Variational inference

Partly based on material developed together with Helge Langseth

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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
  - ...

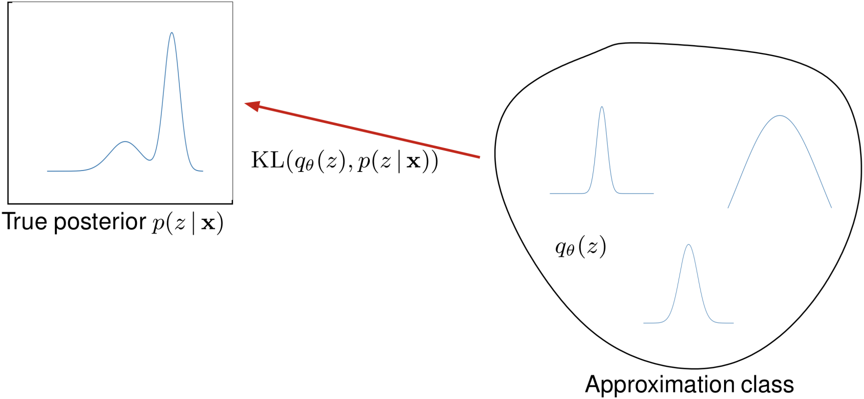
Day 3: Variational inference – cont'd

- Black box variational inference
- Variational inference in Pyro
- Variational auto-encoders

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' $\mathrm{KL}(q_\theta(z), p(z \mid \mathbf{x}))$ is minimized:

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

ELBO: Evidence Lower-BOund

We can rearrange the KL divergence as follows:

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

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

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&= \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 \tfrac{q(\mathbf{z})}{p(\mathbf{z},\mathbf{x})}\right] = \log p(\mathbf{x}) - \mathcal{L}(q)
\end{aligned}$$

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

VI focuses on the ELBO:

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

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:

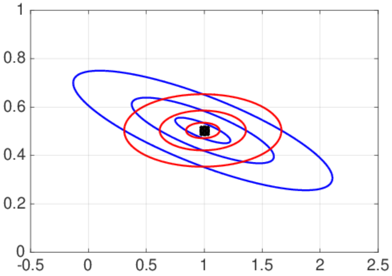
- We can minimize $\mathrm{KL}\left(q(\mathbf{z})||p(\mathbf{z}\,|\,\mathbf{x})\right)$ by maximizing $\mathcal{L}(q)$
- This is **computationally simpler** because it uses $p(\mathbf{z},\mathbf{x})$ instead of $p(\mathbf{z}\,|\,\mathbf{x})$.
- $\mathcal{L}(q)$ is a *lower bound* of the marginal data 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.

Algorithm:

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

Algorithm:

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

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

Solving the VB optimization

Solving the VB equation

We will maximize $\mathcal{L}(q) = \mathbb{E}_q\left[\log \frac{p(\mathbf{z},\mathbf{x})}{q(\mathbf{z})}\right]$ 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{aligned}
\mathcal{L}(q) &= \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]
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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

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

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&= \mathbb{E}_{q_j} \log f_j(z_j) - \mathbb{E}_{q_j}\mathbb{E}_{q_{\neg j}}[\log q(\mathbf{z})]
\end{aligned}$$

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

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

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

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&= -\mathrm{KL}\left(q_j(z_j)||f_j(z_j)\right) + c
\end{aligned}$$

We get the following result:

The ELBO is maximized wrt. q_j 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.

Setup

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

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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 $\boldsymbol{\lambda}_j$ so that $q_j(z_j \mid \boldsymbol{\lambda}_j) \propto \exp\left(\mathbb{E}_{q_{\neg j}}\left[\log p(\mathbf{z}, \mathbf{x})\right]\right)$.
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Calculating $q_j(z_j \mid \boldsymbol{\lambda}_j)$ - an observation

The update-rule can equivalently be expressed as

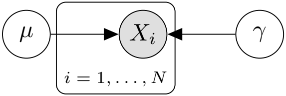
$$\begin{aligned}\log q_j(z_j \mid \boldsymbol{\lambda}_j) &= \mathbb{E}_{q_{\neg j}}[\ln p(\mathbf{z}, \mathbf{x})] + c. \\ &= \sum_{x \in \mathrm{mb}(z_j)} \mathbb{E}_{q_{\neg j}} \log p(x \mid \mathrm{pa}(x)) + \sum_{z \in \mathrm{mb}(z_j)} \mathbb{E}_{q_{\neg j}} \log p(z \mid \mathrm{pa}(z)) + c'.\end{aligned}$$

Note!

- We only need to consider terms that share a factor with z_j – all other terms get absorbed into the constant c.
- $\rightsquigarrow$ 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

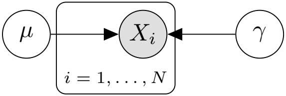


- $X_i \mid \{\mu, \gamma\} \sim \mathcal{N}(\mu, 1/\gamma)$
- $\mu \sim \mathcal{N}(0, \tau^{-1})$
- $\gamma \sim \text{Gamma}(\alpha, \beta)$

The probability model

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

A Gaussian model with unknown mean and precision



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. . . after taking the log

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

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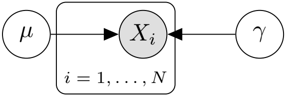

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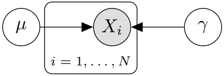
The variational model (full mean field)

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

where

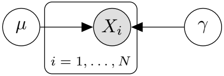
- $q(\mu) = \mathcal{N}(\nu_p, \tau_p^{-1})$
- $q(\gamma) = \text{Gamma}(\alpha_p, \beta_p)$

We choose the variational distribution so that



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

VB for simple Gaussian model: updating $q(\mu)$



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Recall

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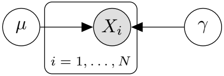

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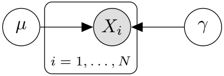

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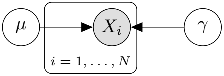

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Recall

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

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

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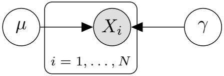

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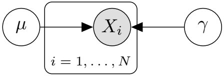

We choose the variational distribution so that

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

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

Recall

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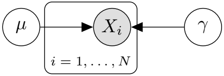

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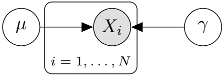
$$
\begin{aligned}
\log q(\mu) &= \mathop{\mathbb{E}}_{\gamma} p(\mathbf{x}, \mu, \gamma | \tau, \alpha, \beta) + c = \sum_{i=1}^{N} \mathop{\mathbb{E}}_{\gamma} (\log p(x_i \,|\, \mu, \gamma^{-1})) + \log p(\mu \,|\, 0, \tau^{-1}) + c \\
&= \sum_{i=1}^{N} \mathop{\mathbb{E}}_{\gamma} \left(-\frac{\gamma}{2} (x_i - \mu)^2 \right) - \frac{\tau}{2} (\mu)^2 + c \\
&= -\frac{1}{2} \mathop{\mathbb{E}}_{\gamma}(\gamma) \left(\sum_{i=1}^{N} x_i^2 + N \cdot \mu^2 - 2\mu \sum_{i=1}^{N} x_i \right) - \frac{\tau}{2} (\mu)^2 + c
\end{aligned}
$$

VB for simple Gaussian model: updating $q(\mu)$



We choose the variational distribution so that

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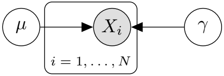
&= -\frac{1}{2} \left(\mathop{\mathbb{E}}_{\gamma}(\gamma) \cdot N + \tau \right) \mu^2 + \left(\mathop{\mathbb{E}}_{\gamma}(\gamma) \sum_{i=1}^{N} x_i \right) \mu + c
\end{aligned}
$$

VB for simple Gaussian model: updating $q(\mu)$



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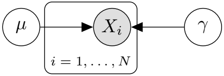

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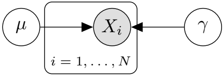
Recall the normal distribution

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

VB for simple Gaussian model: updating $q(\mu)$



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

Recall the normal distribution

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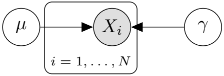


We choose the variational distribution so that

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

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

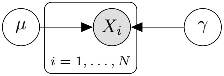
Thus, we see that $q(\mu)$ is normally distributed with

- 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

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

VB for simple Gaussian model: updating $q(\gamma)$



We choose the variational distribution so that

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

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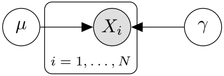

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Recall

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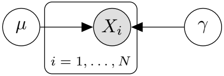

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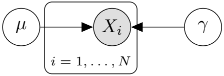

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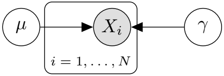

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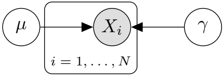
Recall

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

$$\log p(\gamma \,|\, \alpha, \beta) = \text{Gamma}(\alpha, \beta) = \alpha \cdot \log(\beta) + (\alpha - 1)\log(\gamma) - \beta \cdot \gamma - \log(\Gamma(\alpha))$$

VB for simple Gaussian model: updating $q(\gamma)$



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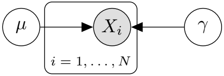
VB for simple Gaussian model: updating $q(\gamma)$



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

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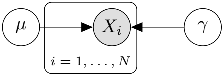
VB for simple Gaussian model: updating $q(\gamma)$



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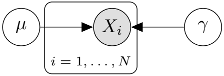
$$= \left(\frac{N}{2} + \alpha - 1 \right) \log(\gamma) - \left(\frac{1}{2} \sum_{i=1}^{N} \mathop{\mathbb{E}}_{\mu}(x_i - \mu)^2 + \beta \right) \cdot \gamma + c$$

VB for simple Gaussian model: updating $q(\gamma)$



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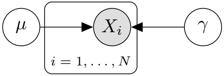
VB for simple Gaussian model: updating $q(\gamma)$



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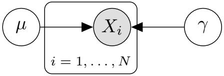

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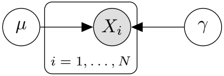
$$\log q(\gamma \,|\, \alpha_p, \beta_p^{-1}) = \alpha_p \cdot \beta_p + (\alpha_p - 1) \log(\gamma) - \beta \cdot \gamma - \log(\Gamma(\alpha_p))$$

VB for simple Gaussian model: updating $q(\gamma)$



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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:

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

Monitoring the ELBO

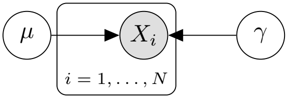
The variational updating rules are guaranteed to never decrease the ELBO $\mathcal{L}(q)$:

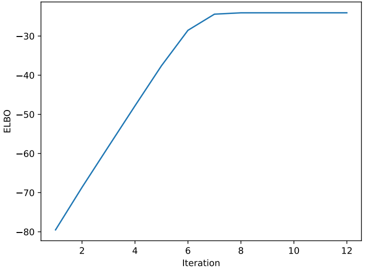
$$\begin{aligned}\mathcal{L}(q) &= \mathop{\mathbb{E}}_{q} \log p(\mathbf{x}, \mu, \gamma \,|\, \tau, \alpha, \beta) - \mathop{\mathbb{E}}_{q} \log q(\mu, \gamma) \\ &= \sum_{i=1}^{N} \mathop{\mathbb{E}}_{q} \log p(x_i \,|\, \mu, \gamma) + \mathop{\mathbb{E}}_{q} \log p(\mu \,|\, 0, \tau^{1}) + \mathop{\mathbb{E}}_{q} \log p(\gamma \,|\, \alpha, \beta) - \mathop{\mathbb{E}}_{q} \log q(\mu) - \mathop{\mathbb{E}}_{q} \log q(\gamma)\end{aligned}$$

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

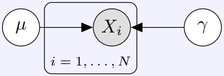
- Assessing convergence
- Doing debugging





Code-task: VB for a simple Gaussian model

Code Task: VB for a simple Gaussian model



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

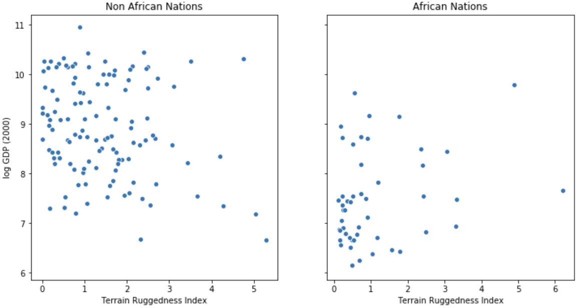
In this task you need to use mean-field, and look for $q(\mu, \gamma) = q(\mu) \cdot q(\gamma)$ that best approximates $p(\mu, \tau \mid x_1, \ldots, x_N)$ wrt. the VB measure $\mathrm{KL}\,(q||p)$.

- Go though the notebook

  `students_simple_model.ipynb`

  and try to link the code to the derivations in the slides.
- 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.

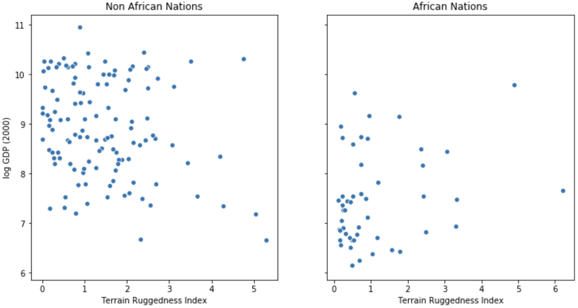
Bayesian linear regression



Relationship between topographic heterogeneity and GDP per capita

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

Real Data Example

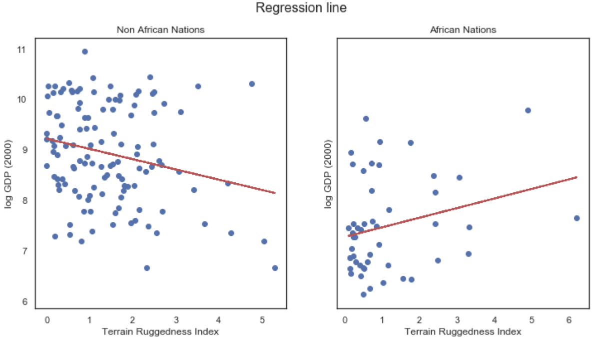


Relationship between topographic heterogeneity and GDP per capita

- 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.

`Day1/students_Bayesian_regression.ipynb`

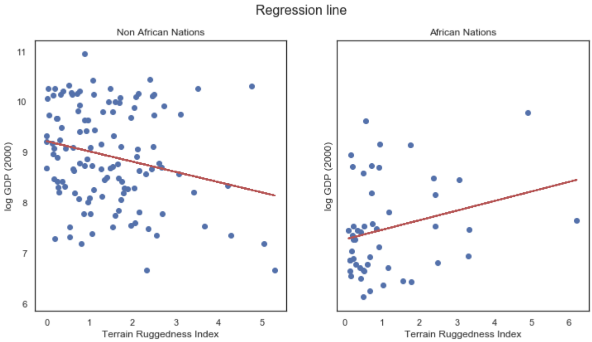
Real Data Example



Linear Regression Model

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

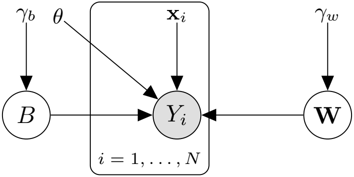
Real Data Example



Bayesian Linear Regression Model

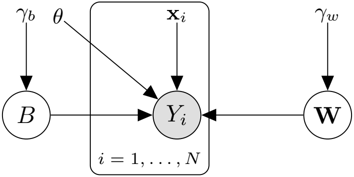
- Modeling data noise (aleatoric uncertainty)
- Modeling uncertainty about the linear coefficients (epistemic uncertainty).

The Bayesian linear regression model



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

The Bayesian linear regression model



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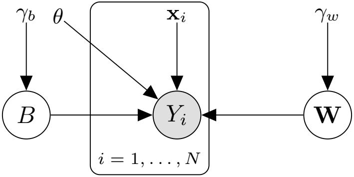
- Num. of data inst: N
- $Y_i \mid \{\mathbf{w}, \mathbf{x}_i, b, \theta\} \sim \mathcal{N}(\mathbf{w}^{\mathsf{T}}\mathbf{x}_i + b, 1/\theta)$
- $\mathbf{W} \sim \mathcal{N}(\mathbf{0}, \gamma_w^{-1}\mathbf{I}_{M\times M})$
- $B \sim \mathcal{N}(0, \gamma_b^{-1})$

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 Bayesian linear regression model



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

The probability model

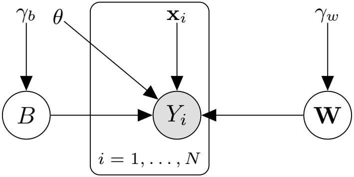
$$p(\cdot \mid \mathbf{x}, \theta, \gamma_w, \gamma_b) = \prod_{i=1}^{N} p(y_i \mid \mathbf{x}_i, \mathbf{w}, b, \theta) p(\mathbf{w} \mid \gamma_w) p(b \mid \gamma_b)$$

The variational updating rules (full mean field) - with some pencil pushing

$q(w_j)$ is normally distributed with

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

The Bayesian linear regression model



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

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 updating rules (full mean field) - with some pencil pushing

$q(b)$ is normally distributed with

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

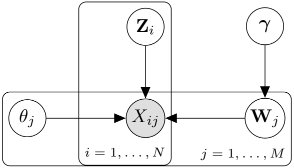
Exercise: Implement the updating rules

Now it is your turn!

- Implement the updating rules in the notebook
  `students_lin_reg.ipynb`
- Play around with the code

Factor analysis

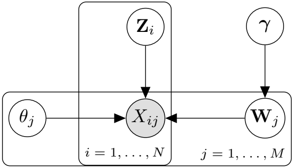
The factor analysis model



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

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

The factor analysis model



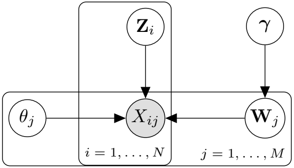
- $X_{ij} \mid \{\mathbf{w}_j, \mathbf{z}_i, \theta_j\} \sim \mathcal{N}(\mathbf{w}_j^\intercal \mathbf{z}_i, 1/\theta_j)$
- $\mathbf{Z}_i \sim \mathcal{N}(\mathbf{0}, \mathbf{I}_{D\times D})$
- $\mathbf{W}_j \sim \mathcal{N}(\mathbf{0}, \gamma^{-1}\mathbf{I}_{D\times D})$
- $\theta_j \sim \text{Gamma}(\alpha_\theta,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

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

The probability model

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

The factor analysis model



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

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

The probability model

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

The variational model

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

The updating rule for $q(\gamma)$

By choosing the variational distribution so that

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

we find that $q(\gamma \,|\, \cdot)$ is gamma distributed with

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

The updating rule for $q(\gamma)$

By choosing the variational distribution so that

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

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

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

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

The updating rule for $q(\gamma)$

By choosing the variational distribution so that

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

we find that $q(\gamma \,|\, \cdot)$ is gamma distributed with

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

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

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

Compare this to the Gibbs sampler:

$$\alpha \leftarrow \alpha_\gamma + \frac{DM}{2} \qquad \beta \leftarrow \beta_\gamma + \frac{1}{2}\sum_{j=1}^{M} \mathbf{w}_j^{\mathsf{T}} \mathbf{w}_j$$

VB uses posterior expectations where Gibbs uses samples!

The variational updating rules

By choosing the variational distribution so that

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

we find that $q(\mathbf{w}_j \mid \cdot)$ is normally distributed with

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

The variational updating rules

By choosing the variational distribution so that

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

we find that $q(\mathbf{w}_j \mid \cdot)$ is normally distributed with

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

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

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

The variational updating rules

By choosing the variational distribution so that

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

we find that $q(\mathbf{w}_j \mid \cdot)$ is normally distributed with

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

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

$$\mathbb{E}(\mathbf{Z}_i \mathbf{Z}_i^\intercal) = \text{Cov}(\mathbf{Z}_i) + \mathbb{E}(\mathbf{Z}_i)\mathbb{E}(\mathbf{Z}_i)^\intercal$$

Compare this to the Gibbs sampler:

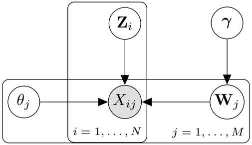
- $\mathbf{Q} \leftarrow \gamma \mathbf{I} + \theta_j \sum_{i=1}^{N} \mathbf{z}_i \mathbf{z}_i^\intercal$
- $\boldsymbol{\mu} \leftarrow \mathbf{Q}^{-1} \left[\theta_j \sum_{i=1}^{N} x_{ij} \mathbf{z}_i\right]$

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

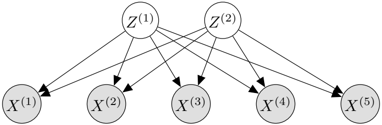
Data

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

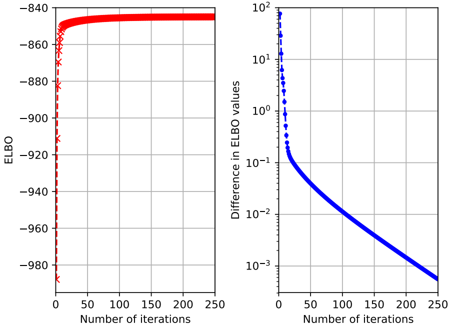
Global model



Local model



Monitoring convergence



Data

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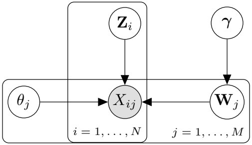
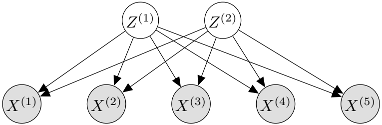
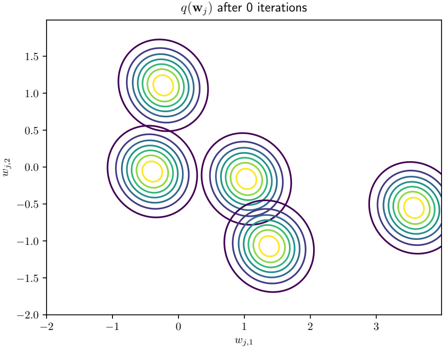
Global model



Local model



Variational posteriors



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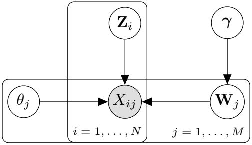
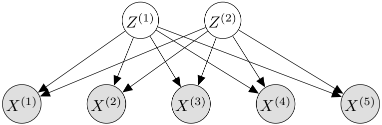
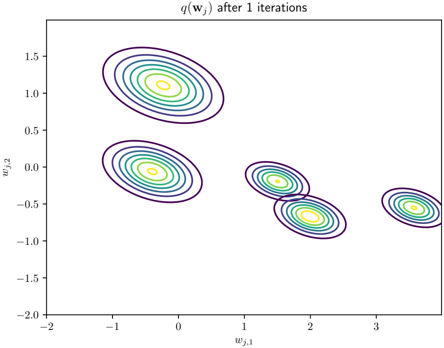
Global model



Local model



Variational posteriors



Data

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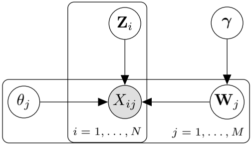
Global model



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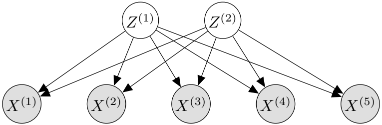
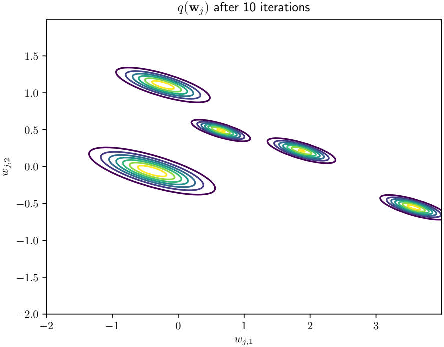


Variational posteriors



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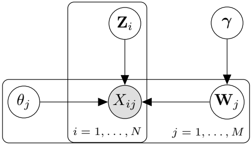
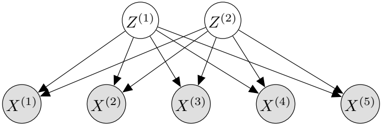
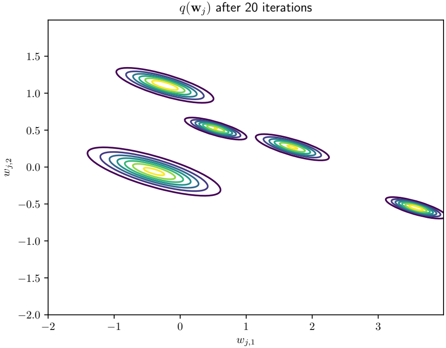


Local model



Variational posteriors



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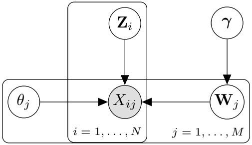
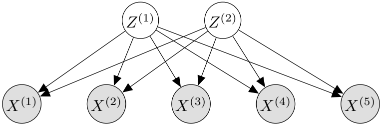
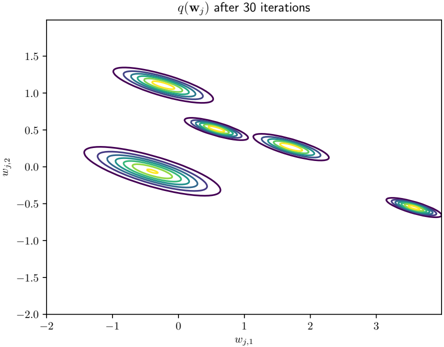
Global model



Local model



Variational posteriors



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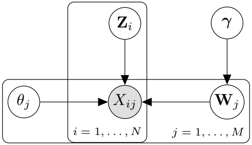

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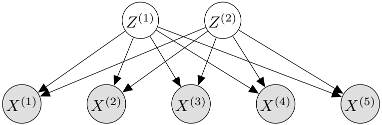
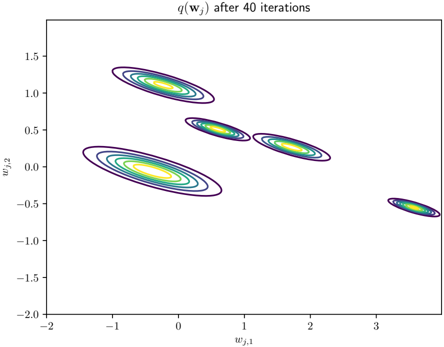


Variational posteriors



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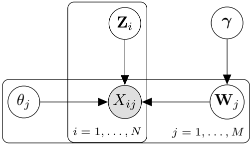
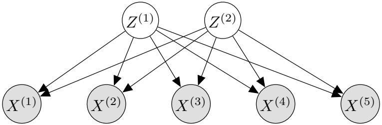
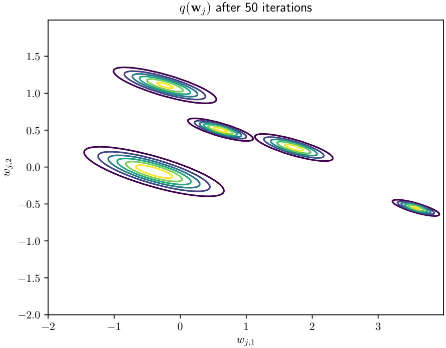
Global model



Local model



Variational posteriors



Data

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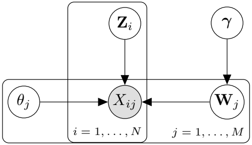
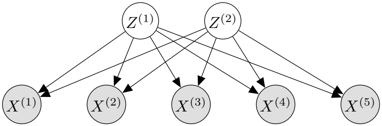
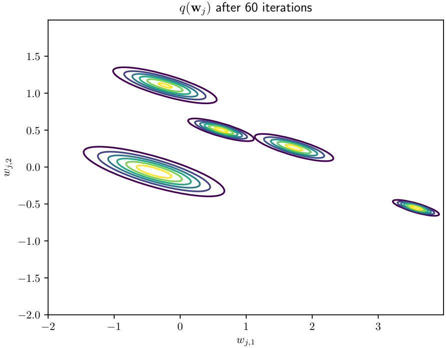
Global model



Local model



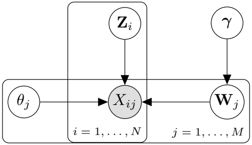
Variational posteriors



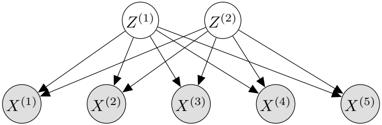
Data

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

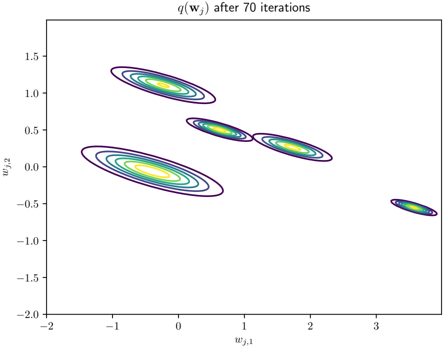
Global model



Local model



Variational posteriors



Data

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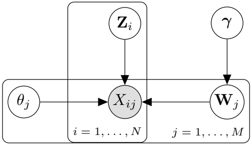
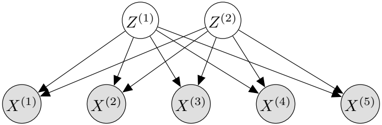
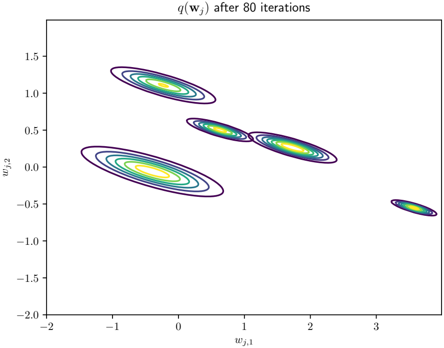
Global model



Local model



Variational posteriors

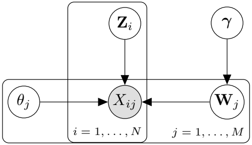


VB for the factor analysis model

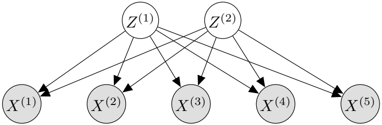
Data

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

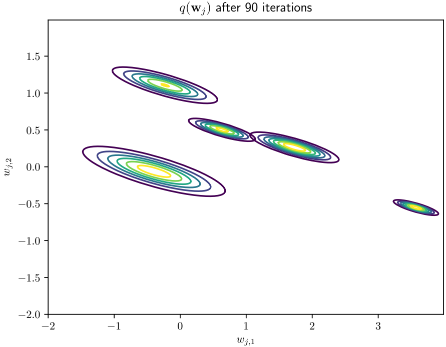
Global model



Local model



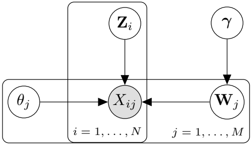
Variational posteriors



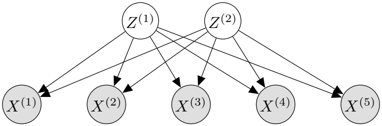
Data

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

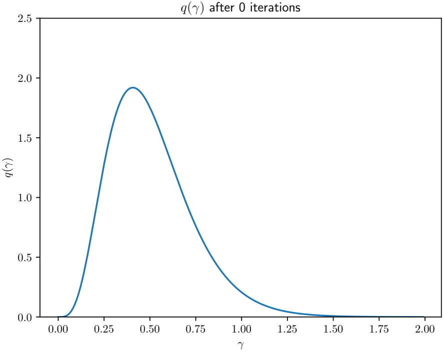
Global model



Local model



Variational posteriors



Data

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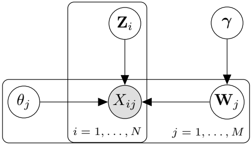
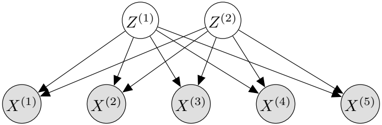
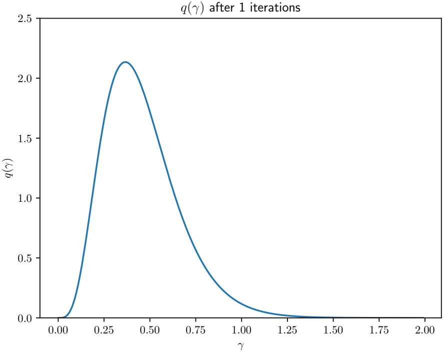
Global model



Local model



Variational posteriors



Data

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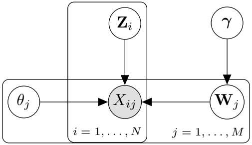
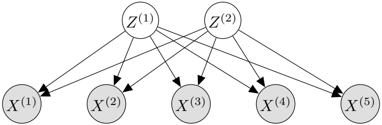
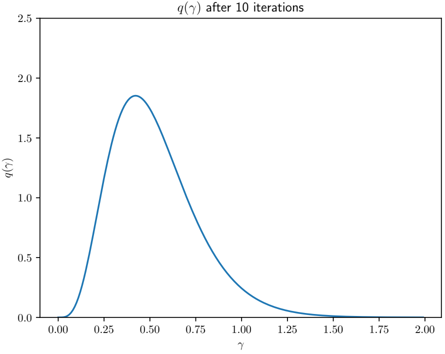
Global model



Local model



Variational posteriors



Data

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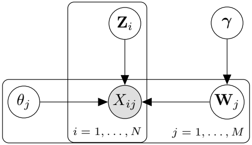
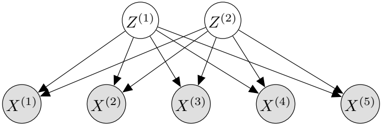
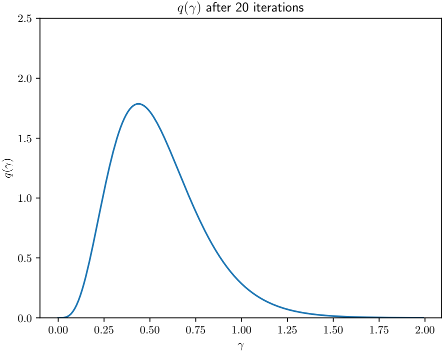
Global model



Local model



Variational posteriors

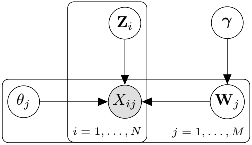


VB for the factor analysis model

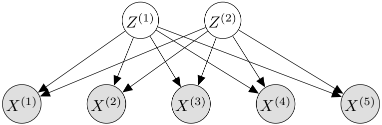
Data

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

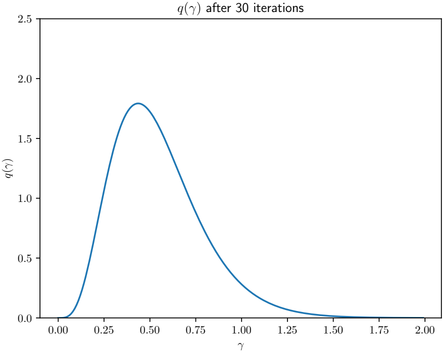
Global model



Local model



Variational posteriors



Data

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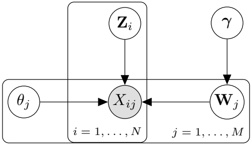
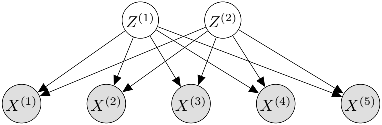
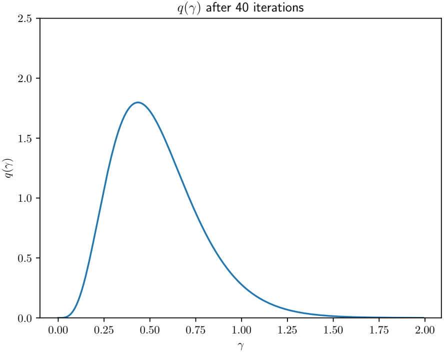
Global model



Local model



Variational posteriors



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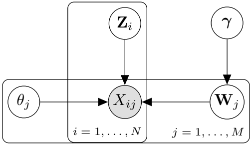
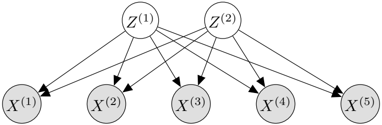
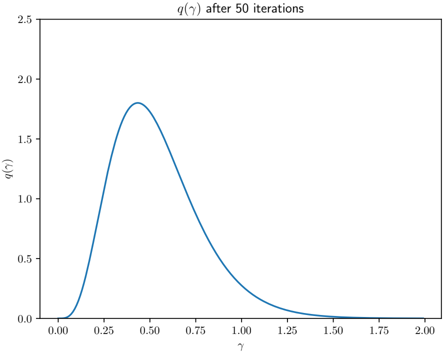
Global model



Local model



Variational posteriors



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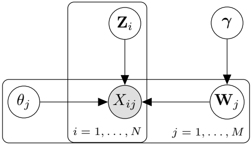
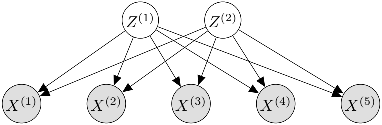
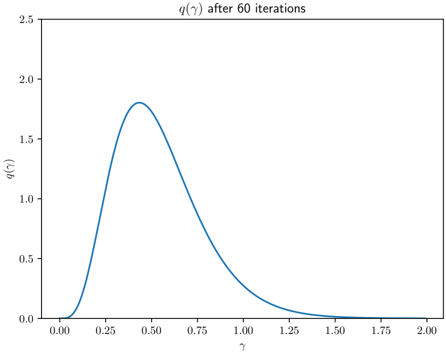


Local model



Variational posteriors



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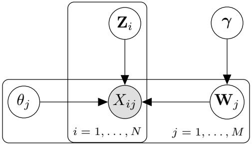
Global model



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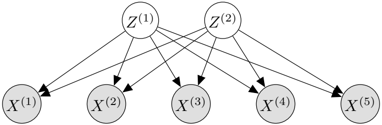
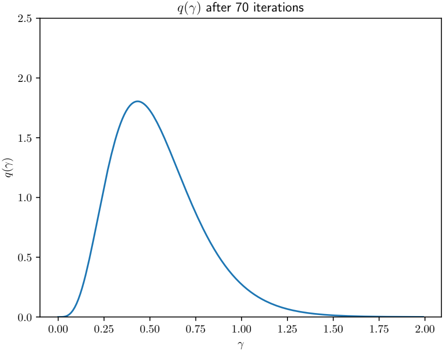


Variational posteriors



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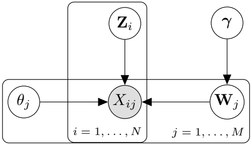
Global model



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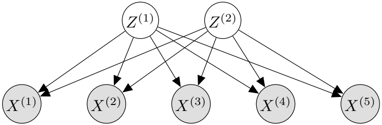
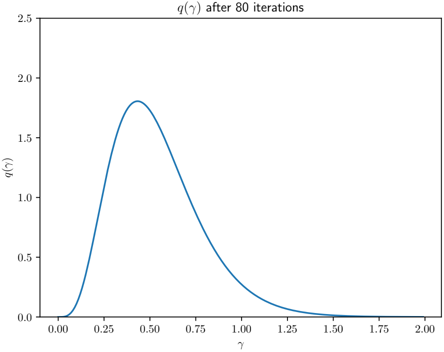


Variational posteriors



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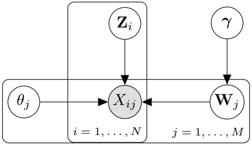
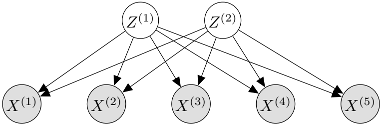
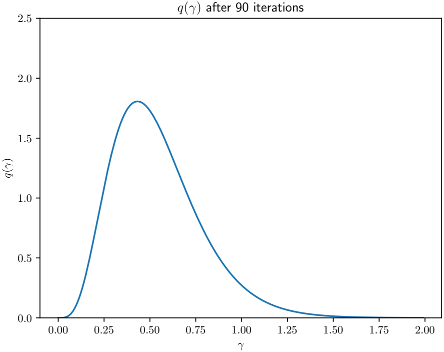


Local model



Variational posteriors



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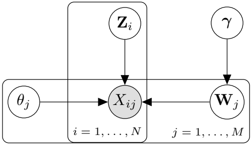
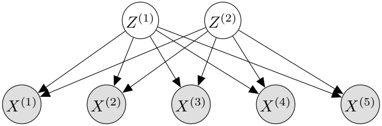
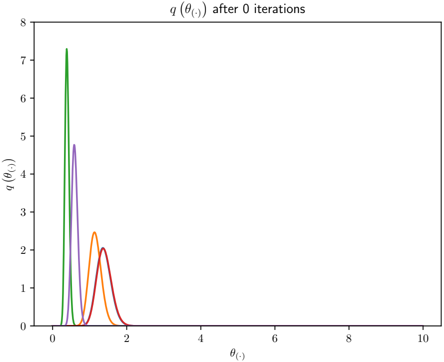
Global model



Local model



Variational posteriors



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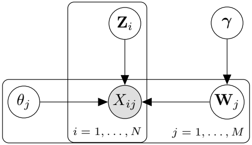
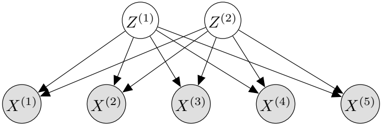
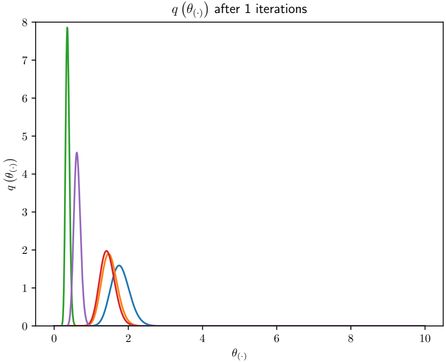


Local model



Variational posteriors



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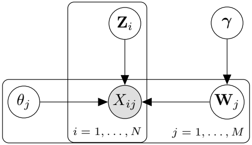
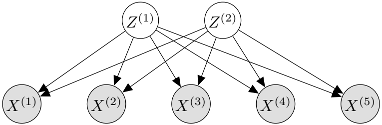
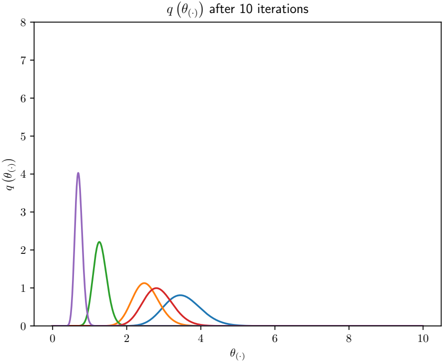
Global model



Local model



Variational posteriors



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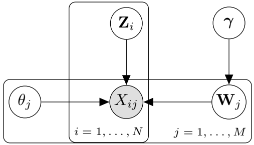
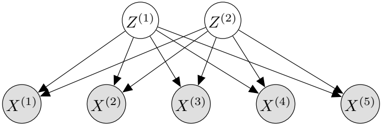
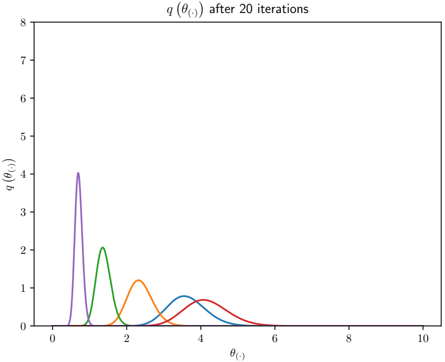
Global model



Local model



Variational posteriors



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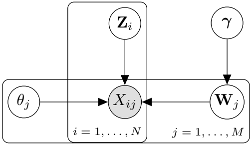
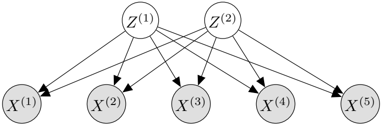
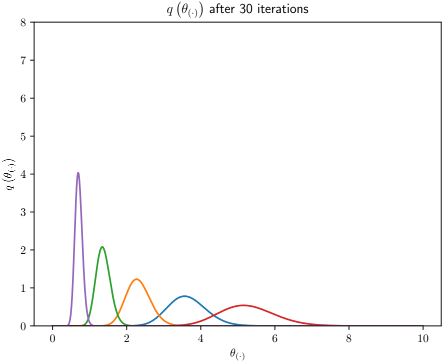


Local model



Variational posteriors



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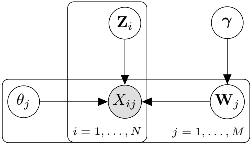
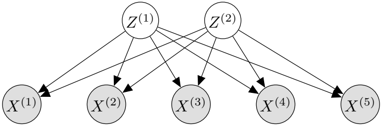
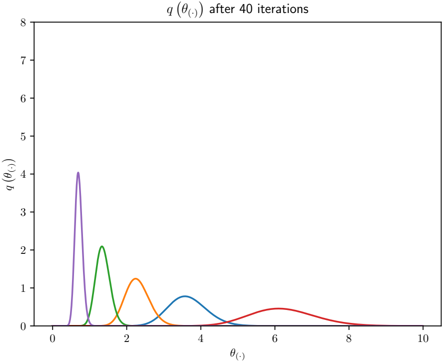
Global model



Local model



Variational posteriors



Data

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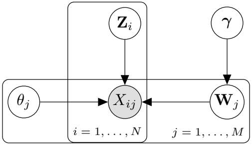
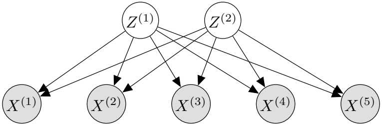
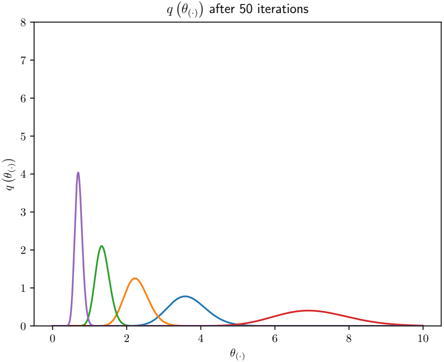
Global model



Local model



Variational posteriors



Data

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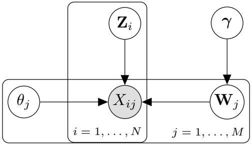
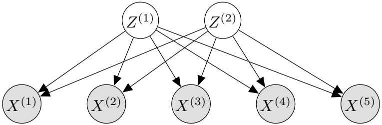
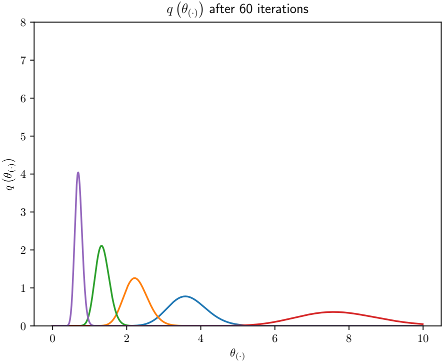
Global model



Local model



Variational posteriors

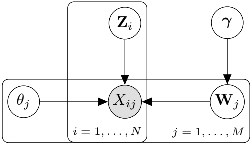


VB for the factor analysis model

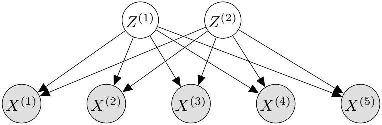
Data

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

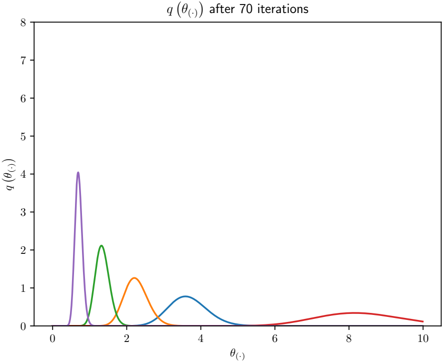
Global model



Local model



Variational posteriors



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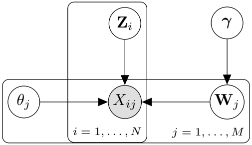
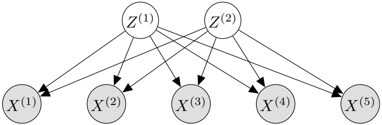
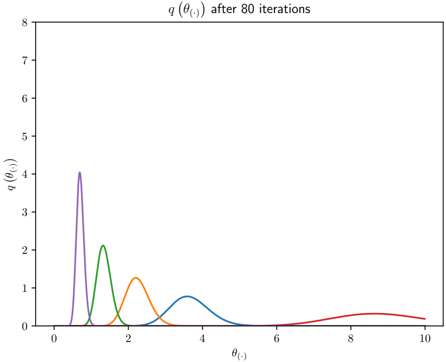
Global model



Local model



Variational posteriors



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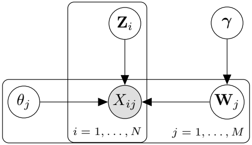
Global model



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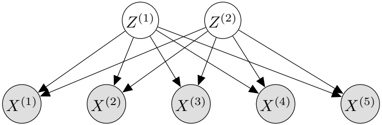
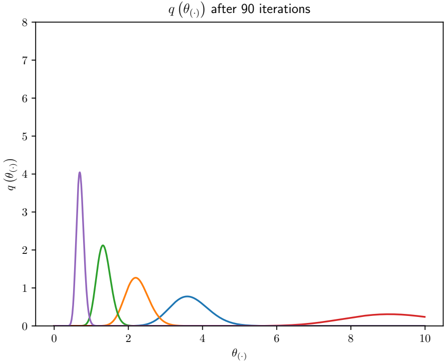


Variational posteriors



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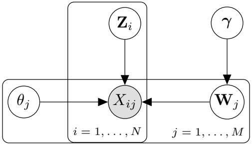
Global model



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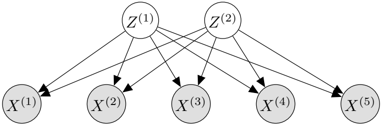
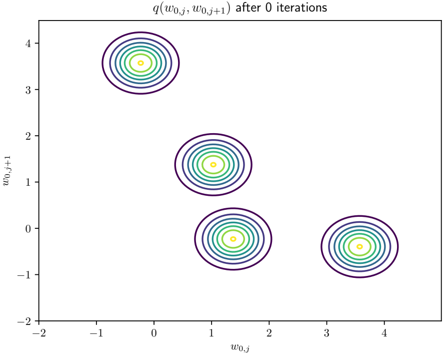


Variational posteriors



Data

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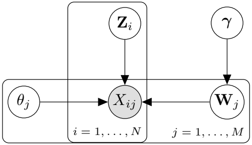
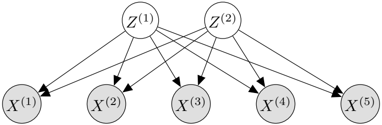
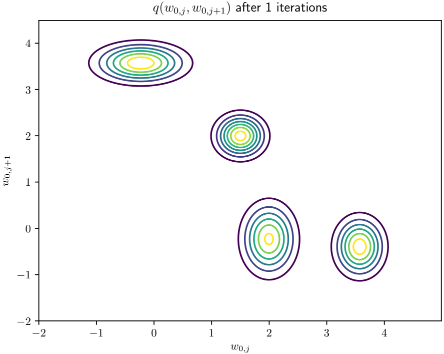
Global model



Local model



Variational posteriors



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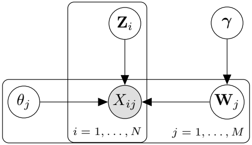

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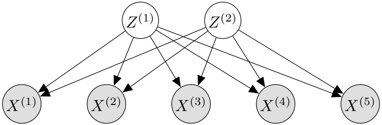

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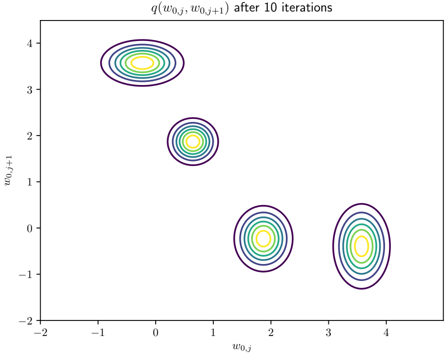

VB for the factor analysis model

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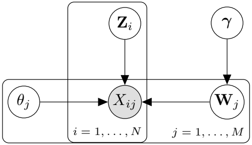

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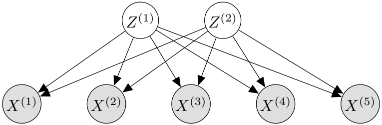

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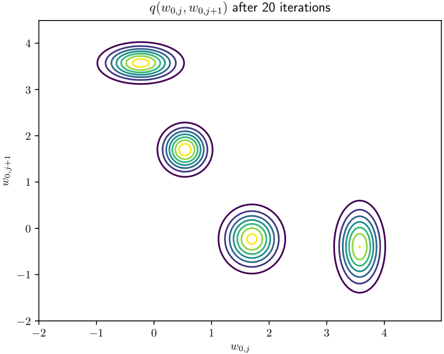

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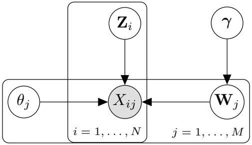

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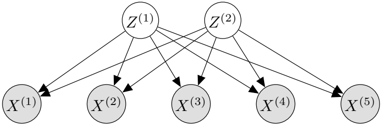

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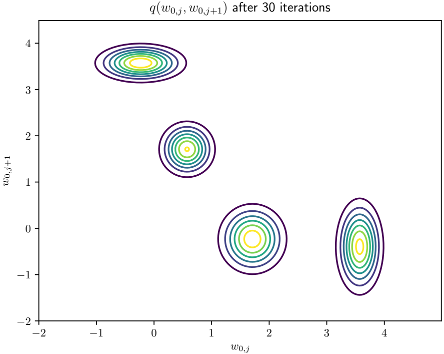

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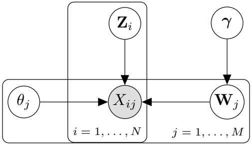

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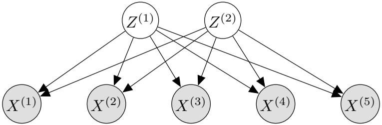

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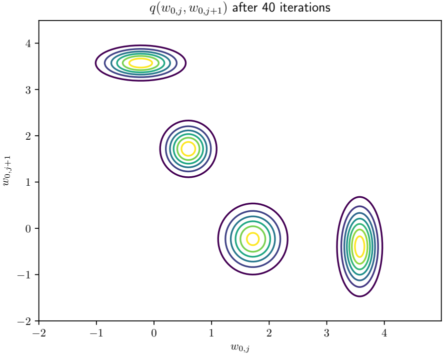

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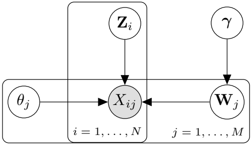

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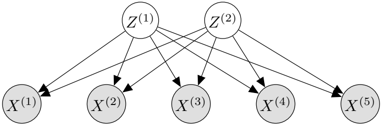

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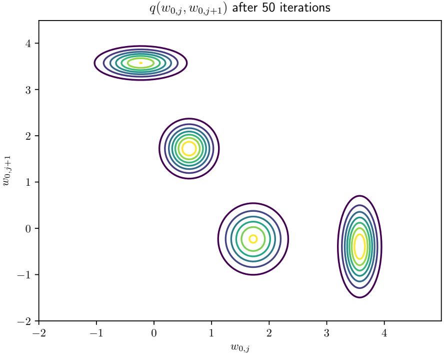

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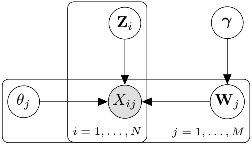

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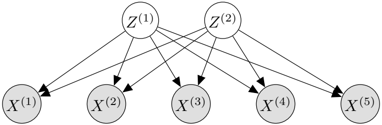

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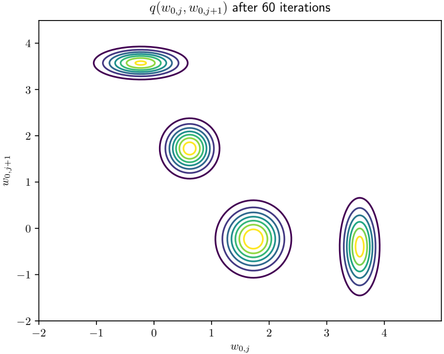

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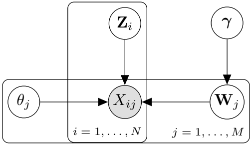

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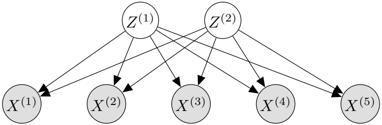

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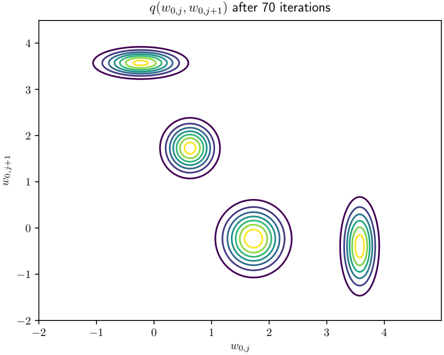

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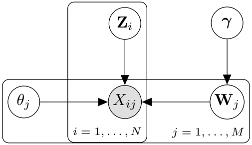

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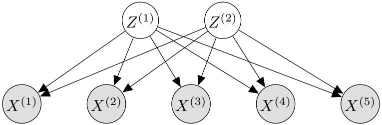

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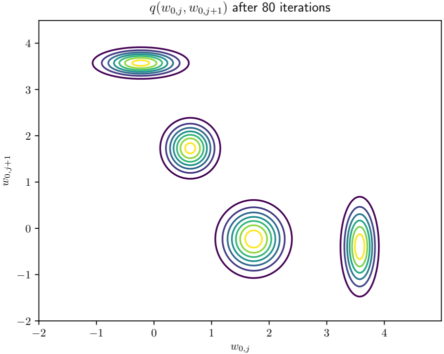

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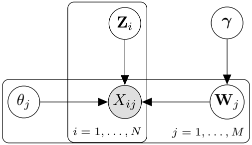

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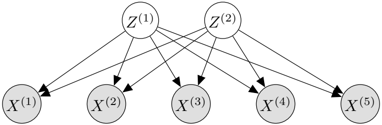

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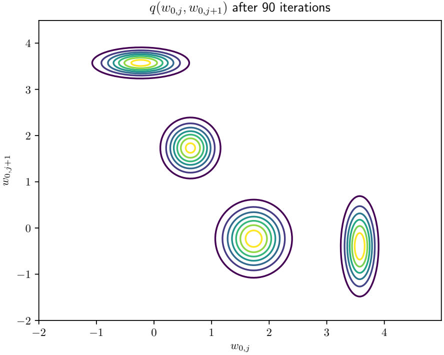

VB for the factor analysis model

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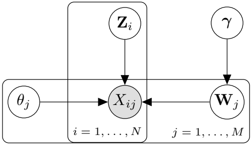
Global model



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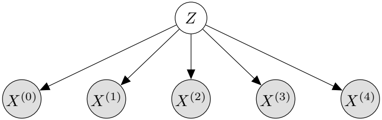
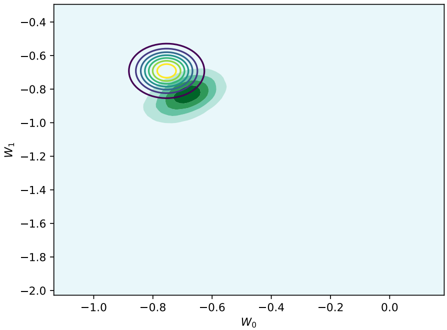


Comparison with Gibbs sampling



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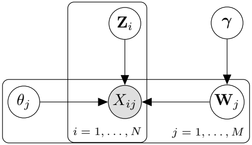

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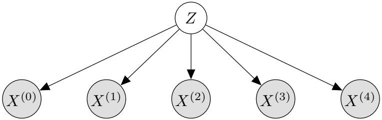

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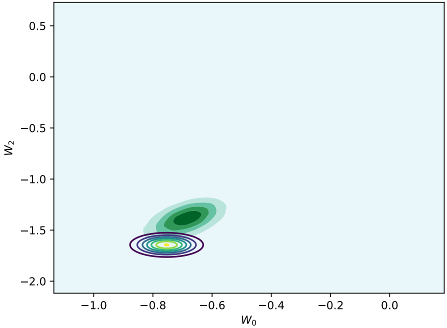

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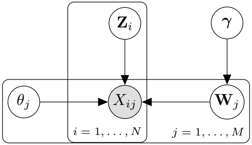

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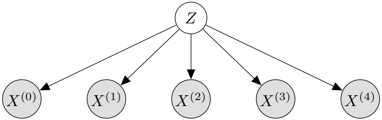

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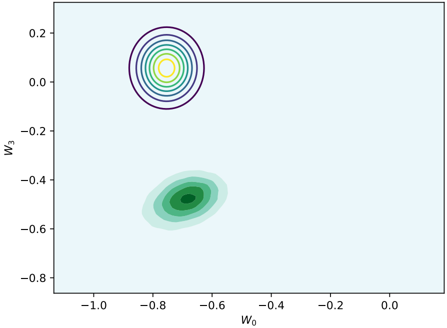

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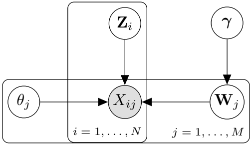

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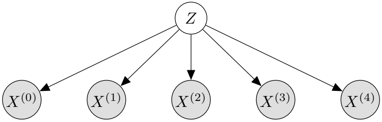

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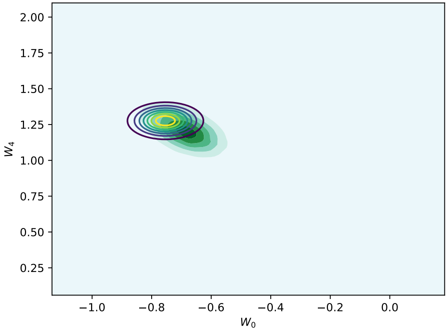

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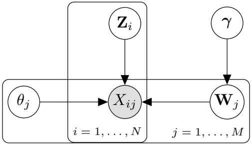

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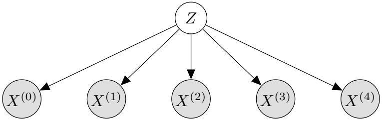

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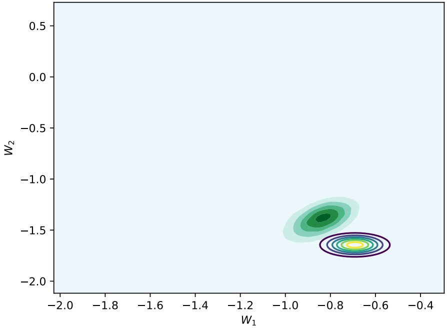

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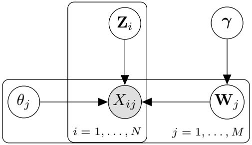

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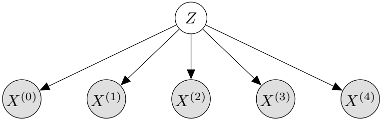

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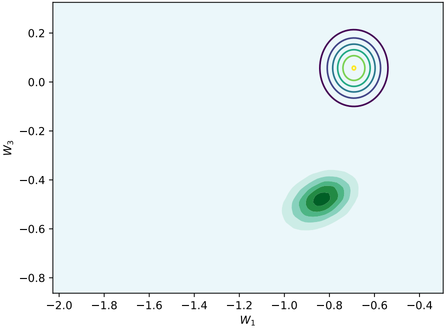

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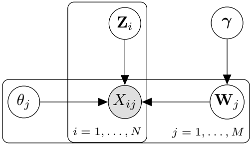

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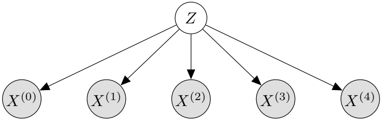

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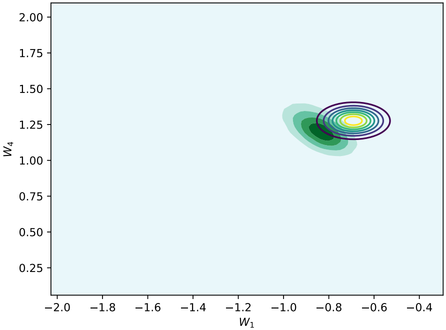

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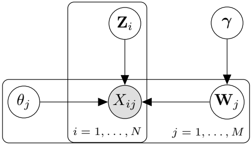

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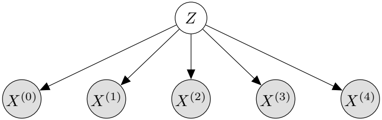

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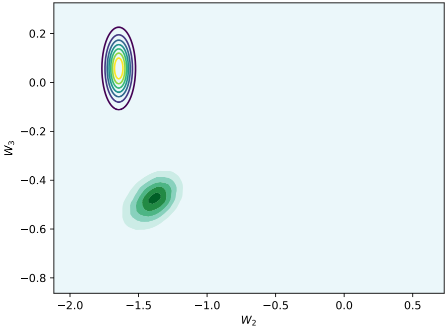

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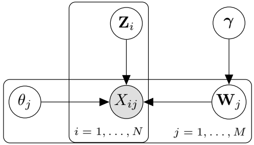

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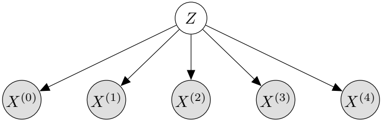

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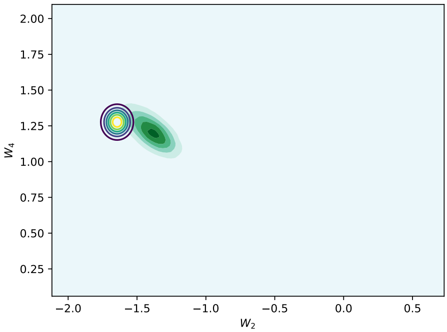

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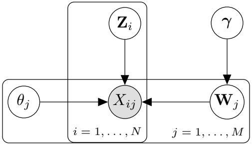

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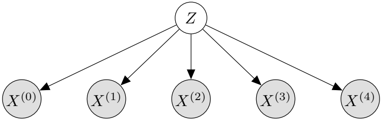

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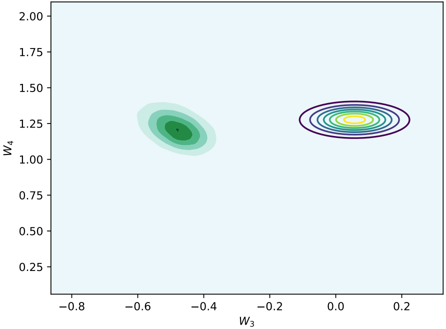

Not seen from the plot, **but** the results strongly dependent on the VI initialization.

Wrapping it all up: The VB algorithm under MF

Algorithm:

- We have observed $\mathbf{X} = \mathbf{x}$, and have access to the full joint $p(\mathbf{z}, \mathbf{x})$.
- We posit a *variational family* of distributions $q_j(\cdot \mid \boldsymbol{\lambda}_j)$, i.e., we choose the distributional form, while wanting to optimize the parameterization $\boldsymbol{\lambda}_j$.
- The posterior approximation is assumed to factorize according to the mean-field assumption, and we use the $\mathrm{KL}\left(q(\mathbf{z}) || p(\mathbf{z} \mid \mathbf{x})\right)$ 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 $\boldsymbol{\lambda}_j$ so that $q_j(z_j \mid \boldsymbol{\lambda}_j) \propto \exp\left(\mathbb{E}_{q_{\neg j}}\left[\log p(\mathbf{z}, \mathbf{x})\right]\right)$.
- Calculate the new $\mathcal{L}(q)$.

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As we just realized, calculations of $\mathbb{E}_{q_{\neg j}}\left[\log p(\mathbf{z}, \mathbf{x})\right]$ and $\mathcal{L}(q)$ 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.