution.

Global model



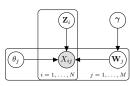
Local model





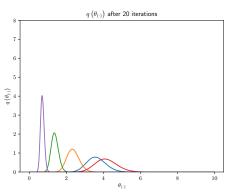
100 data points was randomly sampled from a 5-dim multivariate Gaussian distribution.

Global model



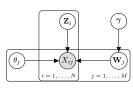
Local model





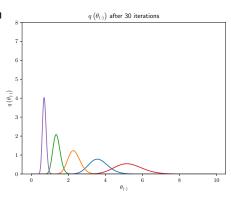
100 data points was randomly sampled from a 5-dim multivariate Gaussian distribution.

Global model



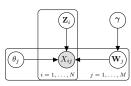
Local model



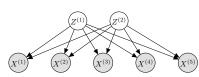


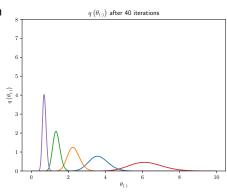
100 data points was randomly sampled from a 5-dim multivariate Gaussian distribution.

Global model



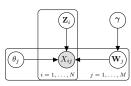
Local model





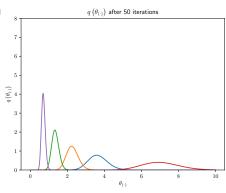
100 data points was randomly sampled from a 5-dim multivariate Gaussian distribution.

Global model



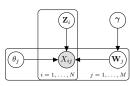
Local model



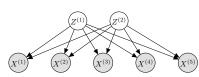


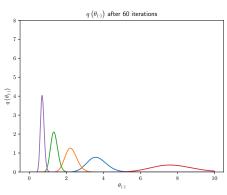
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Global model



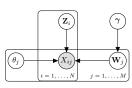
Local model



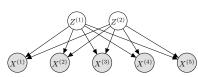


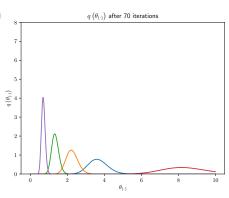
100 data points was randomly sampled from a 5-dim multivariate Gaussian distribution.

Global model



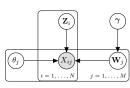
Local model



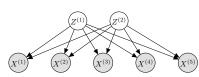


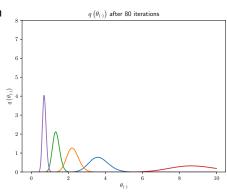
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Global model



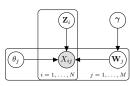
Local model



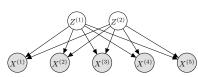


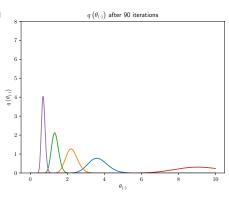
100 data points was randomly sampled from a 5-dim multivariate Gaussian distribution.

Global model



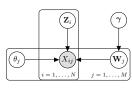
Local model





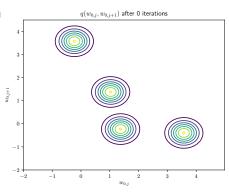
100 data points was randomly sampled from a 5-dim multivariate Gaussian distribution.

Global model



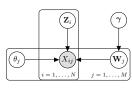
Local model





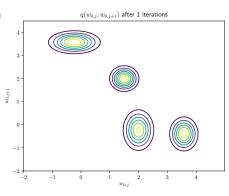
100 data points was randomly sampled from a 5-dim multivariate Gaussian distribution.

Global model



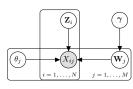
Local model





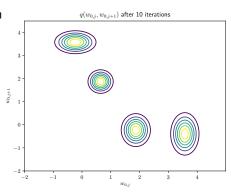
100 data points was randomly sampled from a 5-dim multivariate Gaussian distribution.

Global model



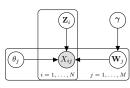
Local model





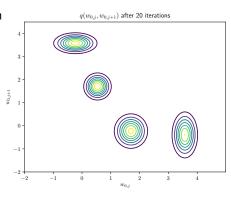
100 data points was randomly sampled from a 5-dim multivariate Gaussian distribution.

Global model



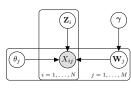
Local model





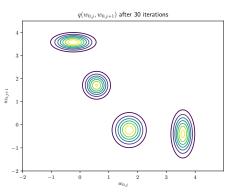
100 data points was randomly sampled from a 5-dim multivariate Gaussian distribution.

Global model



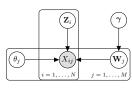
Local model





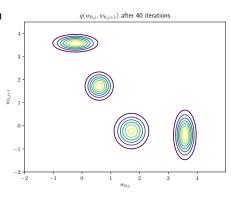
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Global model



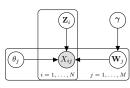
Local model





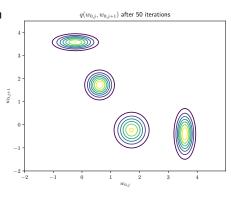
100 data points was randomly sampled from a 5-dim multivariate Gaussian distribution.

Global model



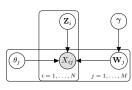
Local model





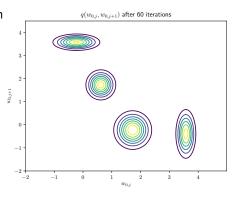
100 data points was randomly sampled from a 5-dim multivariate Gaussian distribution.

Global model



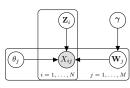
Local model





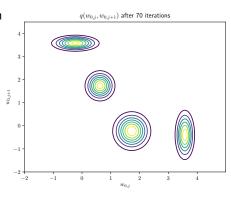
100 data points was randomly sampled from a 5-dim multivariate Gaussian distribution.

Global model



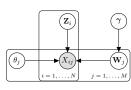
Local model





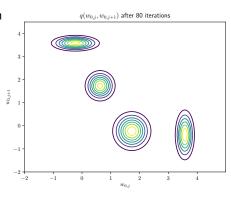
100 data points was randomly sampled from a 5-dim multivariate Gaussian distribution.

Global model



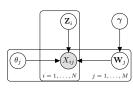
Local model





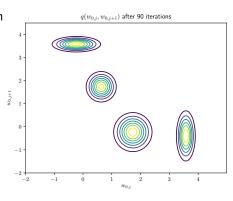
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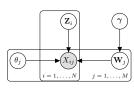
Local model



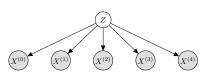


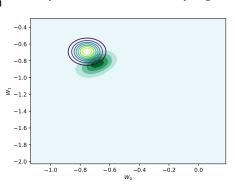
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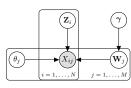
Local model



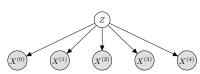


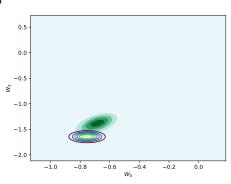
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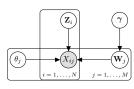
Local model





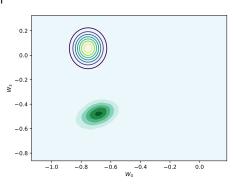
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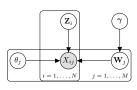
Local model





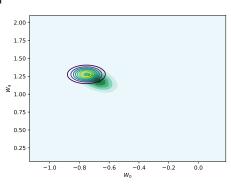
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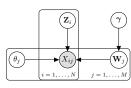
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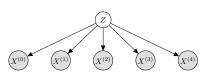


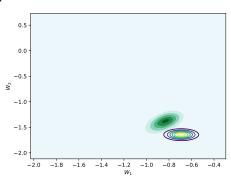
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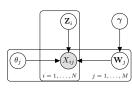
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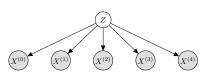


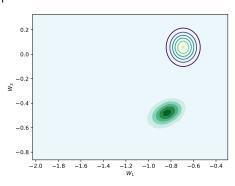
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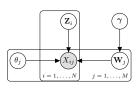
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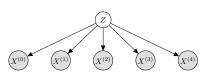


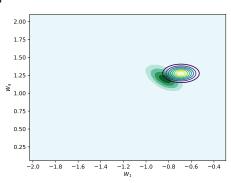
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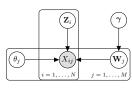
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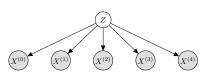


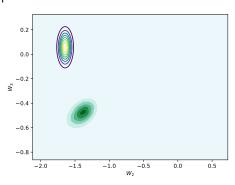
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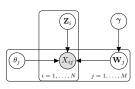
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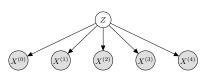


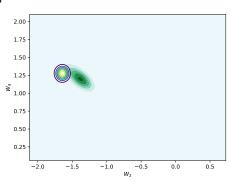
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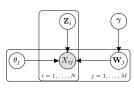
Local model



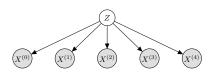


100 data points was randomly sampled from a 5-dim multivariate Gaussian distribution.

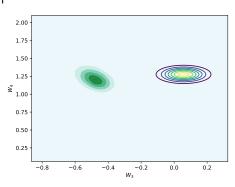
Global model



Local model



Comparison with Gibbs sampling



Not seen from the plot, **but** the results strongly dependent on the VI initialization.

Wrapping it all up: The VB algorithm under MF

Algorithm:

- ullet We have observed ${f X}={f x},$ and have access to the full joint $p({f z},{f x}).$
- We posit a *variational family* of distributions $q_j(\cdot | \lambda_j)$, i.e., we choose the distributional form, while wanting to optimize the parameterization λ_j .
- The posterior approximation is assumed to factorize according to the mean-field assumption, and we use the $\mathrm{KL}\left(q(\mathbf{z})||p(\mathbf{z}\,|\,\mathbf{x})\right)$ as our objective.

Algorithm:

Repeat until negligible improvement in terms of $\mathcal{L}(q)$:

- For each *j*:
 - Calculate $\mathbb{E}_{q_{\neg j}}\left[\log p(\mathbf{z}, \mathbf{x})\right]$ using current estimates for $q_i(\cdot \mid \boldsymbol{\lambda}_i), i \neq j$.
 - Choose λ_j so that $q_j(z_j | \lambda_j) \propto \exp \left(\mathbb{E}_{q_{\neg j}} \left[\log p(\mathbf{z}, \mathbf{x}) \right] \right)$.
- Calculate the new $\mathcal{L}(q)$.

Wrapping it all up: The VB algorithm under MF

Algorithm:

- We have observed X = x, and have access to the full joint p(z, x).
- We posit a *variational family* of distributions $q_j(\cdot | \lambda_j)$, i.e., we choose the distributional form, while wanting to optimize the parameterization λ_j .
- The posterior approximation is assumed to factorize according to the mean-field assumption, and we use the $\mathrm{KL}\left(q(\mathbf{z})||p(\mathbf{z}\,|\,\mathbf{x})\right)$ as our objective.

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- Calculate the new $\mathcal{L}(q)$.

As we just realized, calculations of $\mathbb{E}_{q_{-j}}\left[\log p(\mathbf{z},\mathbf{x})\right]$ and $\mathcal{L}\left(q\right)$ are quite tedious – and apparently must be done separately for each model we make.

This harms the applicability of variational inference, even under the quite restrictive mean field assumption.

Variational inference – Part II Factor analysis

The Exponential Family of distributions

Why consider the Exponential Family

Positives with the Exponential Family:

- It is the only family of distributions with finite-sized sufficient statistics*;
- It is the only family of distributions that has conjugate priors;
- It simplifies the operations of variational inference;
- It has simple mathematical procedures for calculating moments, MLEs, Bayesian posteriors, ...

Negatives:

- Standard distributions are defined using a new parameterization. Can be "unnatural".
- While all the calculations we will do are in principle simple, they are sometimes a bit abstract – due to the massive generality of the construction.

^{*} Under certain regularity conditions...

Definition – univariate exponential family model

Consider a univariate distribution $f_X(x | \theta)$, written as:

$$f_X(x \mid \boldsymbol{\theta}) = \exp\left(h(x) + \boldsymbol{\eta}(\boldsymbol{\theta})^{\mathsf{T}} \mathbf{t}(x) - A(\boldsymbol{\theta})\right)$$

Here we define:

- h(x): log base measure
- $\eta(\theta)$: the natural parameters
- \bullet $\mathbf{t}(x)$: the sufficient statistics
- $A(\theta)$: the log partition function

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Example:

•
$$h(x) = 0$$

$$\bullet \ \boldsymbol{\eta}(p) = \log(p/1 - p)$$

$$\bullet$$
 $\mathbf{t}(x) = x$

•
$$A(p) = -\log(1-p)$$

Members:

Bernoulli (and Multinomial)

$$f_X(x \mid \boldsymbol{\theta}) = \exp \left(h(x) + \boldsymbol{\eta}(\boldsymbol{\theta})^\mathsf{T} \mathbf{t}(x) - A(\boldsymbol{\theta})\right)$$

$$= \exp \left\{\log \left[p/(1-p)\right] \cdot x + \log(1-p)\right\}$$

$$= \left[p/(1-p)\right]^x \cdot (1-p)$$

$$= p^x (1-p)^{1-x}$$

The Bernoulli is in the exponential family

Definition – univariate exponential family model

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Members:

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- h(x): log base measure
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- $A(\theta)$: the log partition function

Example:

•
$$h(x) = -\frac{1}{2}\log(2\pi)$$

•
$$\eta(\mu, \tau) = \left[\tau \mu, -\frac{\tau}{2}\right]^{\mathsf{T}}$$

•
$$\mathbf{t}(x) = \left[x, x^2\right]^\mathsf{T}$$

•
$$A(\theta) = \frac{\tau \mu^2}{2} - \frac{1}{2} \log |\tau|$$
.

$$f_X(x \mid \boldsymbol{\theta})$$

$$f_X(x \mid \boldsymbol{\theta}) = \exp \left\{ \left[\tau \mu, -\frac{\tau}{2} \right] \left[\begin{array}{c} x \\ x^2 \end{array} \right] \right\}$$

Gaussians

$$\begin{bmatrix} & 2 \end{bmatrix} \begin{bmatrix} & x^2 \end{bmatrix}$$

$$-\frac{1}{2}\log(2)$$

Bernoulli (and Multinomial)

$$-\frac{1}{2}\log(2\pi) - (\tau\mu^2/2 - \frac{1}{2}\log\tau)$$

$$=\sqrt{\frac{\tau}{2\pi}}$$

$$= \sqrt{\frac{\tau}{2\pi}} \cdot \exp\left(-\tau(x-\mu)^2/2\right)$$

The Gaussian is in the exponential family

Consider a univariate distribution $f_X(x \mid \theta)$, written as:

$$f_X(x \mid \boldsymbol{\theta}) = \exp \left(h(x) + \boldsymbol{\eta}(\boldsymbol{\theta})^{\mathsf{T}} \mathbf{t}(x) - A(\boldsymbol{\theta})\right)$$

Here we define:

- h(x): log base measure
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- $A(\theta)$: the log partition function

Members:

- Bernoulli (and Multinomial)
- Gaussians
- Gamma + Inverse Gamma
- ...

Example:

•
$$h(x) = 0$$

$$\bullet \ \boldsymbol{\eta}(\alpha,\beta) = [-\beta,(\alpha-1)]^{\mathsf{T}}$$

$$\bullet \mathbf{t}(x) = [x, \log(x)]^{\mathsf{T}}$$

•
$$A(\boldsymbol{\theta}) = \log(\Gamma(\alpha)) - \alpha \log(\beta)$$

$$f_X(x \mid \theta) = \exp \left(0 + \left[-\beta, (\alpha - 1)\right] \left[x, \log(x)\right]^{\mathsf{T}} + \alpha \log(\beta) - \log(\Gamma(\alpha))\right)$$
$$= \frac{\beta^{\alpha}}{\Gamma(\alpha)} x^{(\alpha - 1)} \exp(-\beta x)$$

The Gamma is in the exponential family

Multivariate distributions

Consider a multi-variate distribution $f_{\mathbf{X}}(\mathbf{x} \,|\, \boldsymbol{\theta})$, and assume it can be written as:

$$f_{\mathbf{X}}(\mathbf{x} \mid \boldsymbol{\theta}) = \exp \left(h(\mathbf{x}) + \boldsymbol{\eta}(\boldsymbol{\theta})^{\mathsf{T}} \mathbf{t}(\mathbf{x}) - A(\boldsymbol{\theta})\right)$$

We define $h(\mathbf{x})$ (the log base measure) and $\mathbf{t}(\mathbf{x})$ (the sufficient statistics) as taking vector-inputs, but otherwise the definition is identical to the univariate case.

Example:

Consider a d-dimensional ${\bf x}$ with expectation ${\boldsymbol \mu}$ and inverse covariance ${\bf Q}={\bf \Sigma}^{-1}.$

Define

- $h(\mathbf{x}) = -\frac{d}{2}\log(2\pi)$
- $oldsymbol{\circ} oldsymbol{\eta}(oldsymbol{\mu}, \mathbf{Q}) = \left[\mathbf{Q}oldsymbol{\mu}, -rac{1}{2}\mathbf{Q}
 ight]^{\mathsf{T}}$
- $\bullet \ \mathbf{t}(\mathbf{x}) = \left[\mathbf{x}, \mathbf{x} \mathbf{x}^{\mathsf{T}}\right]^{\mathsf{T}}$
- $A(\boldsymbol{\theta}) = \frac{1}{2} \boldsymbol{\mu}^{\mathsf{T}} \mathbf{Q} \boldsymbol{\mu} \frac{1}{2} \log |\mathbf{Q}|.$

This gives us the multivariate Gaussian distribution; $f_{\mathbf{X}}(\mathbf{x}) = \mathcal{N}(\mathbf{x} \mid \boldsymbol{\mu}, \mathbf{Q}^{-1})$.

Multivariate exponential family model

Multivariate distributions

Consider a multi-variate distribution $f_{\mathbf{X}}(\mathbf{x} \mid \boldsymbol{\theta})$, and assume it can be written as:

$$f_{\mathbf{X}}(\mathbf{x} \mid \boldsymbol{\theta}) = \exp\left(h(\mathbf{x}) + \boldsymbol{\eta}(\boldsymbol{\theta})^{\mathsf{T}} \mathbf{t}(\mathbf{x}) - A(\boldsymbol{\theta})\right)$$

We define $h(\mathbf{x})$ (the log base measure) and $\mathbf{t}(\mathbf{x})$ (the sufficient statistics) as taking vector-inputs, but otherwise the definition is identical to the univariate case.

Notational simplification:

Notice how η take the role of the parameters θ , and – for the model we consider – a one-to-one mapping between η and θ .

For instance, $\boldsymbol{\eta} = [\boldsymbol{\eta}_1, \boldsymbol{\eta}_2]^{\mathsf{T}} = [\boldsymbol{\Sigma}^{-1} \boldsymbol{\mu}, -\frac{1}{2} \boldsymbol{\Sigma}^{-1}]$ in the Gaussian distribution, meaning

$$oldsymbol{ heta} = [oldsymbol{\mu}, oldsymbol{\Sigma}]^{\mathsf{T}} = \left[-rac{1}{2} oldsymbol{\eta}_2^{-1} oldsymbol{\eta}_1, -rac{1}{2} oldsymbol{\eta}_2^{-1}
ight]^{\mathsf{T}}.$$

Given that θ and η are interchangable, we will simplify notation, and use this form:

$$f_{\mathbf{X}}(\mathbf{x} \mid \boldsymbol{\eta}) = \exp\left(h(\mathbf{x}) + \boldsymbol{\eta}^{\mathsf{T}} \mathbf{t}(\mathbf{x}) - A(\boldsymbol{\eta})\right)$$

Code Task: Translation between moment-based and ExpFam representations

In this task you will translate between moment-based representations and the corresponding ExpFam representations. The task is fairly straight-forward, but is intended to give you "hands-on" experience with ExpFam representation.

Start from

students_translator.ipynb

You will see that there are some supporting functions there, and a translation for univariate Gaussians (to show how the supporting functions work).

Your task is to implement the same for the Gamma distribution. If time, other ExpFam distributions can of course be given the same treatment.

Remember the definition or the Exponential Family:

$$f_X(x \mid \boldsymbol{\eta}) = \exp\left(h(\mathbf{x}) + \boldsymbol{\eta}^{\mathsf{T}} \mathbf{t}(\mathbf{x}) - A(\boldsymbol{\eta})\right)$$

Derivatives of the log normalizer:

 $\nabla^k A(\eta)$ has an interesting form:

•
$$\nabla A(\boldsymbol{\eta}) = \frac{\mathrm{d}A(\boldsymbol{\eta})}{\mathrm{d}\boldsymbol{\eta}} = \mathbb{E}\left[\mathbf{t}\left(\mathbf{X}\right)\right]$$

Proof:

$$\begin{split} \frac{\mathrm{d}A(\boldsymbol{\eta})}{\mathrm{d}\boldsymbol{\eta}} &= \frac{\mathrm{d}}{\mathrm{d}\boldsymbol{\eta}} \log \int_{\mathbf{x}} \exp \left(h(\mathbf{x}) + \boldsymbol{\eta}^\mathsf{T} \mathbf{t}(\mathbf{x})\right) \mathrm{d}\mathbf{x} \\ &= \frac{\frac{\mathrm{d}}{\mathrm{d}\boldsymbol{\eta}} \int_{\mathbf{x}} \exp \left(h(\mathbf{x}) + \boldsymbol{\eta}^\mathsf{T} \mathbf{t}(\mathbf{x})\right) \mathrm{d}\mathbf{x}}{\int_{\mathbf{x}} \exp \left(h(\mathbf{x}) + \boldsymbol{\eta}^\mathsf{T} \mathbf{t}(\mathbf{x})\right) \mathrm{d}\mathbf{x}} \\ &= \frac{\int_{\mathbf{x}} \mathbf{t}(\mathbf{x}) \exp \left(h(\mathbf{x}) + \boldsymbol{\eta}^\mathsf{T} \mathbf{t}(\mathbf{x})\right) \mathrm{d}\mathbf{x}}{\exp \left(A(\boldsymbol{\eta})\right)} \\ &= \int \mathbf{t}(\mathbf{x}) \exp \left(h(\mathbf{x}) + \boldsymbol{\eta}^\mathsf{T} \mathbf{t}(\mathbf{x}) - A(\boldsymbol{\eta})\right) \mathrm{d}\mathbf{x} = \mathbb{E}\left[\mathbf{t}\left(\mathbf{X}\right)\right] \end{split}$$

Remember the definition or the Exponential Family:

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- $\nabla A(\boldsymbol{\eta}) = \frac{\mathrm{d}A(\boldsymbol{\eta})}{\mathrm{d}\boldsymbol{\eta}} = \mathbb{E}\left[\mathbf{t}\left(\mathbf{X}\right)\right]$
- $\nabla^2 A(\boldsymbol{\eta}) = \mathbb{E}\left[(\mathbf{t}(\mathbf{X}) \mathbb{E}\left[\mathbf{t}(\mathbf{X})\right])^2 \right] = \mathbb{V}\left[\mathbf{t}(\mathbf{X})\right]$
 - ullet ... which also shows that $A(\eta)$ is convex.

Proofs for k > 1 are more of the same manipulations (left out for simplicity).