Variational inference (cont'd)

Solving VB and Starting ExpFam

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Introduction

Plan for this weeks

Day 1: Bayesian networks – Definition and inference

- Definition of Bayesian networks: Syntax and semantics
- Exact inference
- Approximate inference using MCMC

Day 2: Variational inference – Introduction and basis

- Approximate inference through the *Kullback-Leibler divergence*
- *Variational Bayes*
- The *mean-field* approach to Variational Bayes

Day 3: Variational Bayes – cont'd

- Solving the VB equations
- Introducing Exponential families

Day 4: Scalable Variational Bayes

- Variational message passing
- Stochastic gradient ascent
- Stochastic variational inference

Day 5: Current approaches and extensions

- Variational Auto Encoders
- Black Box variational inference
- Probabilistic Programming Languages

Recap from last time

- Exact inference, in particular for Bayesian inference of latent-variable models, is computationally very expensive.
- Approximate inference using simulation, like MCMC, importance sampling, . . . :
  - Have asymptotic guarantees
  - Have a non-deterministic behaviour
  - Can be memory-expensive in particular for “difficult models” where we need to store the full sample to approximate inference
  - Can be time-expensive (slow convergence properties for a “difficult” model and/or evidence).
- Approximate inference using projections, $\hat{q} = \arg\min_{q \in \mathcal{Q}} \Delta(p; q)$:
  - Behavior depends on choices of $\mathcal{Q}$ and $\Delta(\cdot; \cdot)$.
  - We look mostly at the **variational objective**: $\Delta(p; q) = \mathrm{KL}\left(q||p\right)$.
  - . . . and make the **mean-field assumption**: $q \in \mathcal{Q} \Leftrightarrow q(\mathbf{z}) = \prod_j q_j(z_j)$.

ELBO: Evidence Lower-BOund

- Notice how we can rearrange the terms to find:

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

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

- Since $\log p(\mathbf{x})$ is constant wrt. q and $\mathrm{KL}\left(q||p\right) \geq 0$ it follows:
  - We can minimize $\mathrm{KL}\left(q(\mathbf{z}\,|\,\mathbf{x})||p(\mathbf{z}\,|\,\mathbf{x})\right)$ by maximizing $\mathcal{L}\left(q\right)$.
  - $\mathcal{L}\left(q\right)$ is a *lower bound* of the marginal data likelihood $p(\mathbf{x})$, hence the variational objective makes sense in a learning setting.

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:
  - 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.

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

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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}} \left[\log q(\mathbf{z})\right]
\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

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

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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&= \mathbb{E}_{q_j} \log f_j(z_j) - \mathbb{E}_{q_j} \left[\log q_j(z_j)\right] + c \\
&= -\mathrm{KL}\left(q_j(z_j) || f_j(z_j)\right) + c
\end{aligned}
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&= \mathbb{E}_{q_j}\log f_j(z_j) - \mathbb{E}_{q_j}\left[\log q_j(z_j)\right] + c \\
&= -\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.

VB w/ MF: algorithm

Setup

- We have observed $\mathbf{X} = \mathbf{x}$, and can calculate the full joint $p(\mathbf{z}, \mathbf{x})$.
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- 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 $q_j(z_j \mid \boldsymbol{\lambda}_j)$

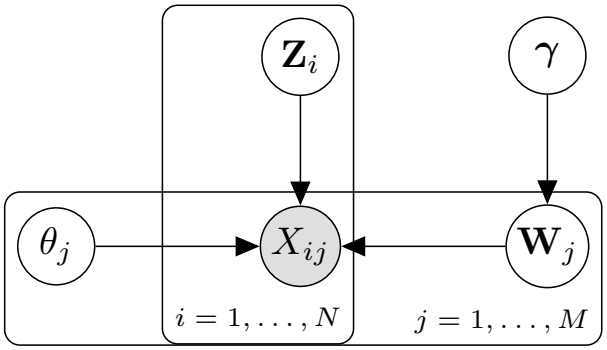
The update-rule can equivalently be expressed as

$$\log q_j(z_j \mid \boldsymbol{\lambda}_j) = \mathbb{E}_{q_{\neg j}}[\ln p(\mathbf{z}, \mathbf{x})] + c.$$

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!

The factor analysis model revisited and refined



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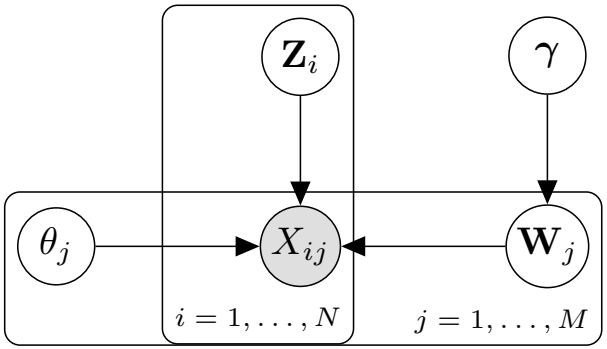

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The probability model

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

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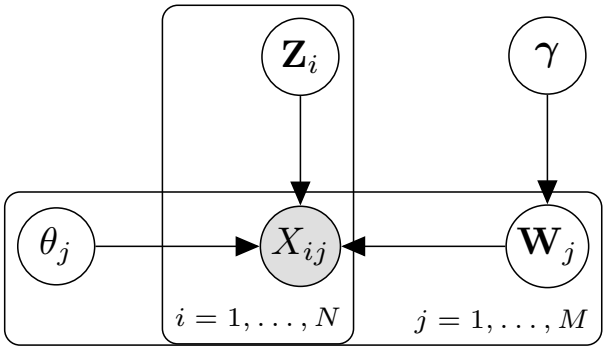

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. . . after taking the log

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

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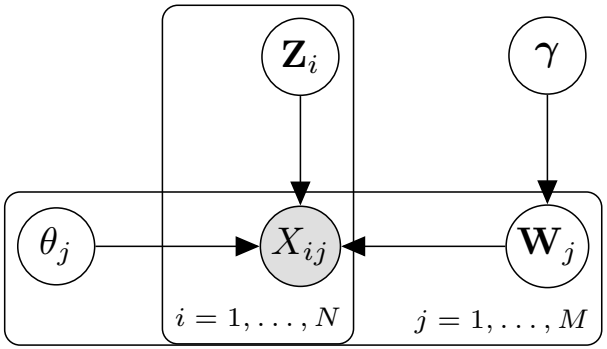

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The variational model

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

VB for the factor analysis model: updating $q(\gamma)$

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

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

VB for the factor analysis model: updating $q(\gamma)$

We choose the variational distribution so that

$$\log q(\gamma \mid \cdot) = \mathbb{E}_{q_{\neg\gamma}} [\log p(\cdot)] + c = \log p(\gamma) + \sum_{j=1}^{M} \mathbb{E}_{q_{\neg j}} \log p(\mathbf{w}_j \mid \gamma) + c$$

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

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

Recall the (generic) gamma distribution

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

VB for the factor analysis model: updating $q(\gamma)$

We choose the variational distribution so that

$$\log q(\gamma \mid \cdot) = \mathbb{E}_{q_{\neg\gamma}} [\log p(\cdot)] + c = \log p(\gamma) + \sum_{j=1}^{M} \mathbb{E}_{q_{\neg j}} \log p(\mathbf{w}_j \mid \gamma) + c$$

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

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

Recall the (generic) gamma distribution

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

VB for the factor analysis model: updating $q(\gamma)$

We choose the variational distribution so that

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

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

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

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

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

VB for the factor analysis model: updating $q(\gamma)$

We choose the variational distribution so that

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

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

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

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

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

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

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

VB for the factor analysis model: updating $q(\gamma)$

We choose the variational distribution so that

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

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

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

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

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

Compare this to the Gibbs sampler:

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

VB uses posterior expectations where Gibbs uses samples!

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

We choose the variational distribution so that

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

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

We choose the variational distribution so that

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

Recall

$$\log p(\cdot)$$

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

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

We choose the variational distribution so that

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

Recall

$$\log p(\cdot)$$

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

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

We choose the variational distribution so that

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

Recall

$$\log p(\cdot)$$

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

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

We choose the variational distribution so that

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

The (multivariate) normal distribution

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

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

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

We choose the variational distribution so that

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

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

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

We choose the variational distribution so that

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

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

The (multivariate) normal distribution

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

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

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

We choose the variational distribution so that

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

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

Expanding the square

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

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

We choose the variational distribution so that

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

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

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

Expanding the square

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

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

We choose the variational distribution so that

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

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

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

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

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

We choose the variational distribution so that

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

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

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

We choose the variational distribution so that

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

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

Recall the (generic) multivariate normal distribution

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

$$= -\frac{D}{2}\log(2\pi) + \frac{1}{2}\log|\mathbf{Q}] - \frac{1}{2}\mathbf{y}^\mathsf{T}\mathbf{Q}\mathbf{y} + \mathbf{y}^\mathsf{T}\mathbf{Q}\boldsymbol{\mu} - \frac{1}{2}\boldsymbol{\mu}^\mathsf{T}\mathbf{Q}\boldsymbol{\mu})$$

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

We choose the variational distribution so that

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

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

Thus we see 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 $\boldsymbol{\mu} \leftarrow \mathbf{Q}^{-1}\left[\mathbb{E}(\theta_j)\sum_{i=1}^{N} x_{ij}\mathbb{E}(\mathbf{Z}_i)\right]$

Recall the (generic) multivariate normal distribution

$$\log p(\mathbf{y} \mid \boldsymbol{\mu}, \mathbf{Q}) = \log \mathcal{N}(\mathbf{y} \mid \boldsymbol{\mu}, \mathbf{Q}^{-1}) = -\frac{D}{2}\log(2\pi) + \frac{1}{2}\log|\mathbf{Q}] - \frac{1}{2}(\mathbf{y}-\boldsymbol{\mu})^\intercal\mathbf{Q}(\mathbf{y}-\boldsymbol{\mu})^\intercal)$$

$$= -\frac{D}{2}\log(2\pi) + \frac{1}{2}\log|\mathbf{Q}] - \frac{1}{2}\mathbf{y}^\intercal\mathbf{Q}\mathbf{y} + \mathbf{y}^\intercal\mathbf{Q}\boldsymbol{\mu} - \frac{1}{2}\boldsymbol{\mu}^\intercal\mathbf{Q}\boldsymbol{\mu})$$

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

We choose the variational distribution so that

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

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

Thus we see 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 $\mathbb{E}(\mathbf{Z}_i \mathbf{Z}_i^\intercal)$

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

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

We choose the variational distribution so that

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

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

Thus we see 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 $\boldsymbol{\mu} \leftarrow \mathbf{Q}^{-1} \left[\mathbb{E}(\theta_j) \sum_{i=1}^{N} x_{ij} \mathbb{E}(\mathbf{Z}_i) \right]$

Compare this to the Gibbs sampler:

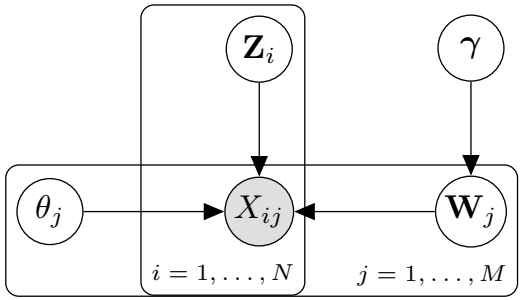
- $\mathbf{Q} \leftarrow \gamma\mathbf{I} + \theta_j \sum_{i=1}^{N} \mathbf{z}_i \mathbf{z}_i^\intercal$
- $\boldsymbol{\mu} \leftarrow \mathbf{Q}^{-1} \left[\theta_j \sum_{i=1}^{N} x_{ij} \mathbf{z}_i \right]$

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

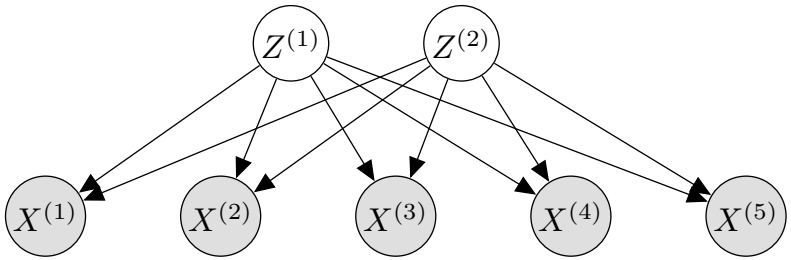
Data

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

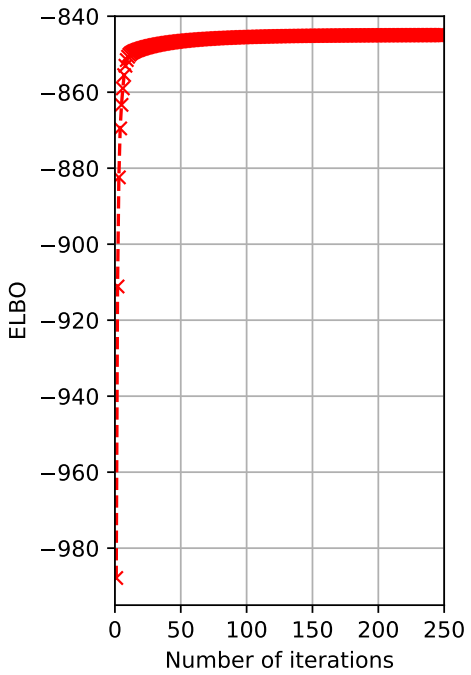
Global model

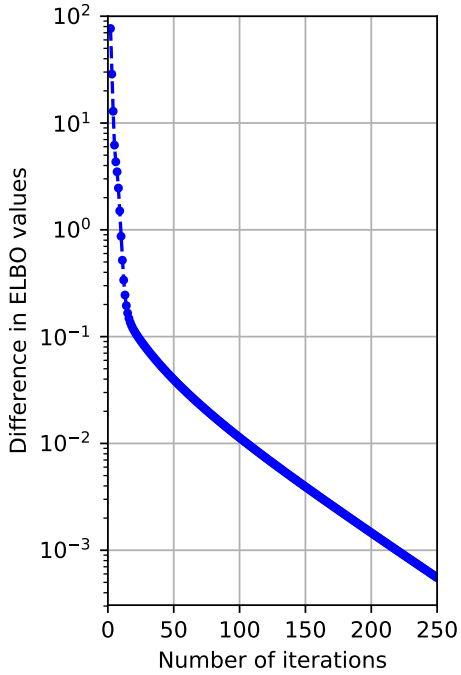


Local model



Monitoring convergence

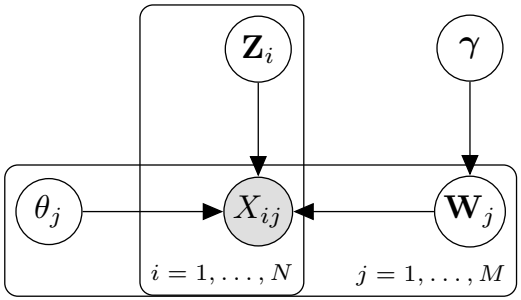




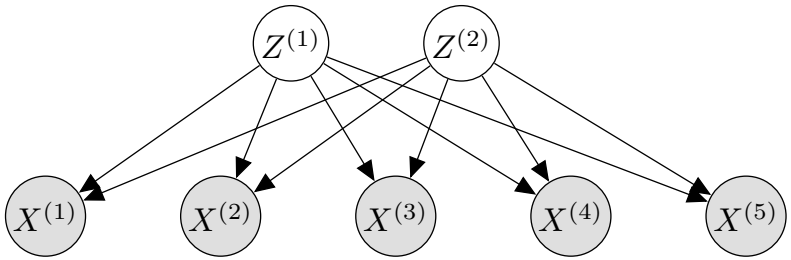
Data

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

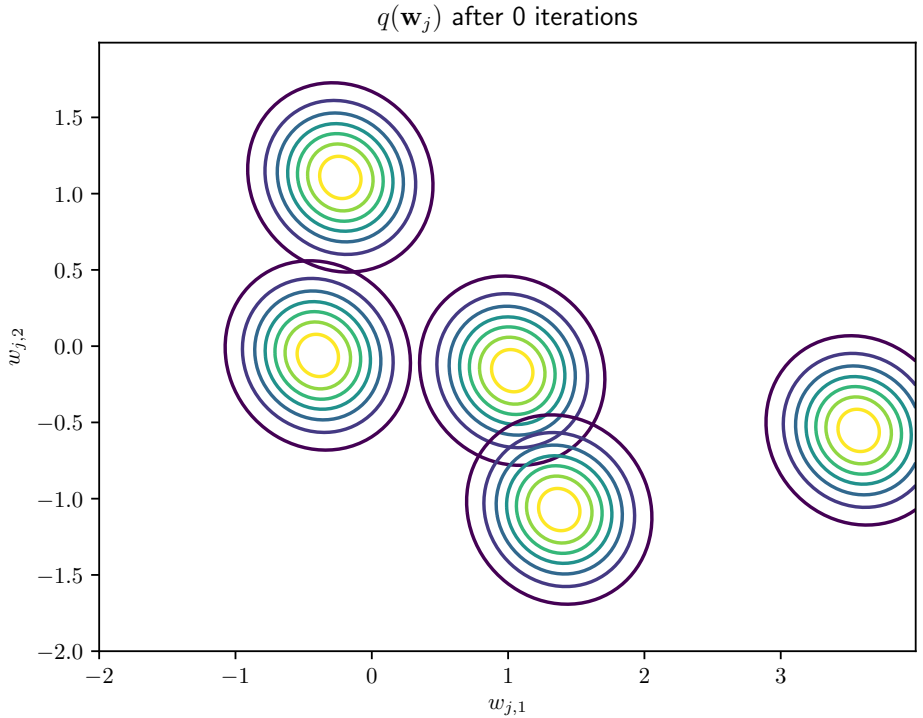
Global model



Local model



Variational posteriors



Data

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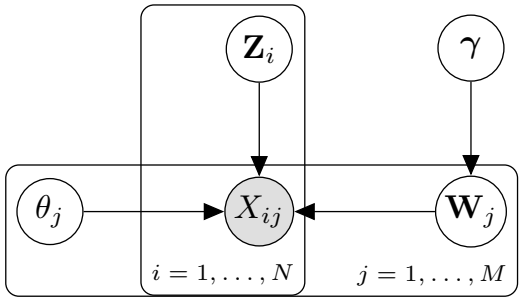
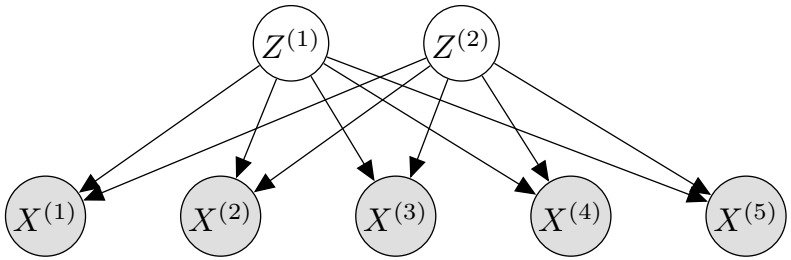
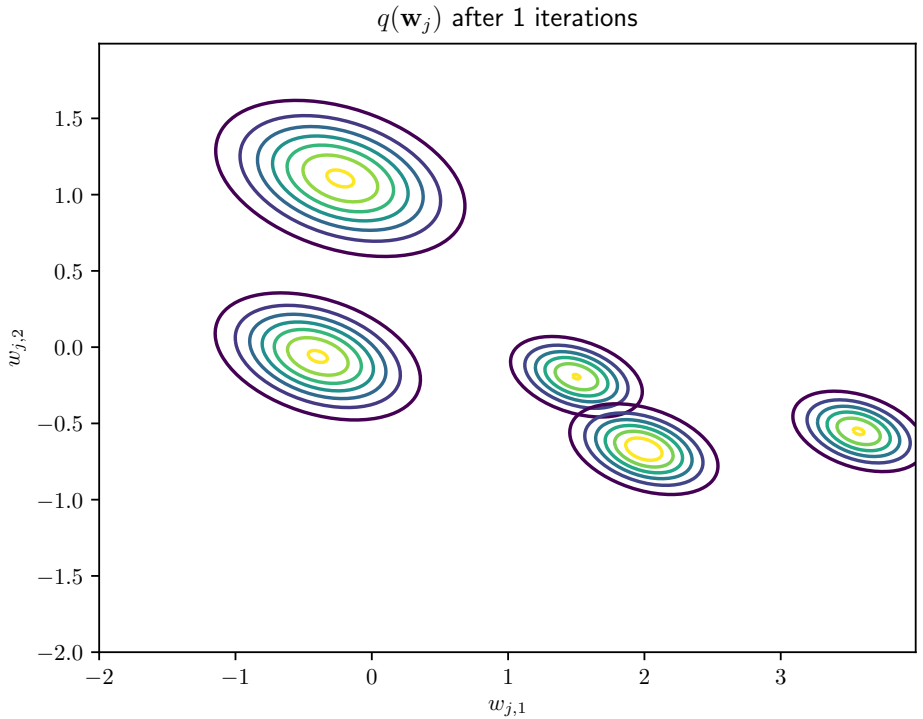
Global model



Local model



Variational posteriors



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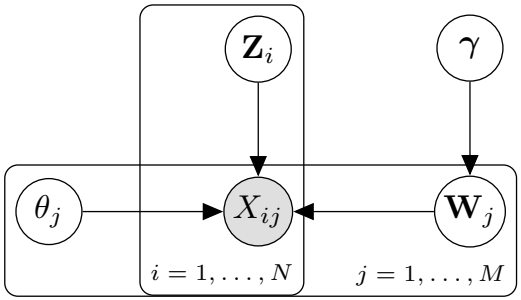
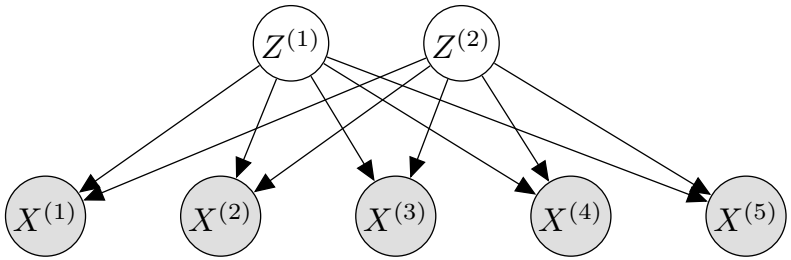
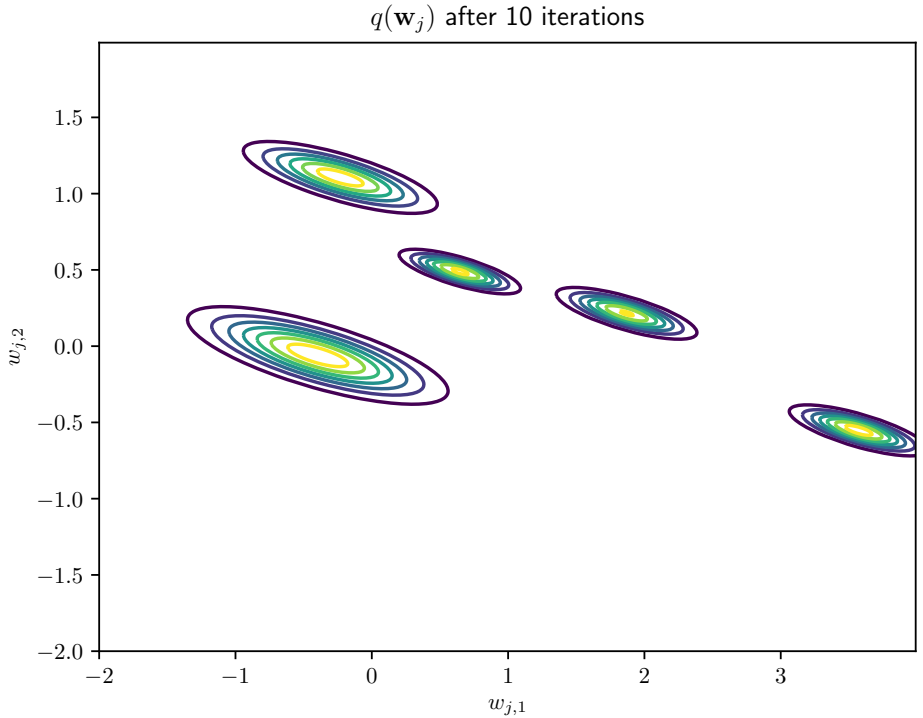
Global model



Local model



Variational posteriors



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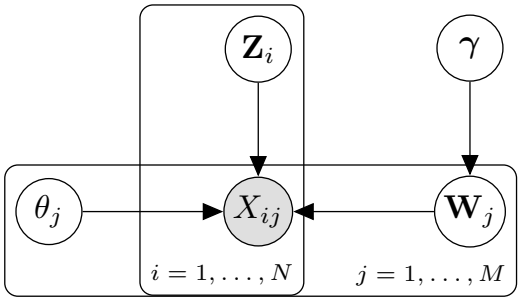
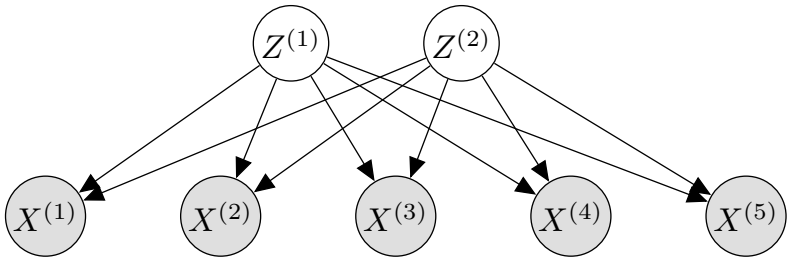
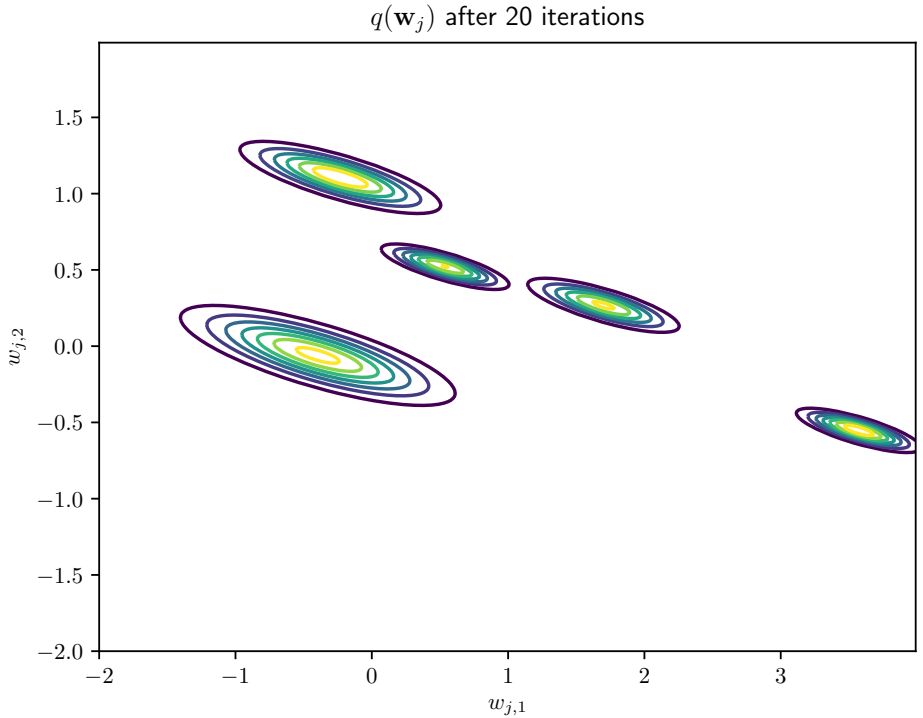


Local model



Variational posteriors



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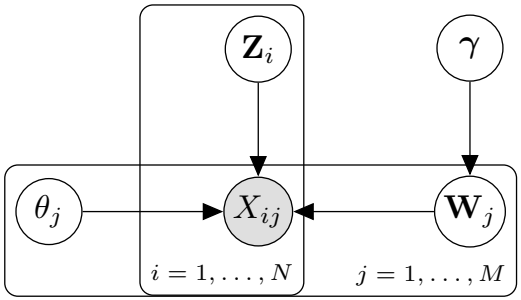
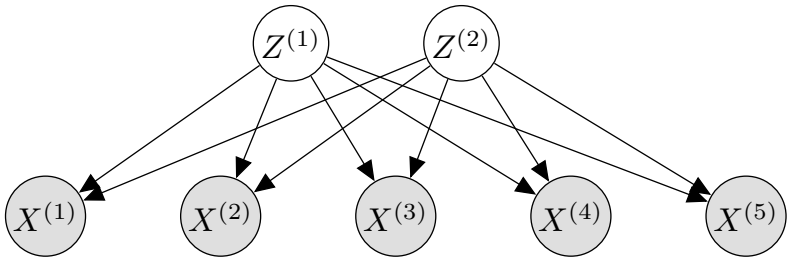
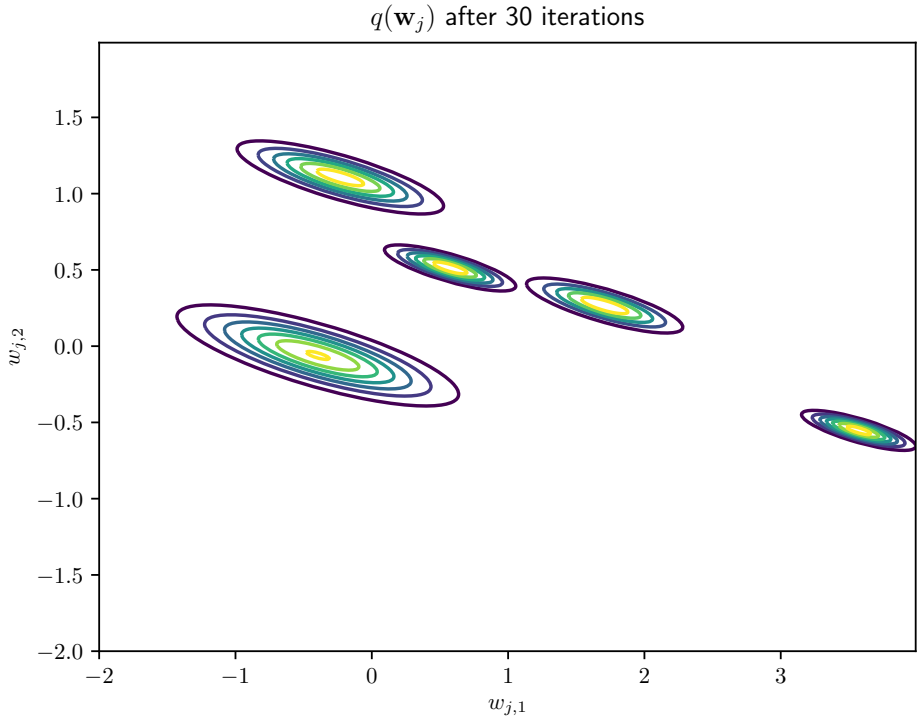
Global model



Local model



Variational posteriors



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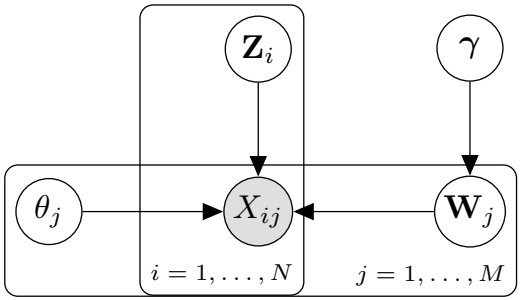
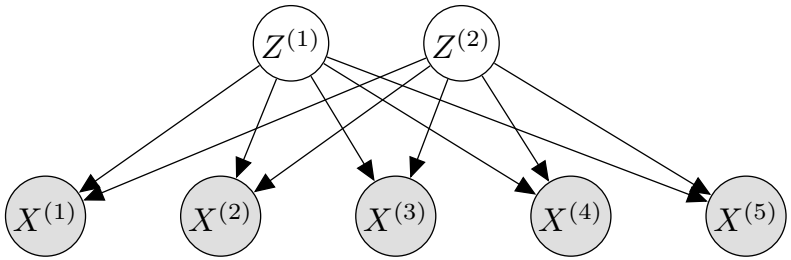
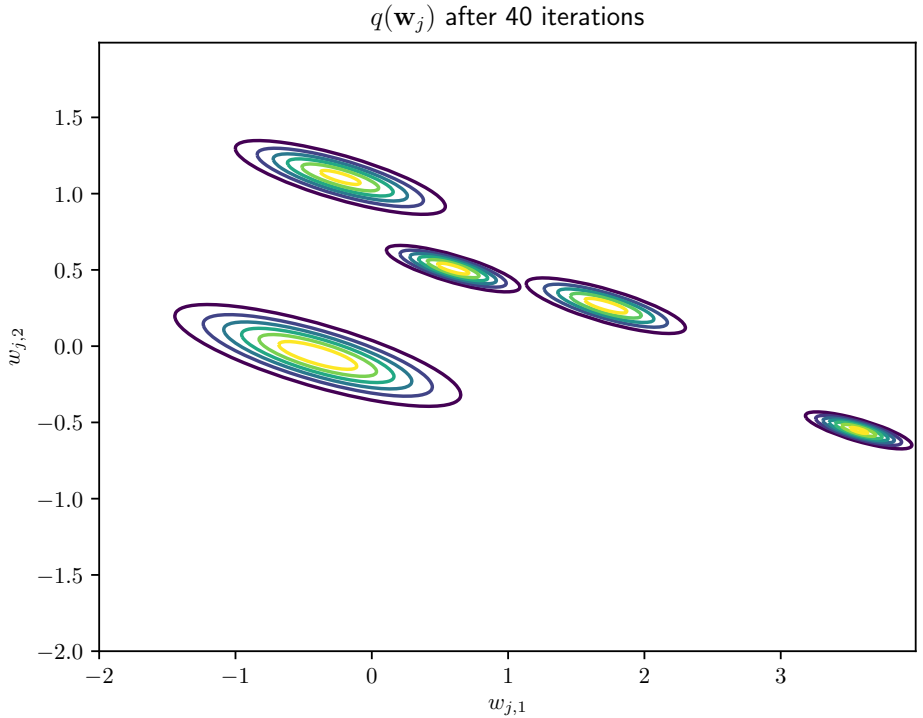


Local model



Variational posteriors



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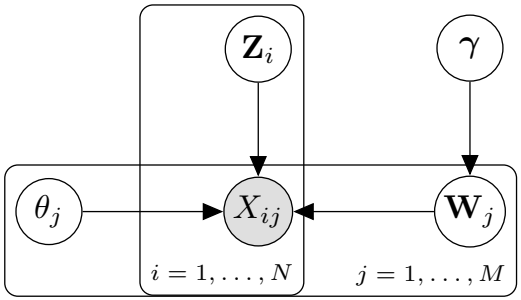
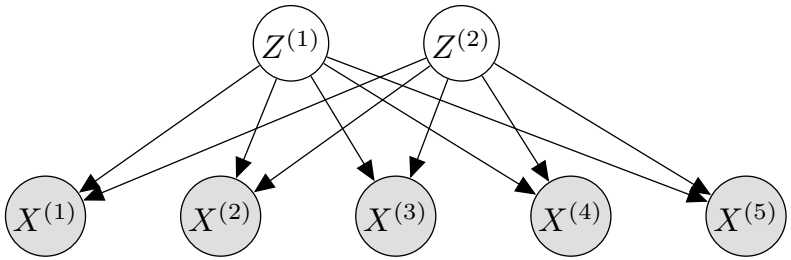
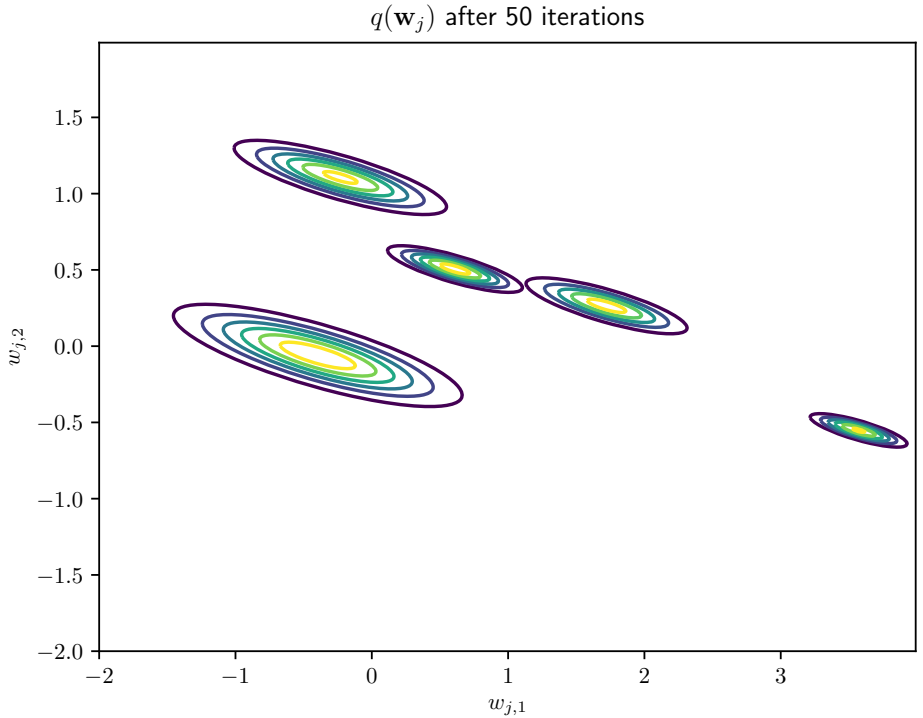
Global model



Local model



Variational posteriors



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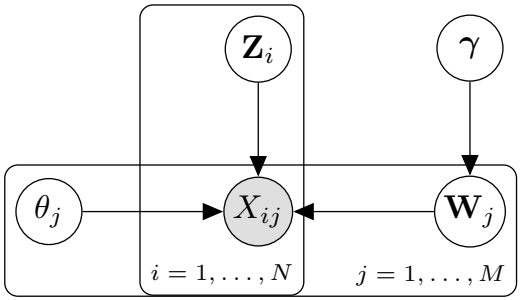
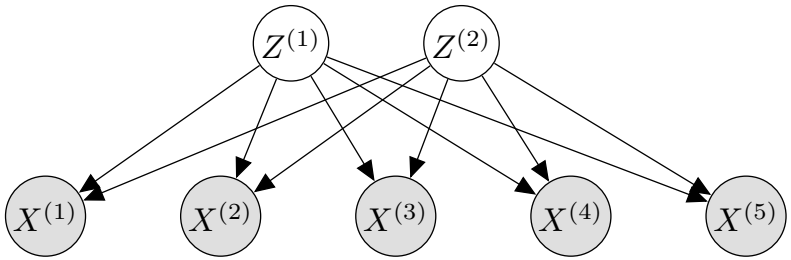
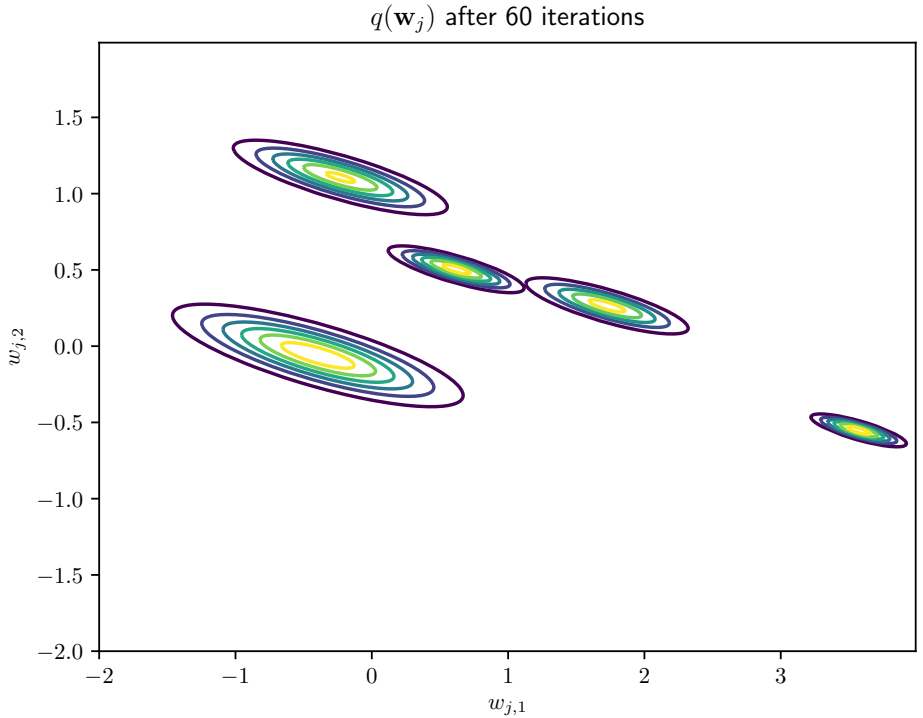
Global model



Local model



Variational posteriors



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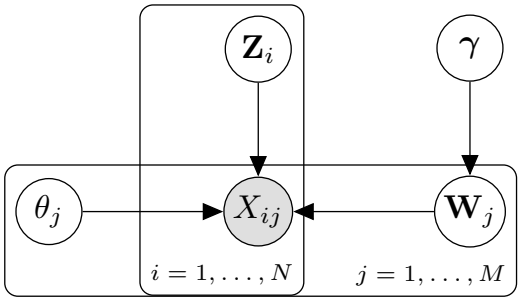
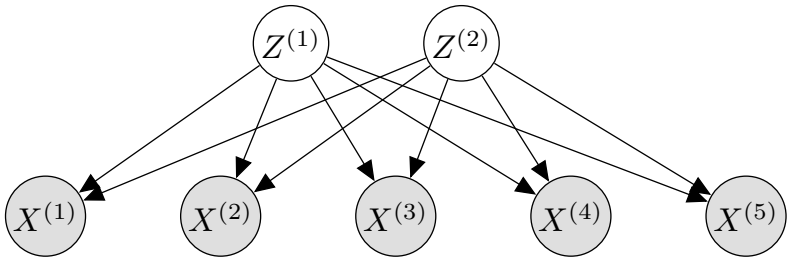
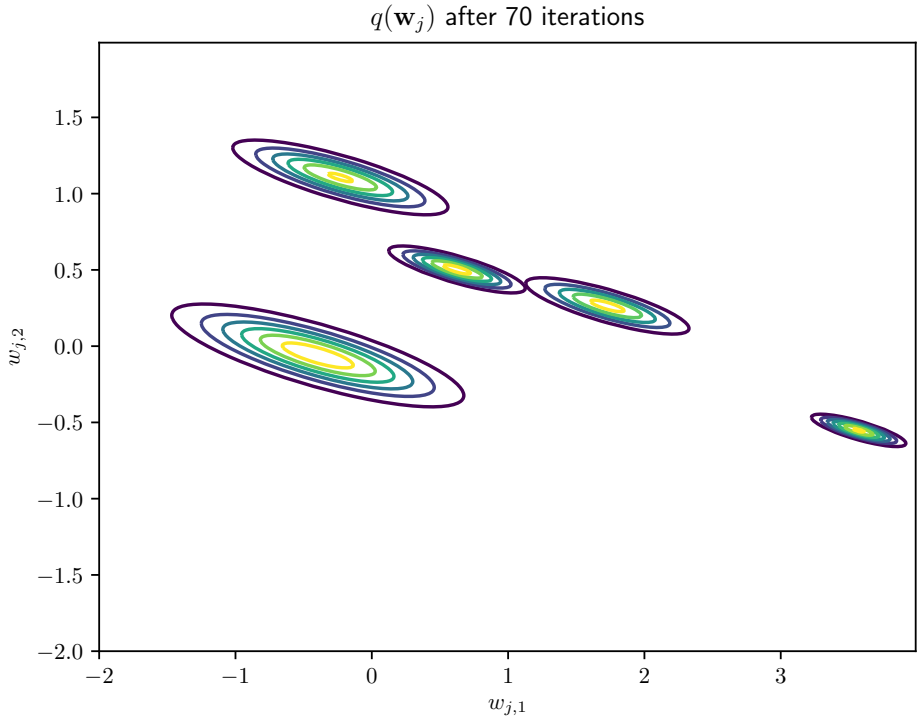


Local model



Variational posteriors



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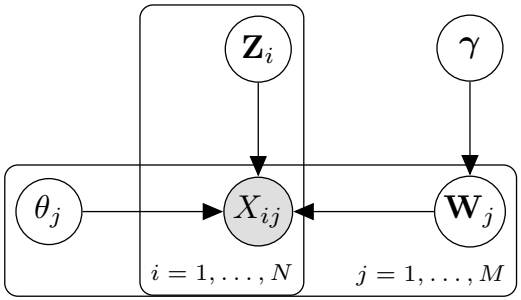
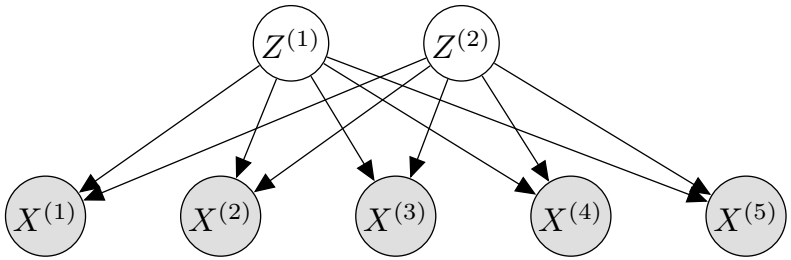
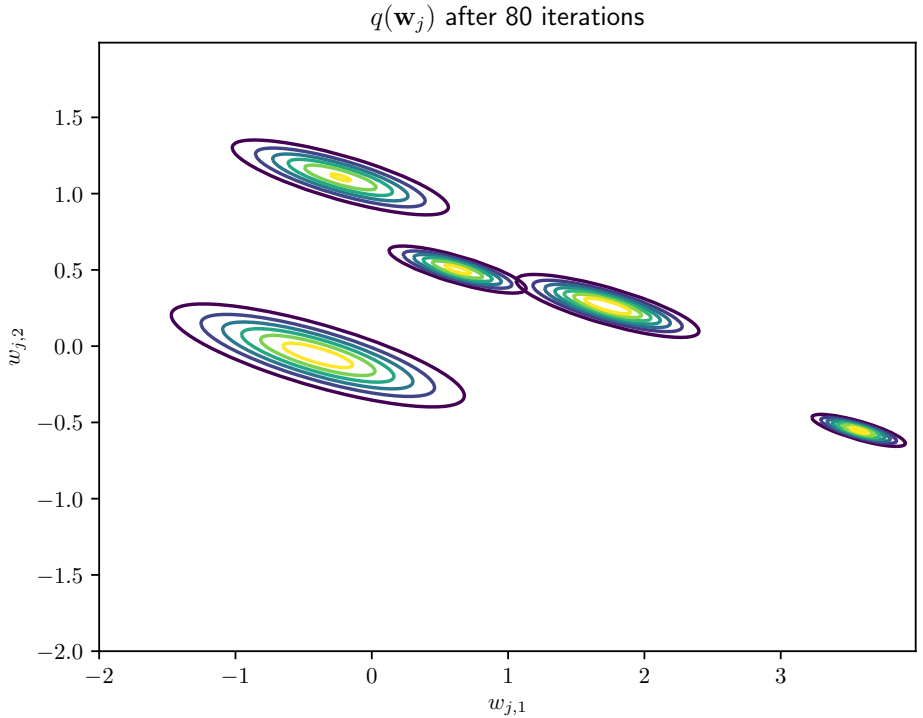


Local model



Variational posteriors



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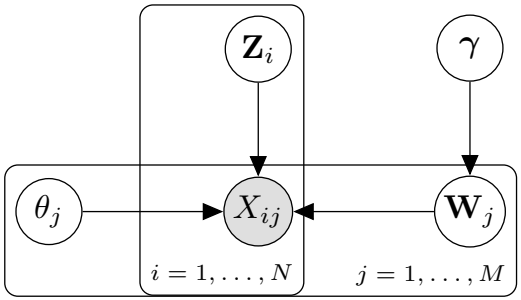
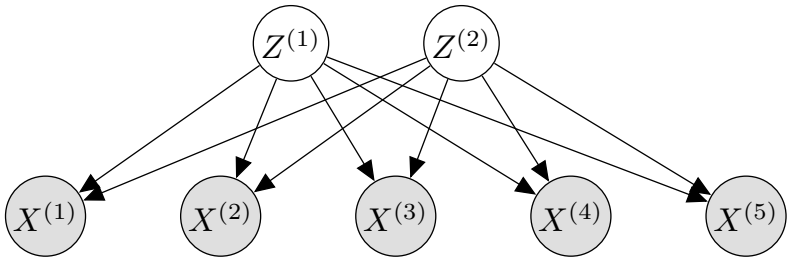
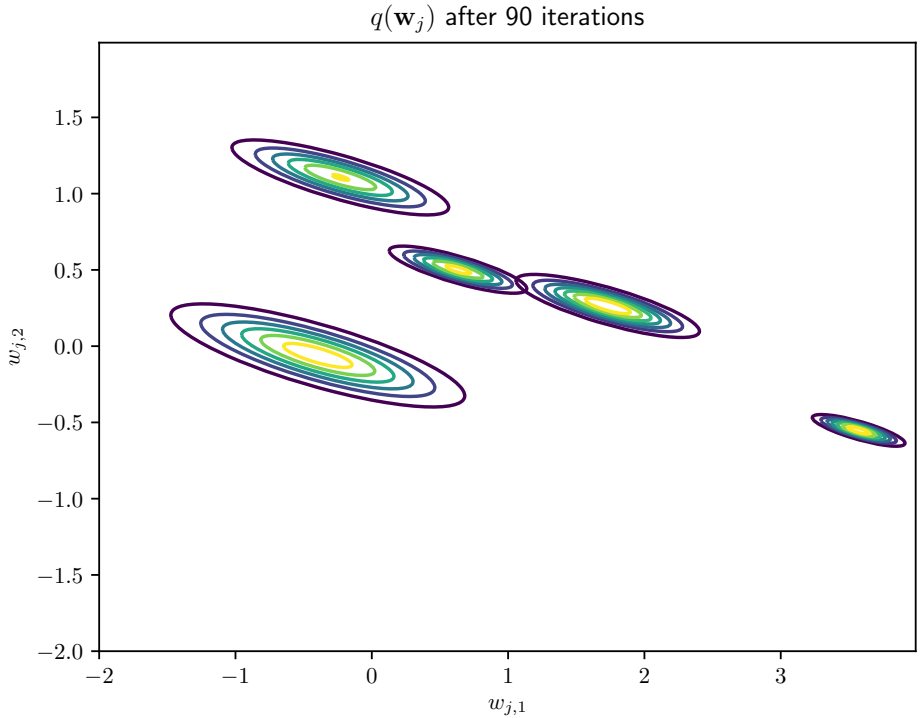


Local model



Variational posteriors



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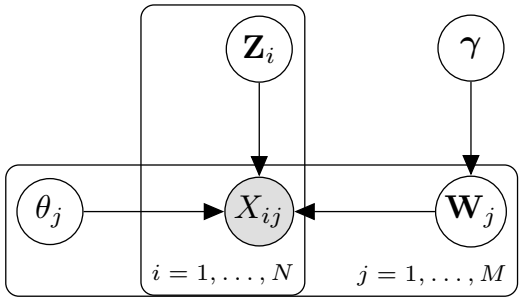
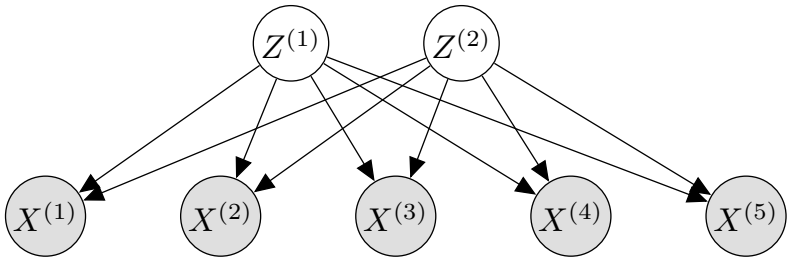
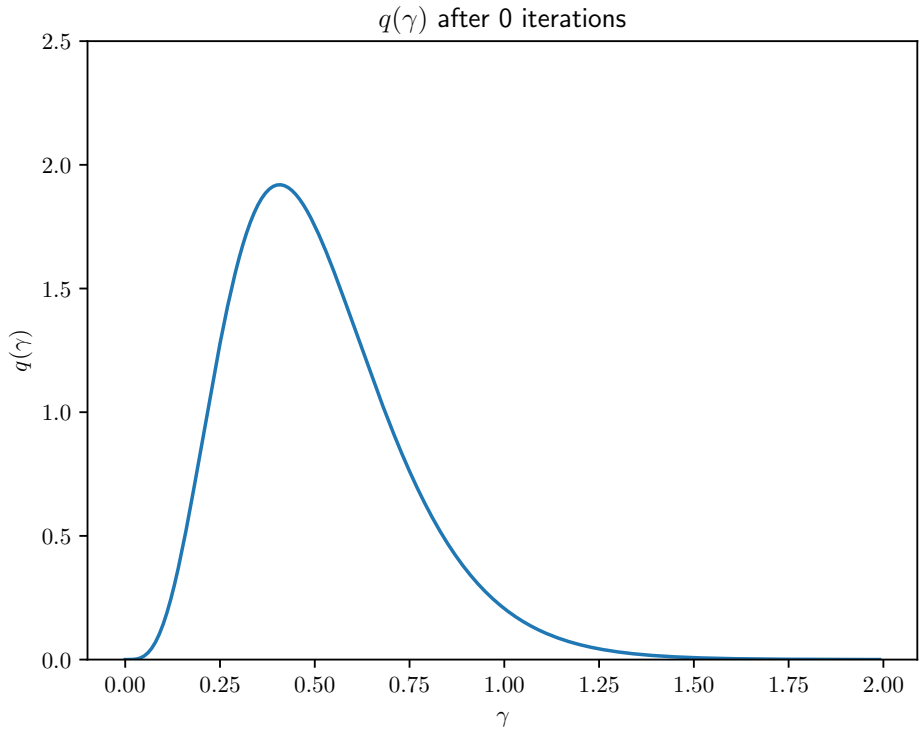


Local model



Variational posteriors



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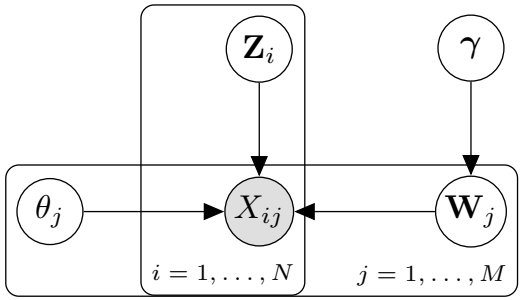
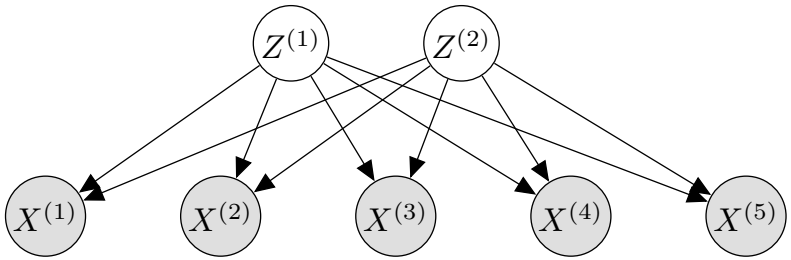
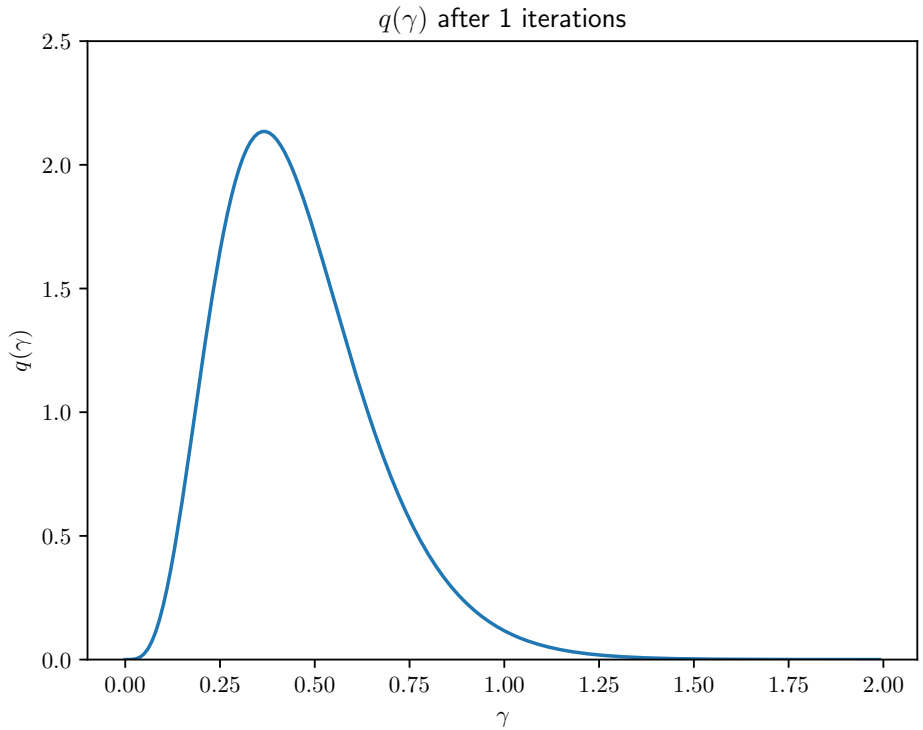


Local model



Variational posteriors



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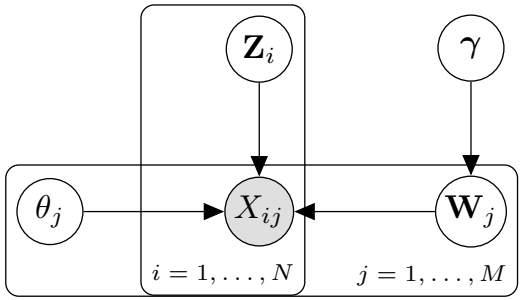
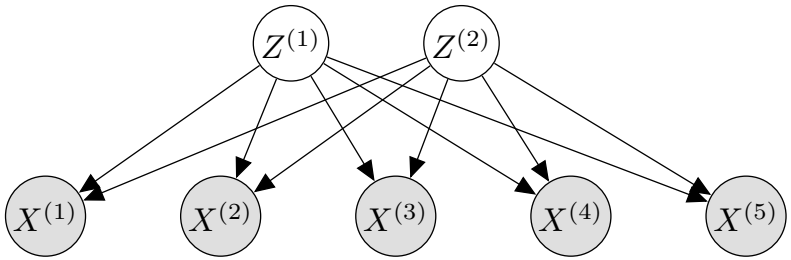


Local model



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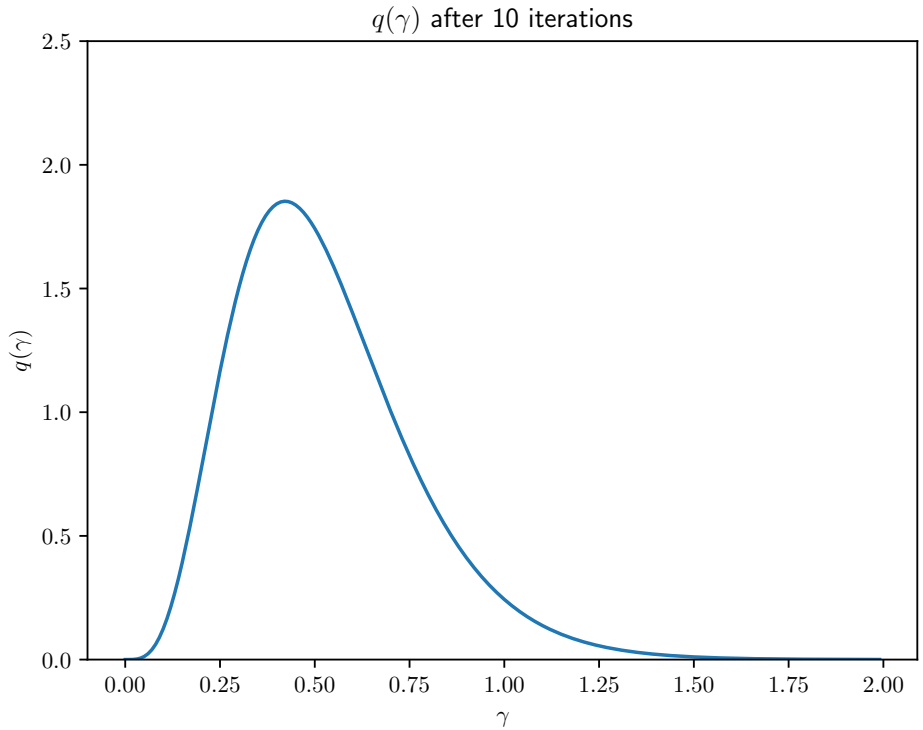

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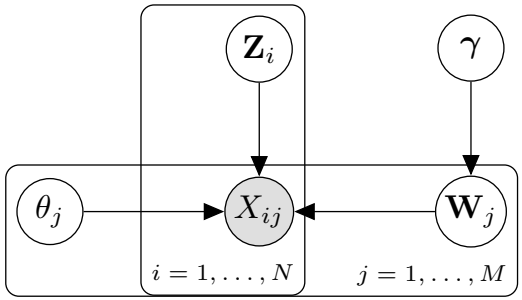
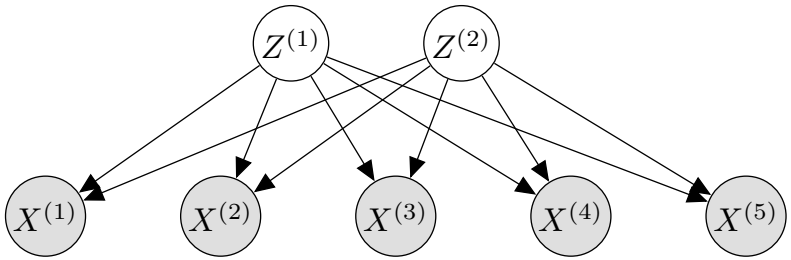


Local model



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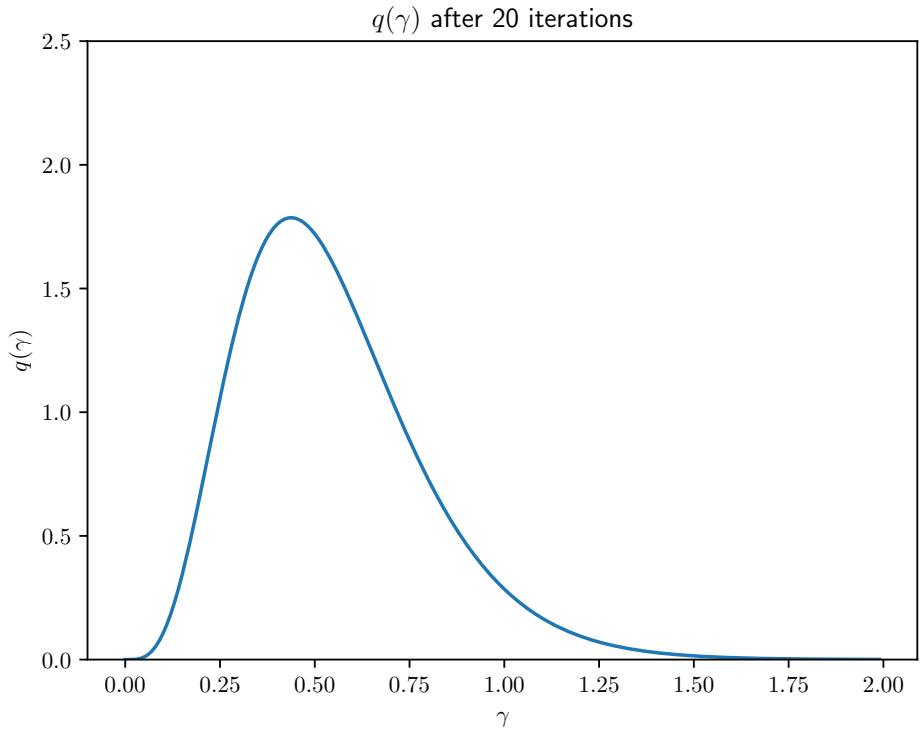

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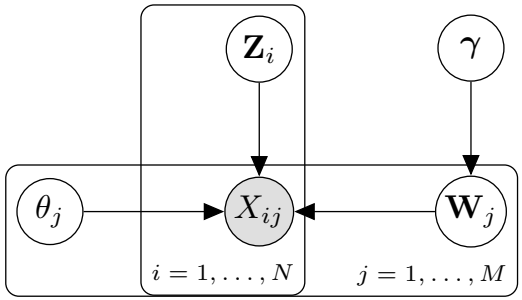
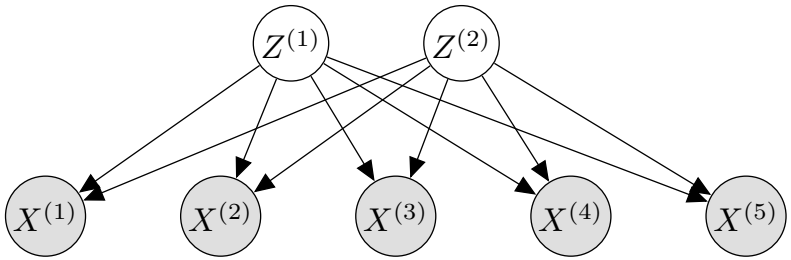
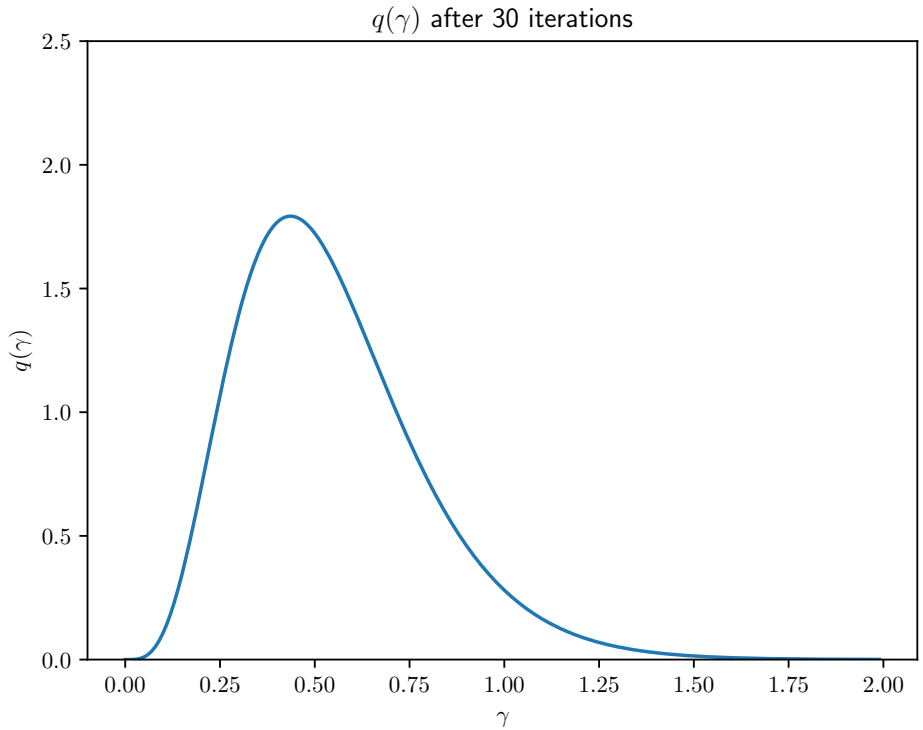


Local model



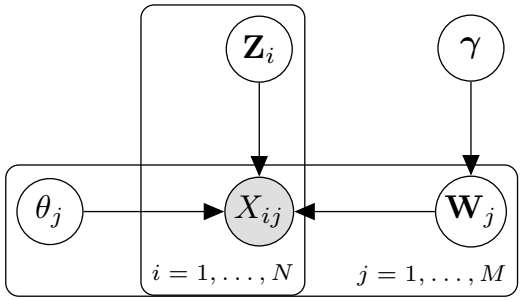
Variational posteriors



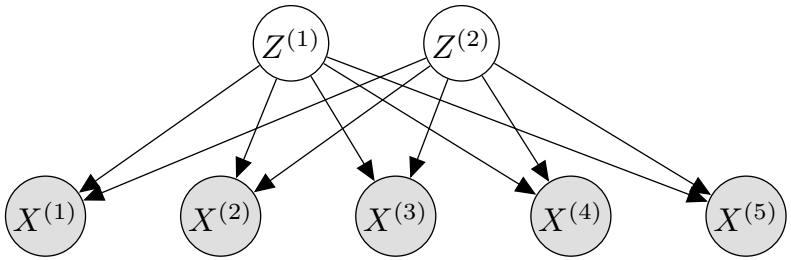
Data

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

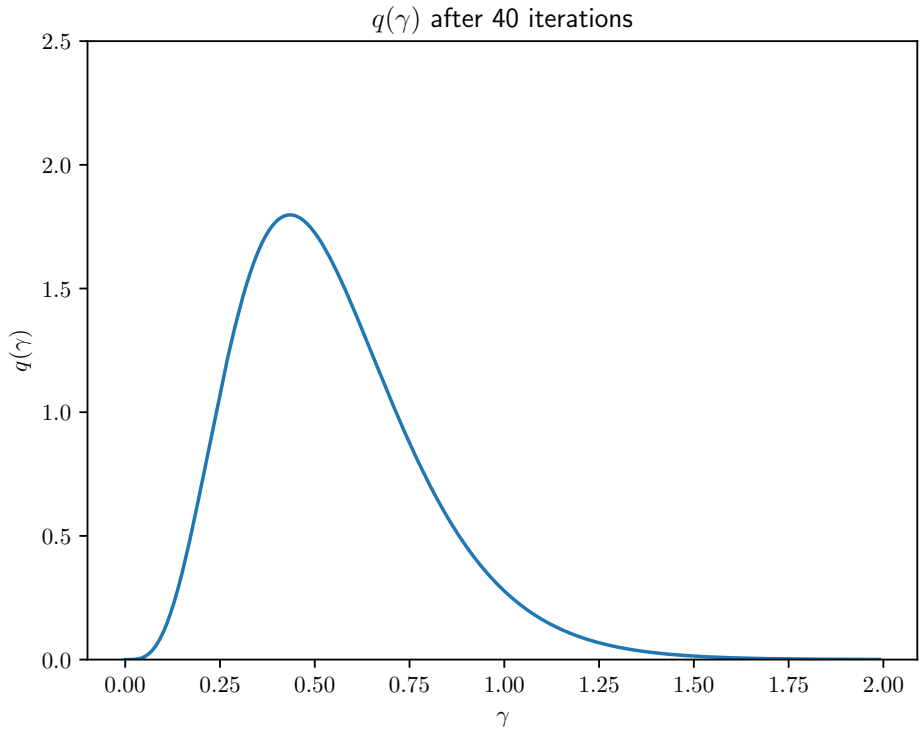
Global model



Local model



Variational posteriors



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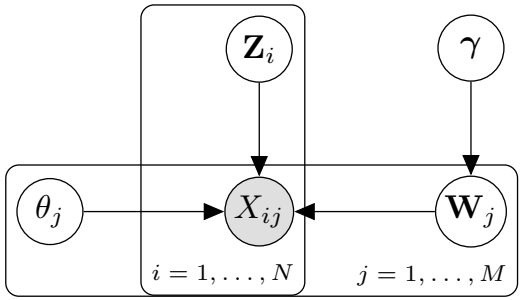

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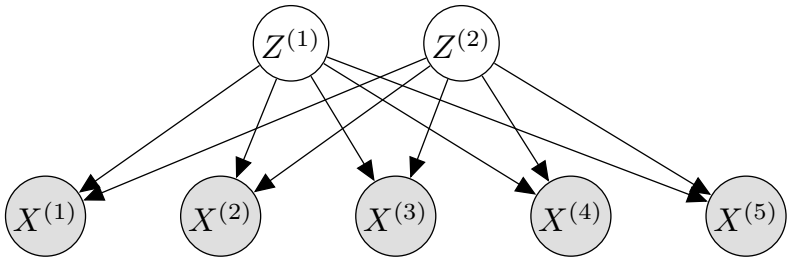
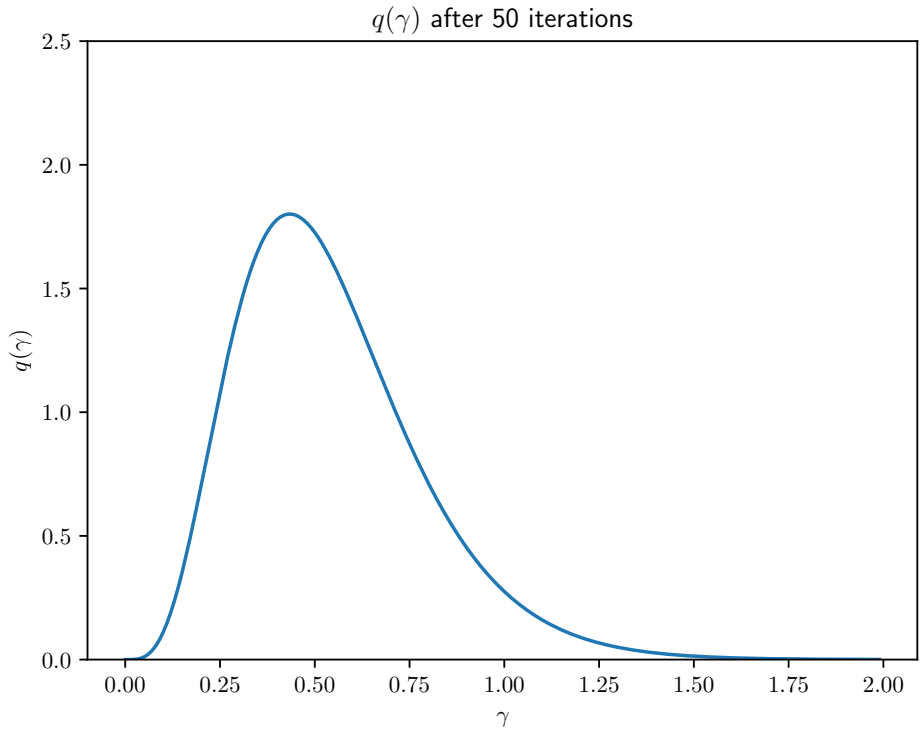


Variational posteriors



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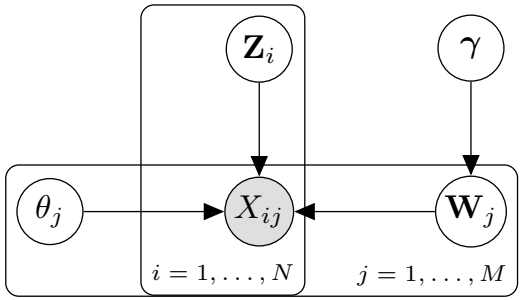
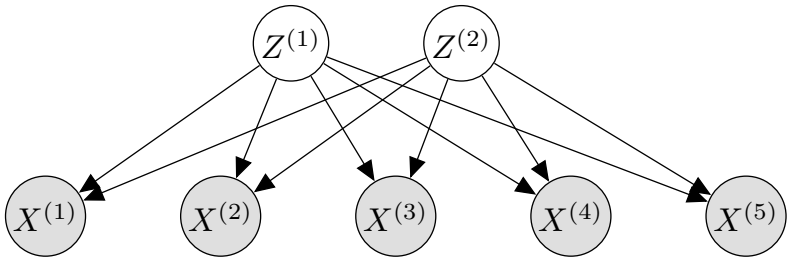
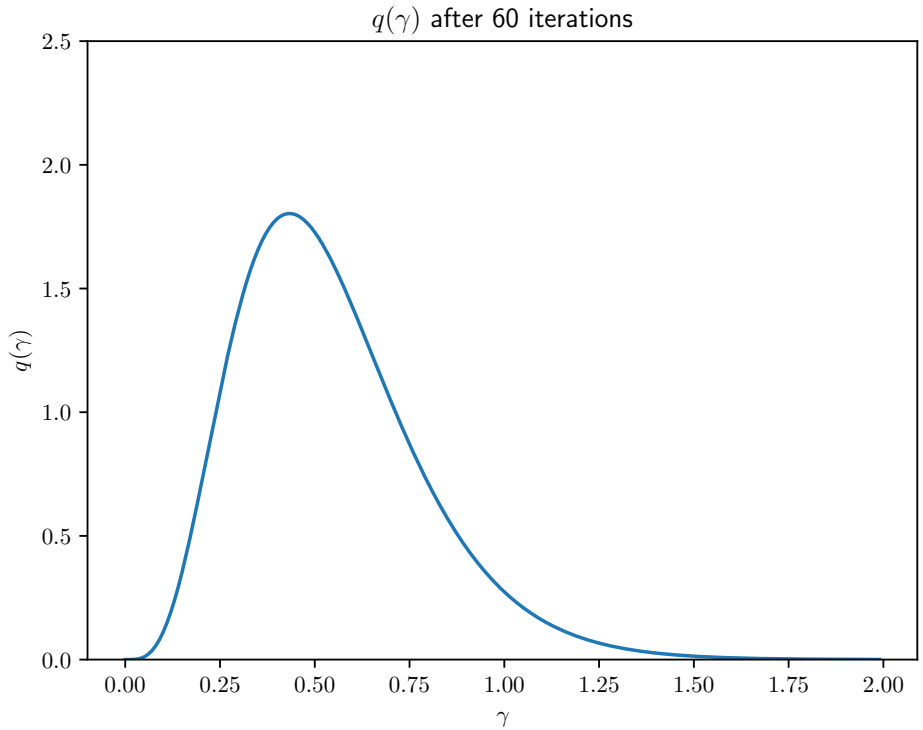


Local model



Variational posteriors



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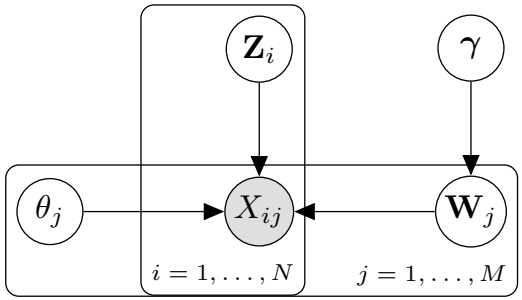
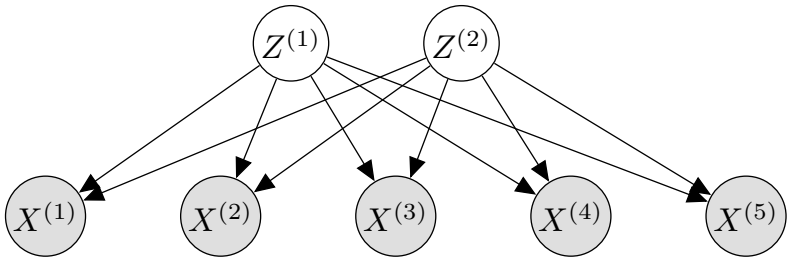
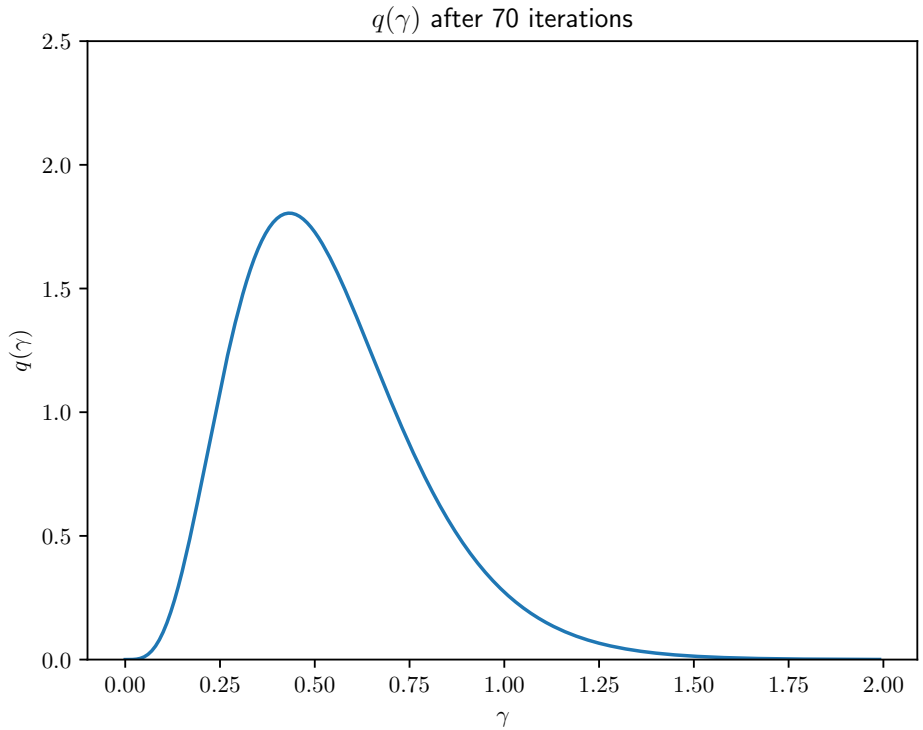


Local model



Variational posteriors



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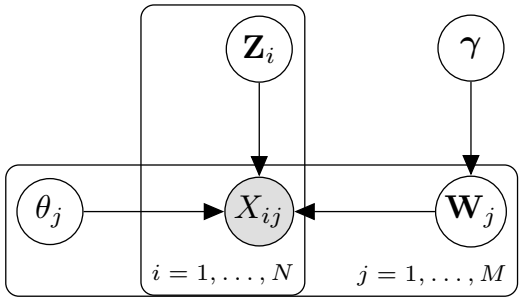

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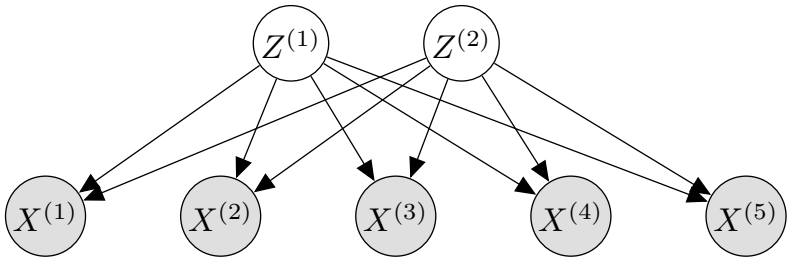
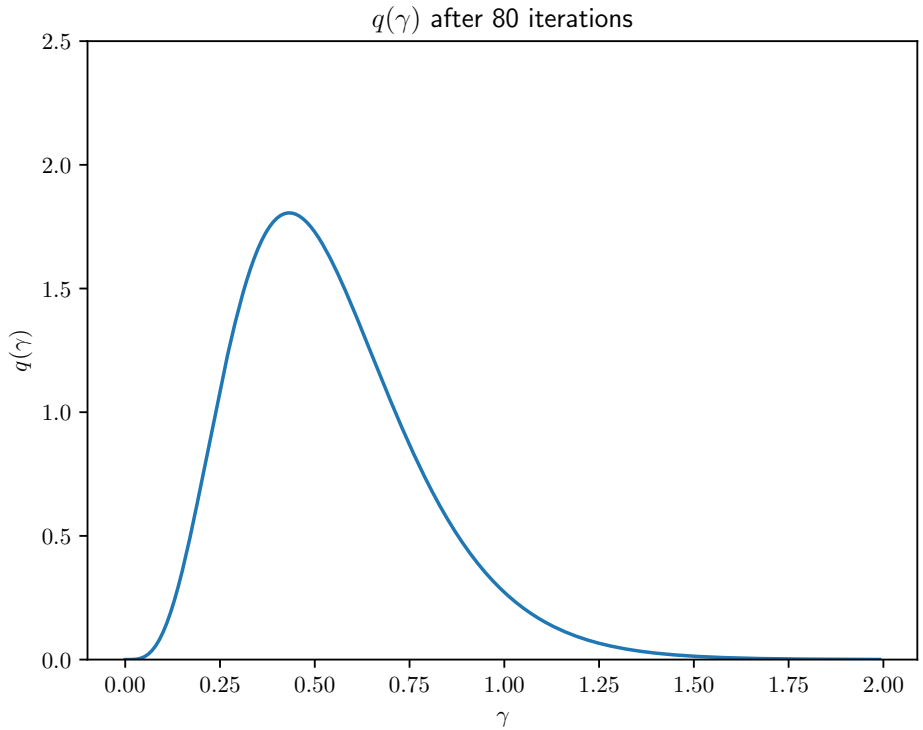


Variational posteriors



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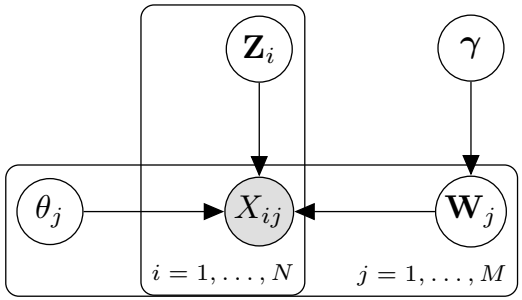
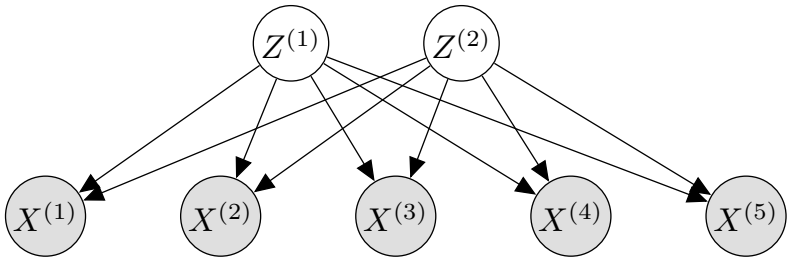
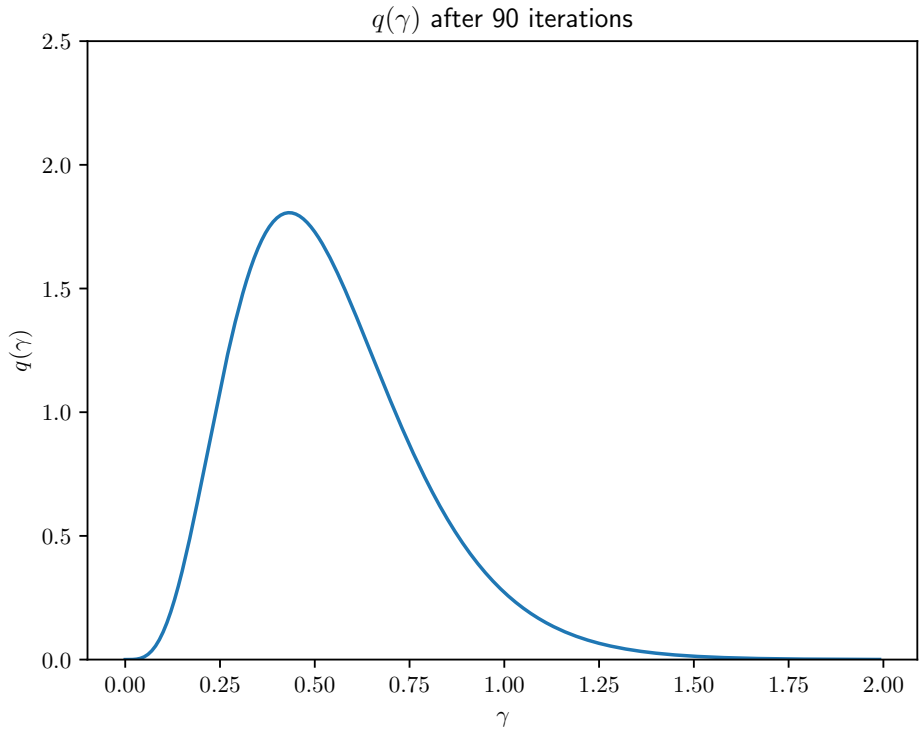


Local model



Variational posteriors



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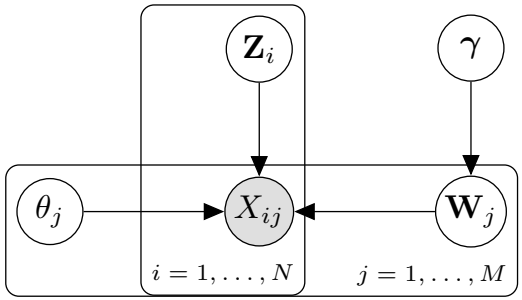

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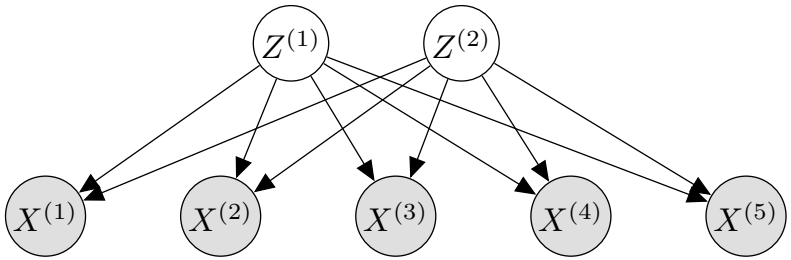
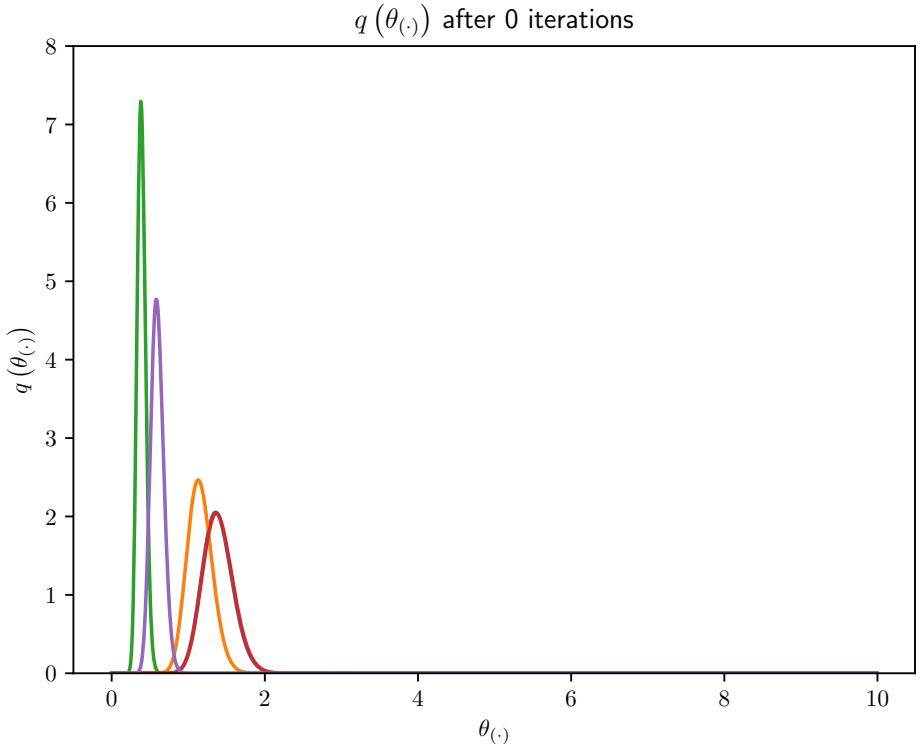


Variational posteriors



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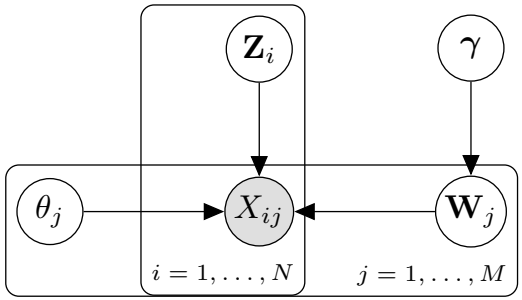

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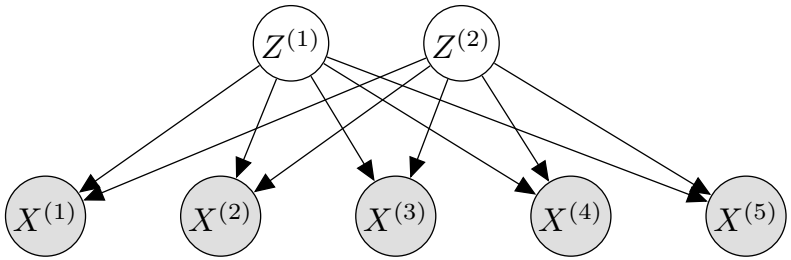
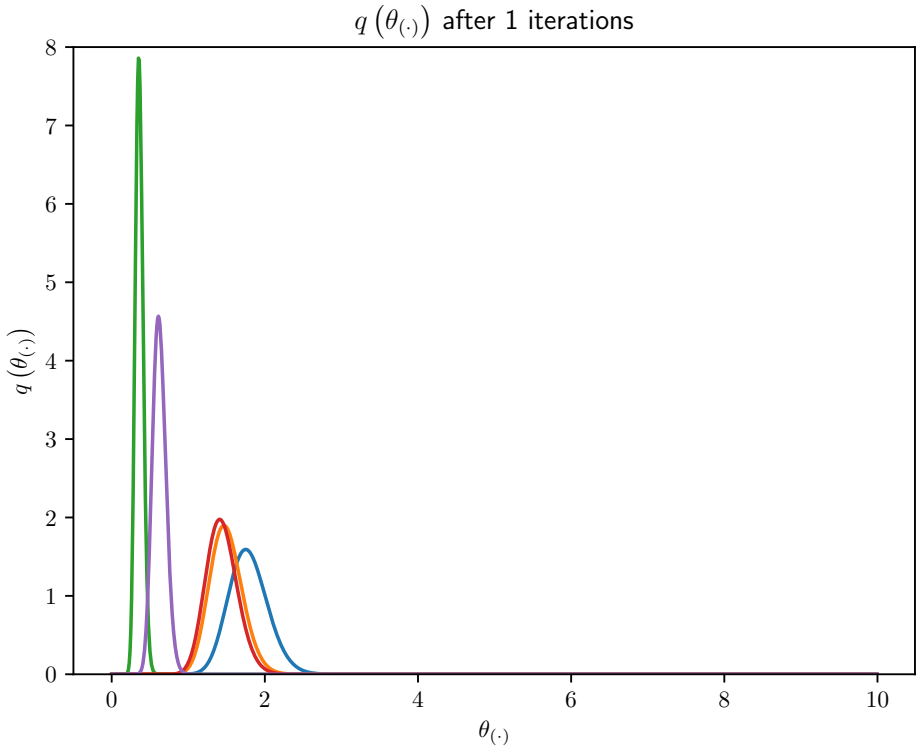


Variational posteriors



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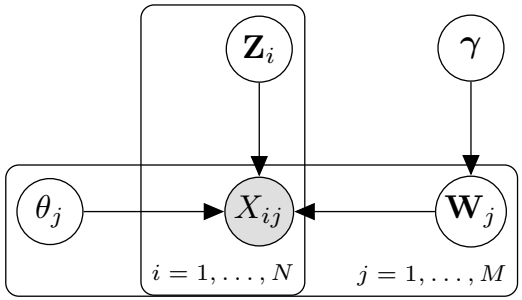
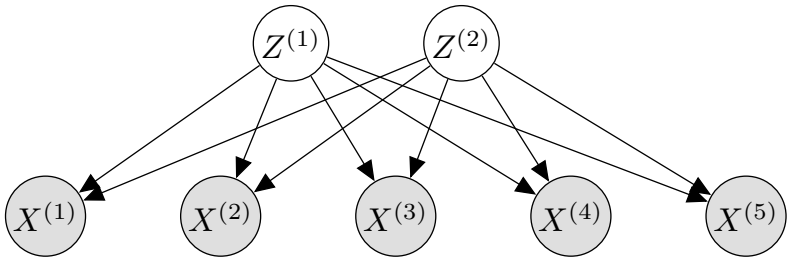
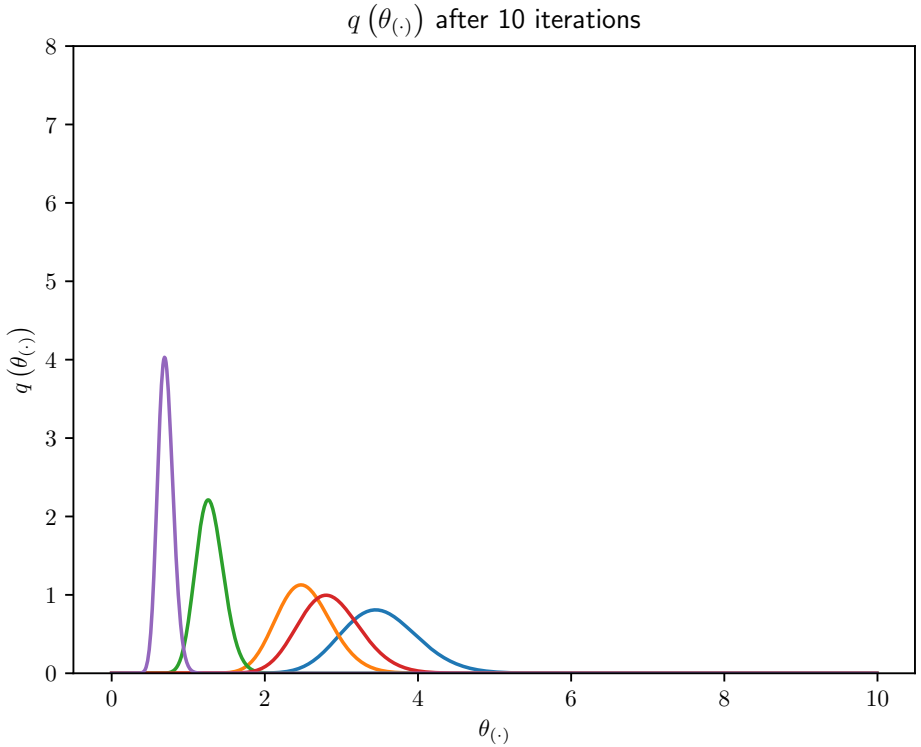


Local model



Variational posteriors



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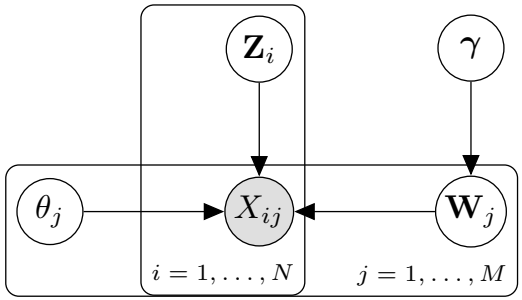
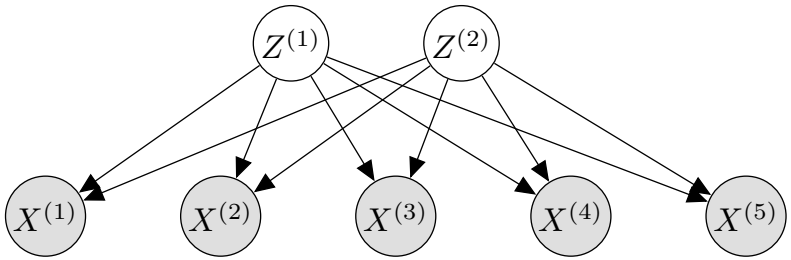
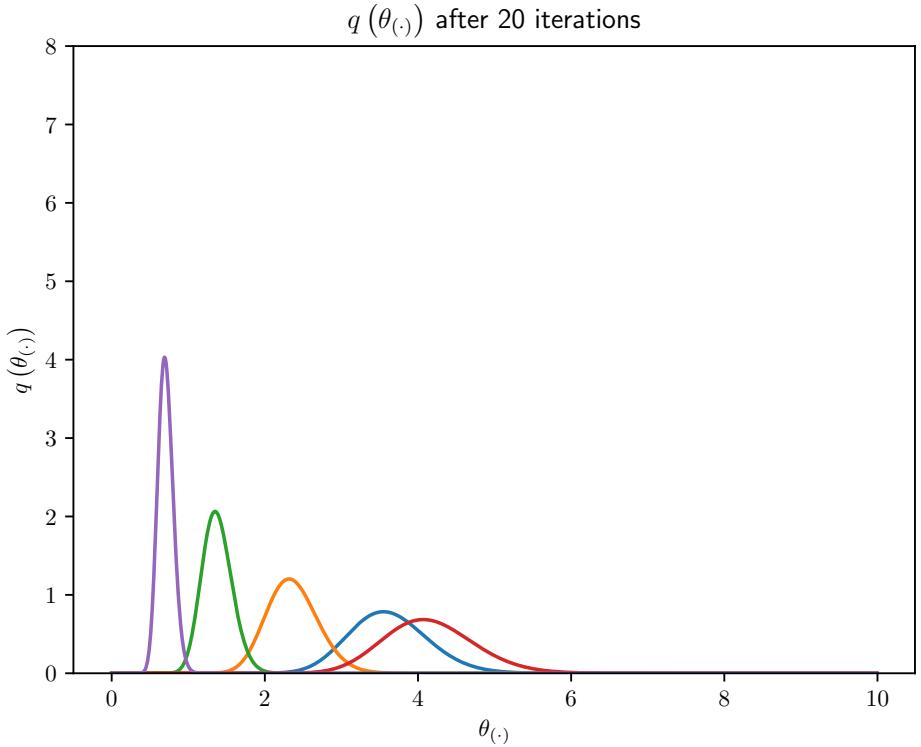


Local model



Variational posteriors



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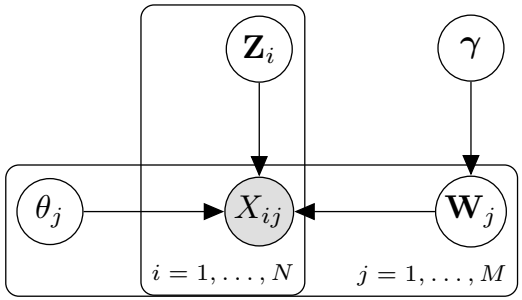
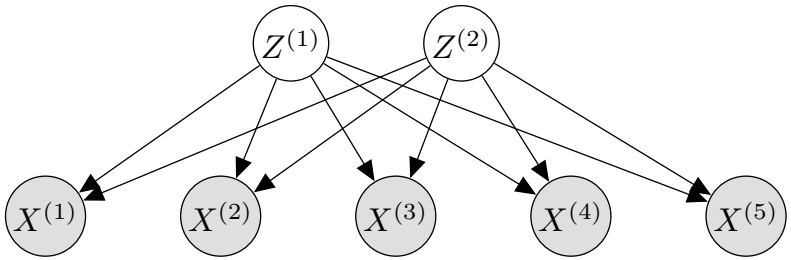
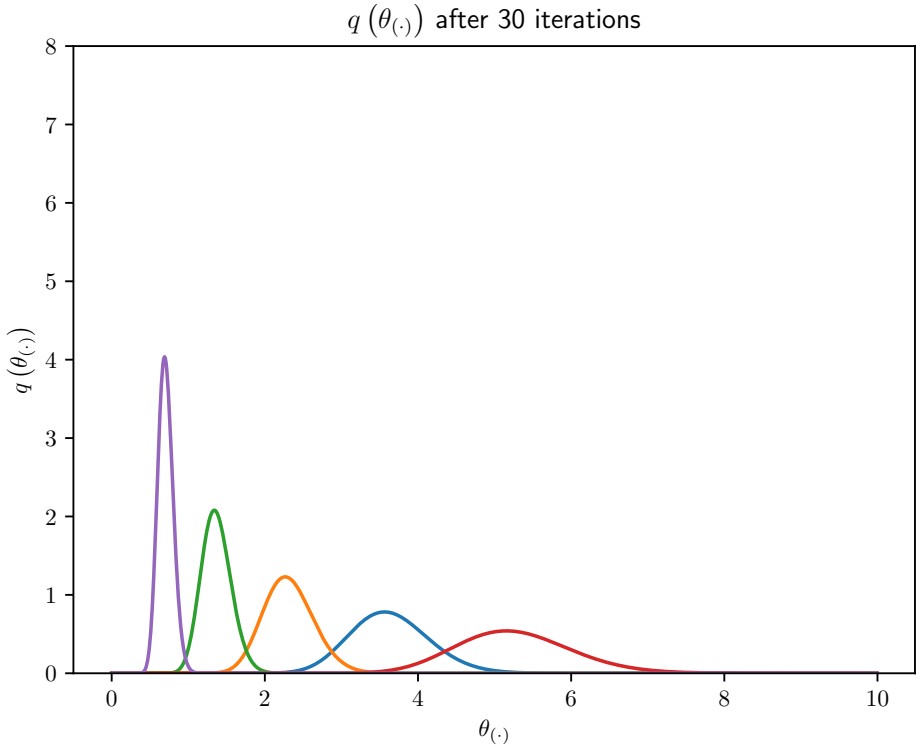


Local model



Variational posteriors



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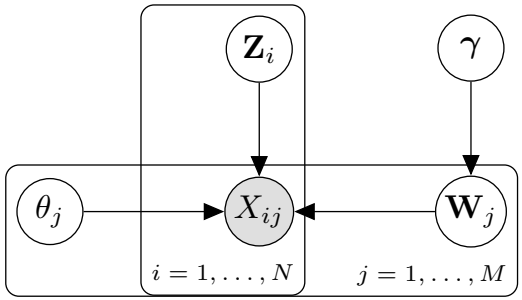

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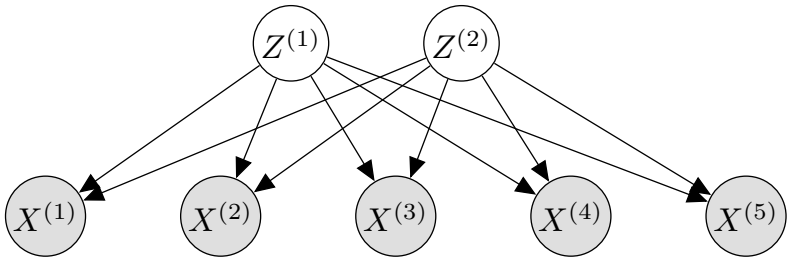
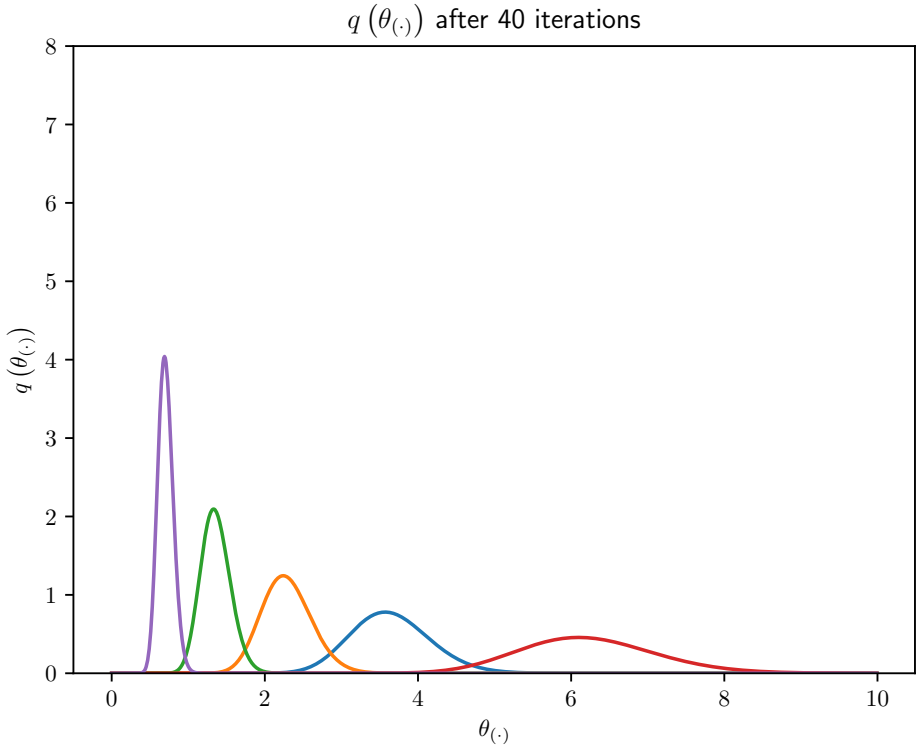


Variational posteriors



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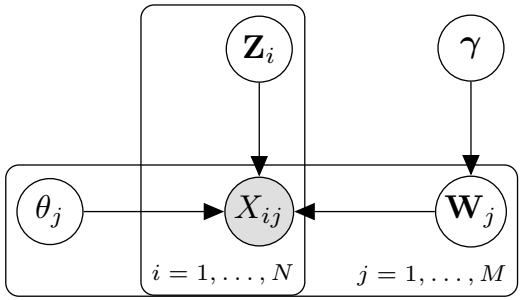
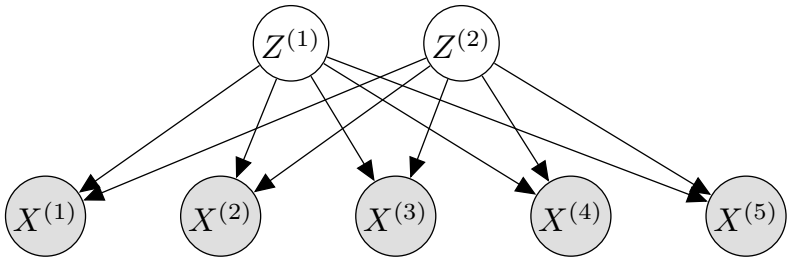


Local model



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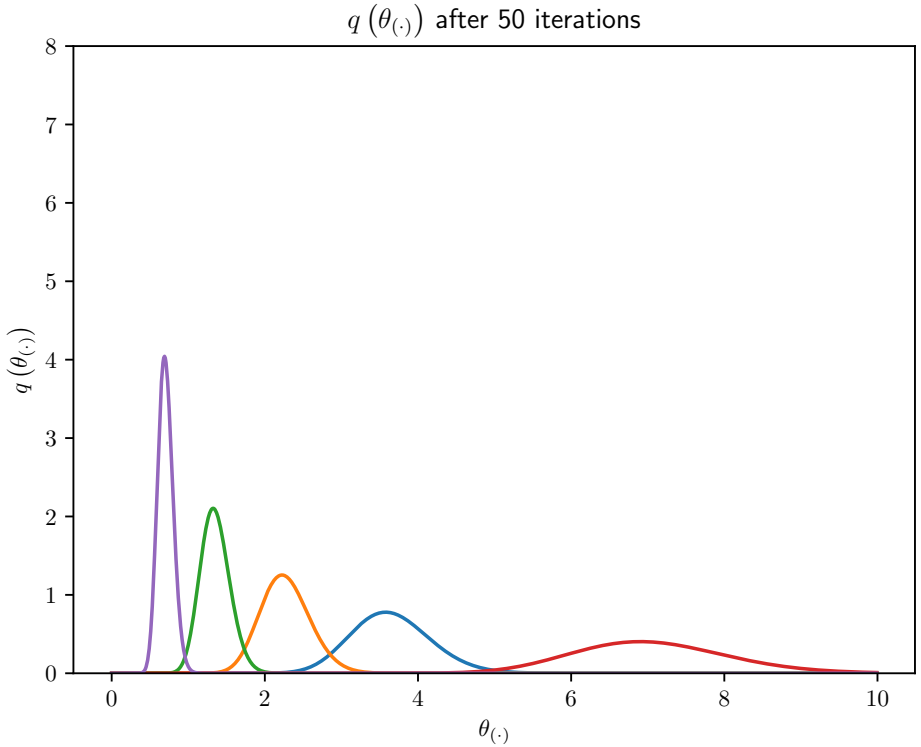

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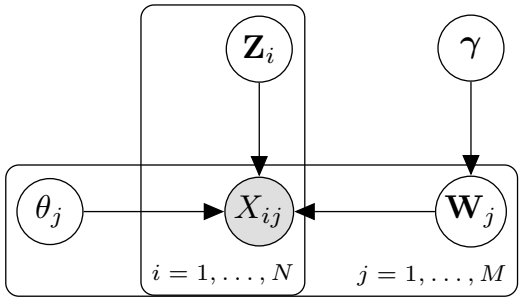

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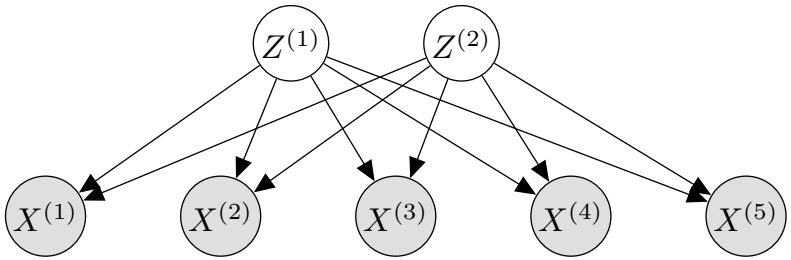

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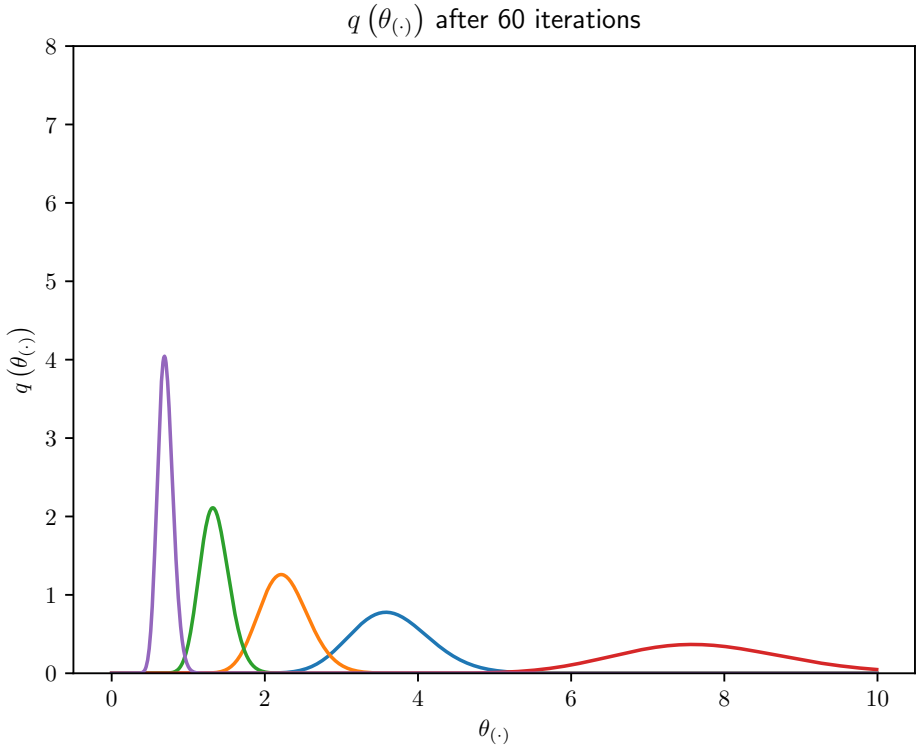

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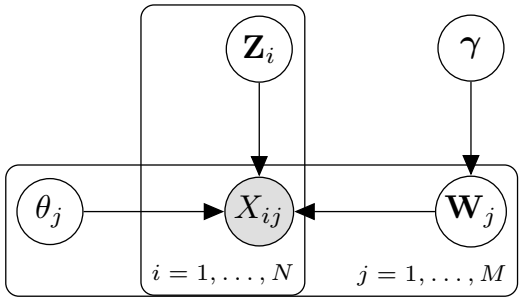

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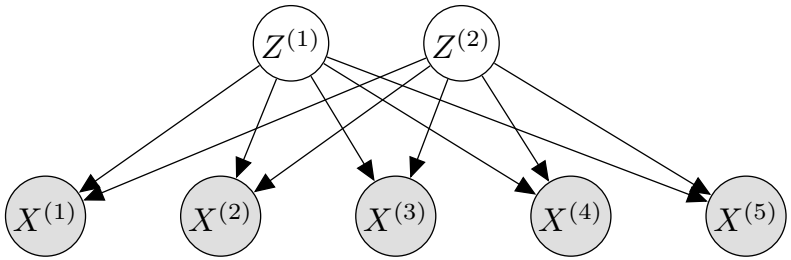

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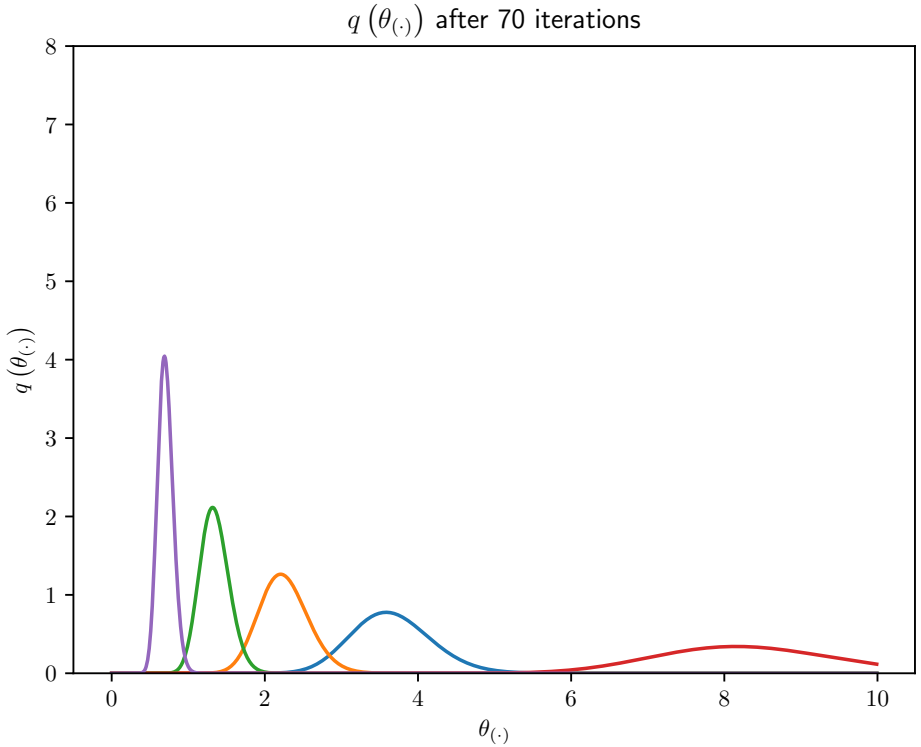

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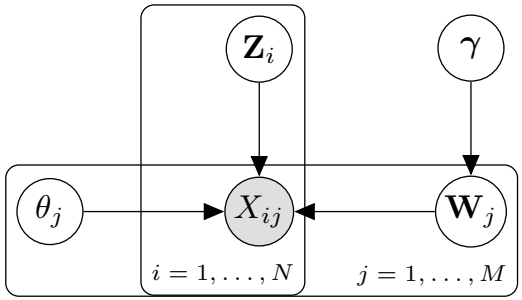
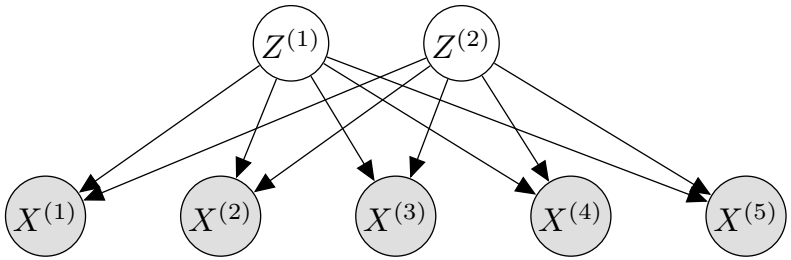
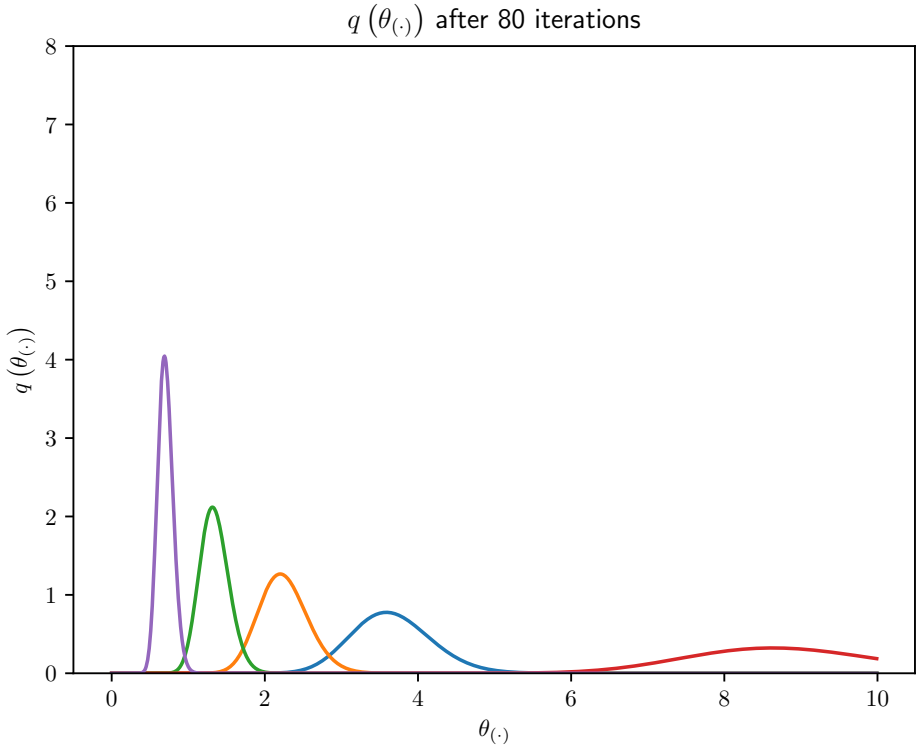
Global model



Local model



Variational posteriors



Data

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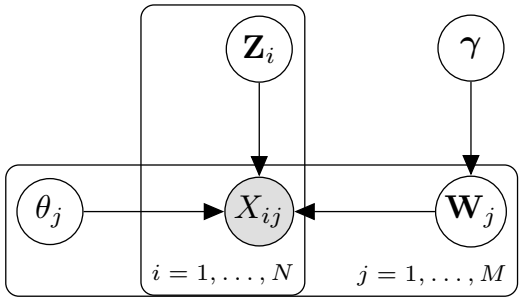
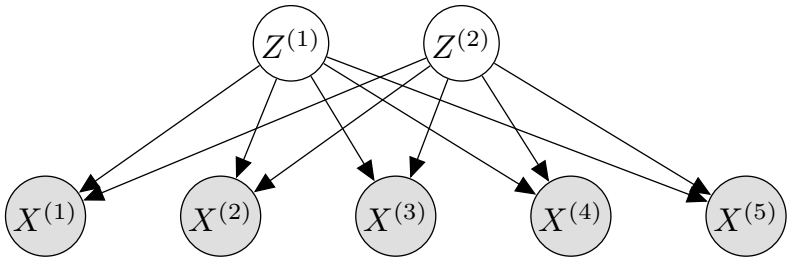
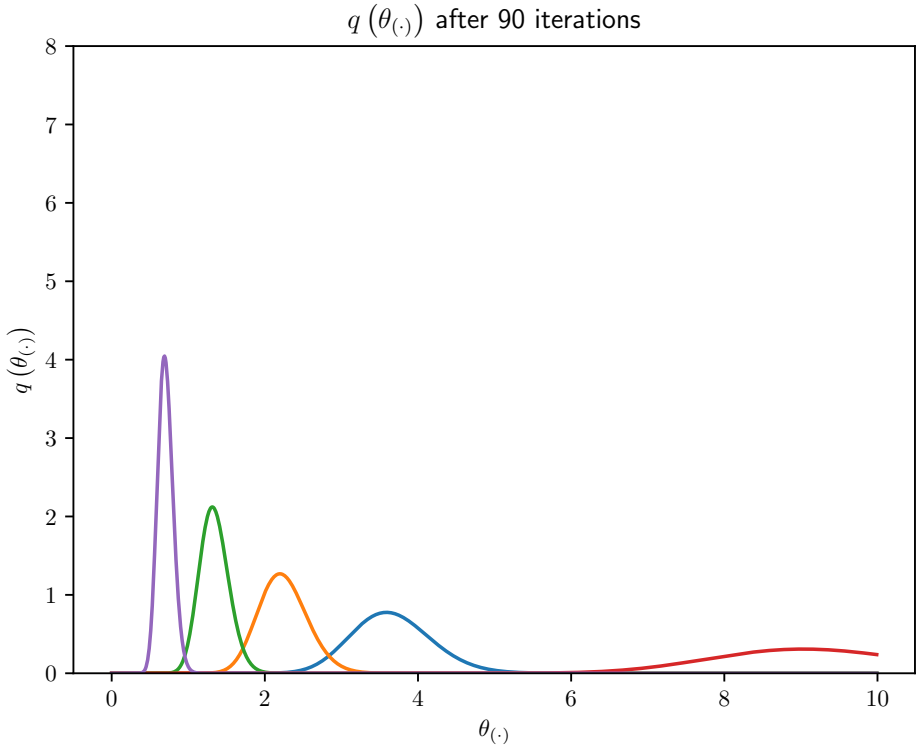
Global model



Local model



Variational posteriors



Data

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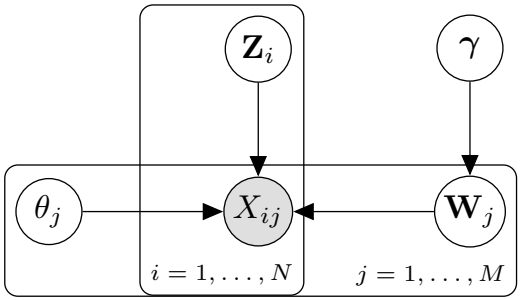
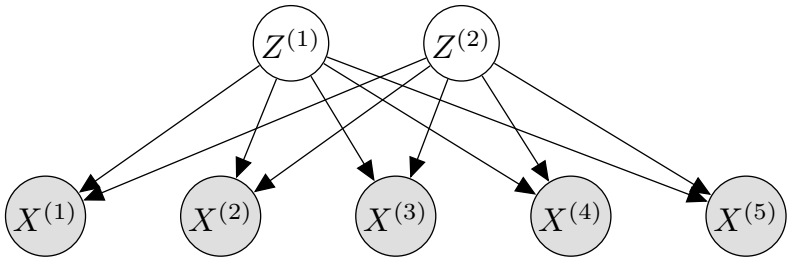
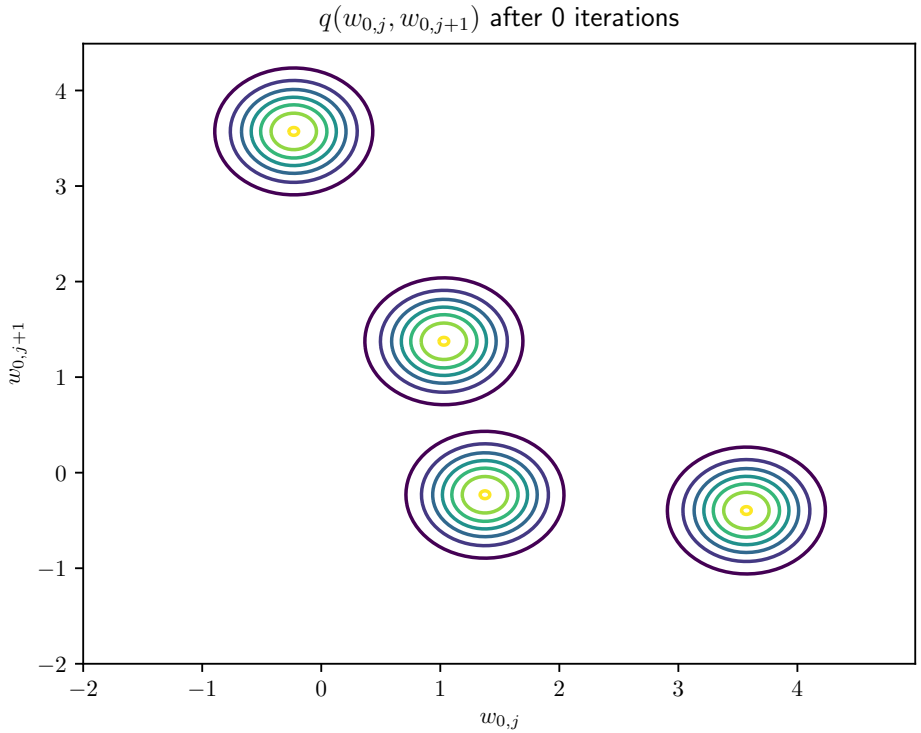


Local model



Variational posteriors



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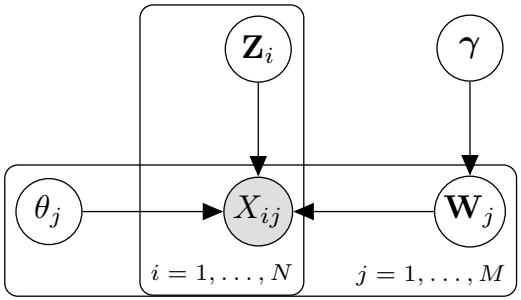
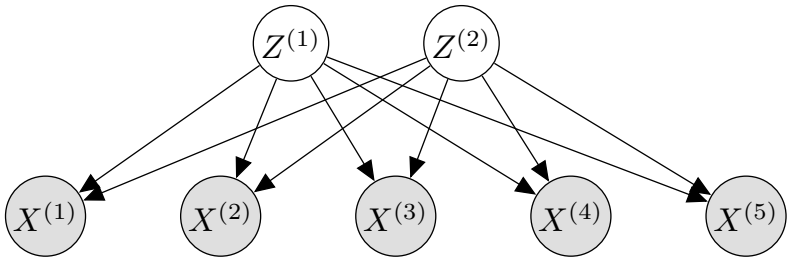
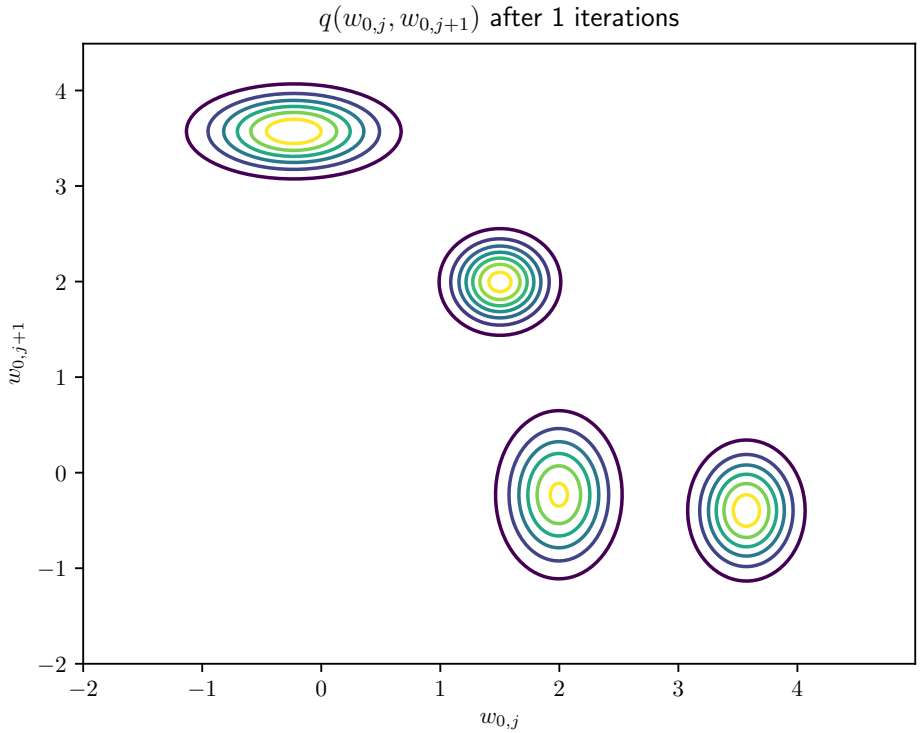
Global model



Local model



Variational posteriors



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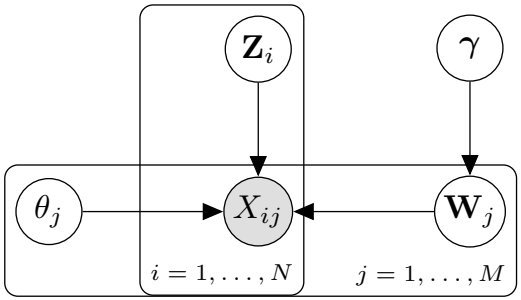
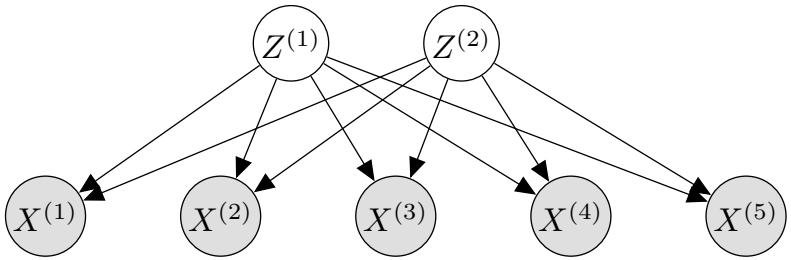
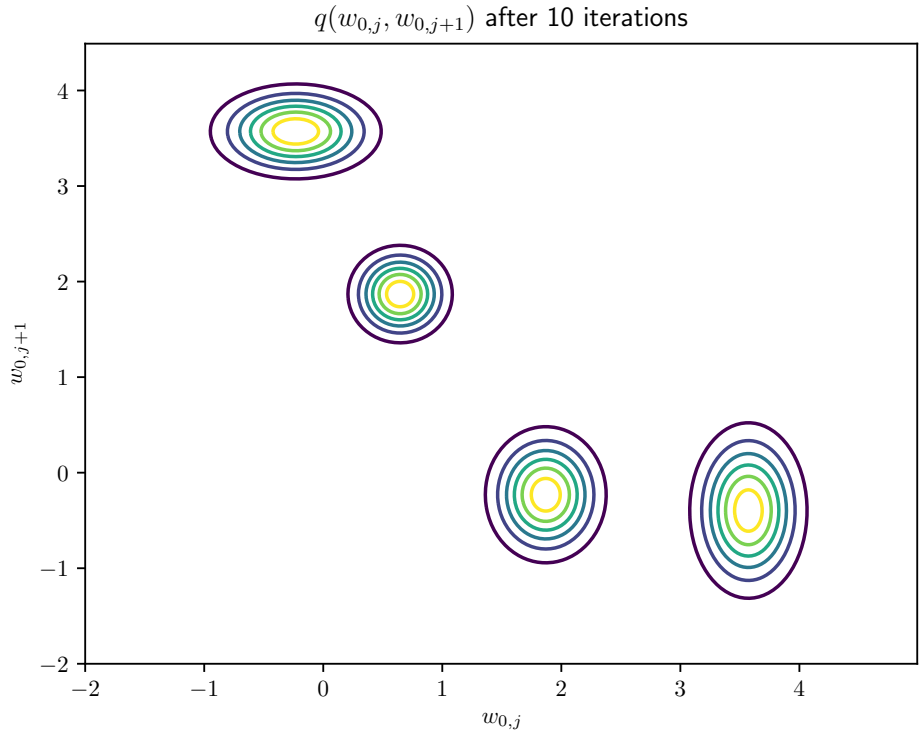
Global model



Local model



Variational posteriors



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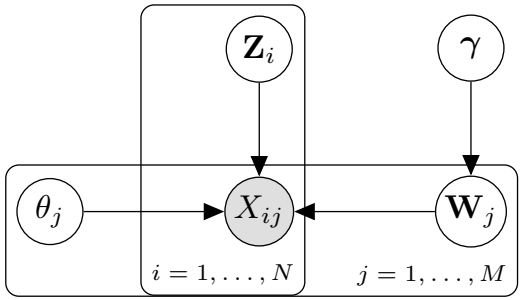
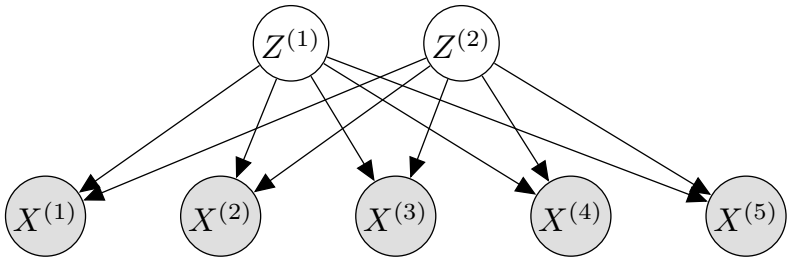
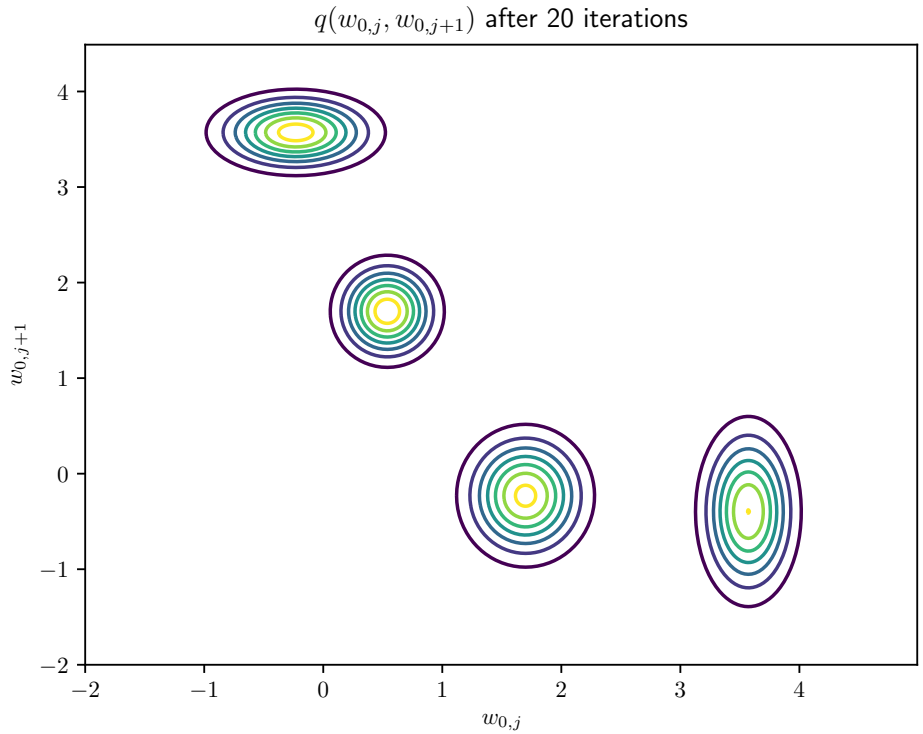


Local model



Variational posteriors



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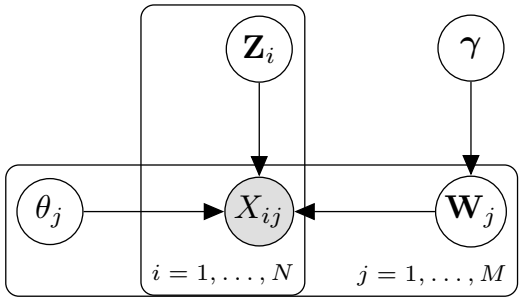
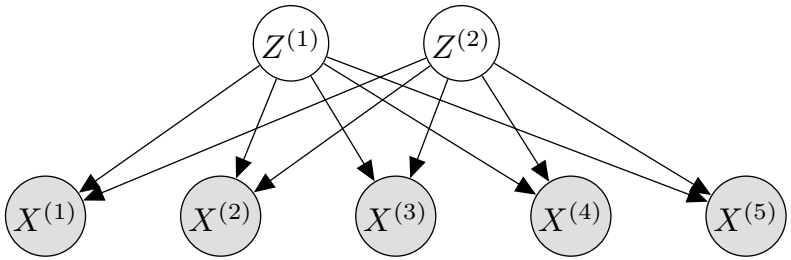
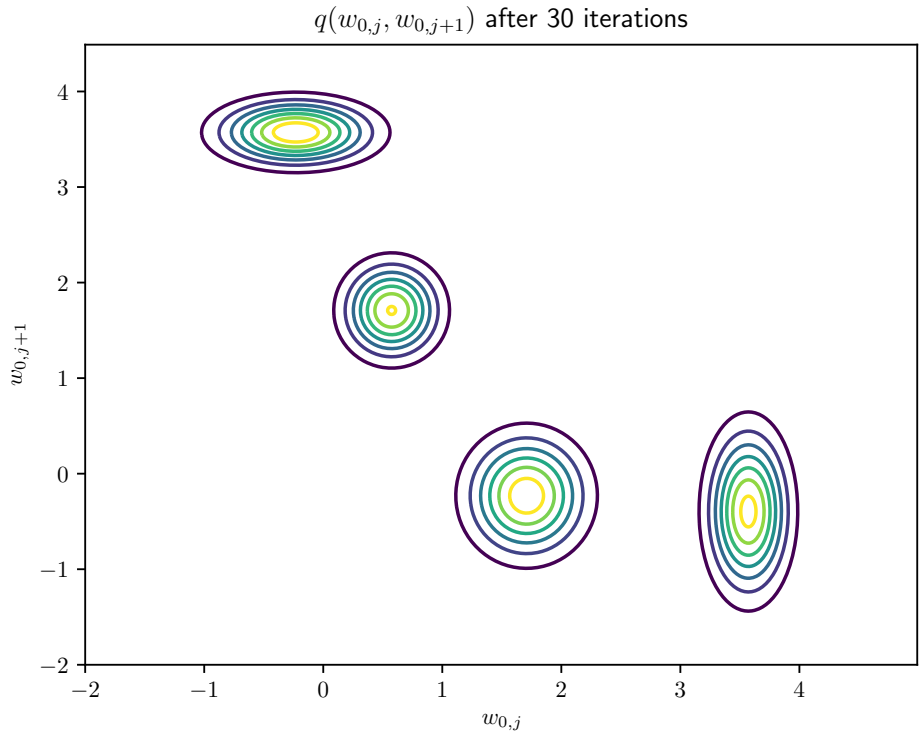
Global model



Local model



Variational posteriors



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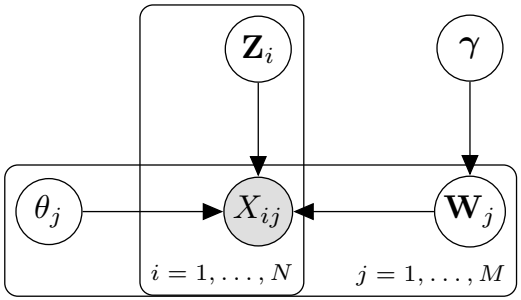
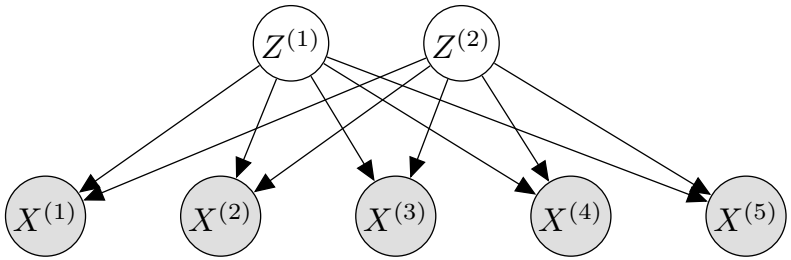


Local model



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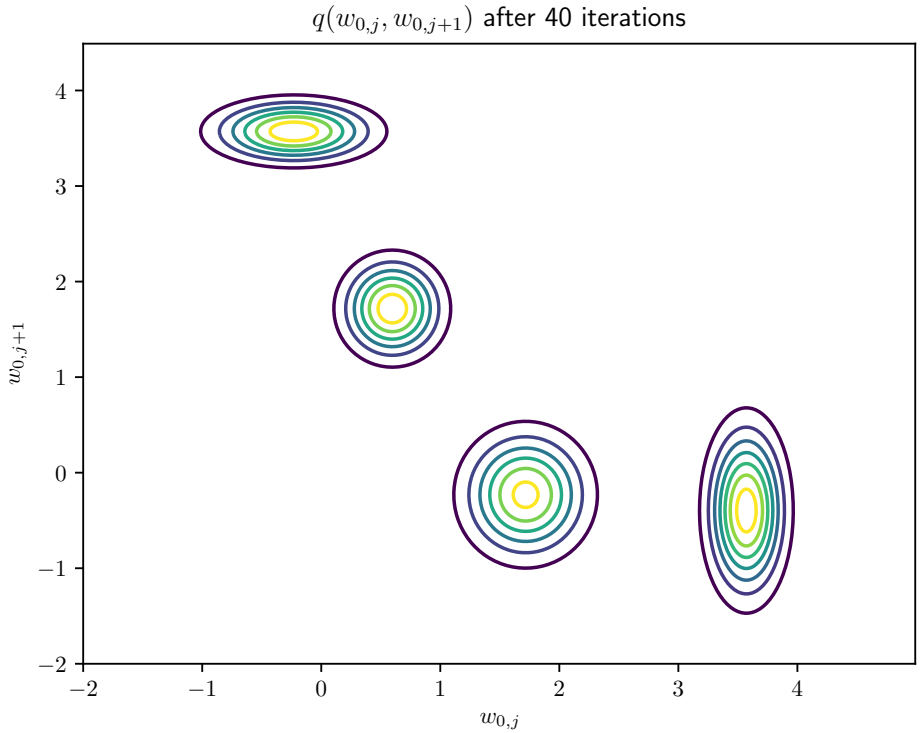

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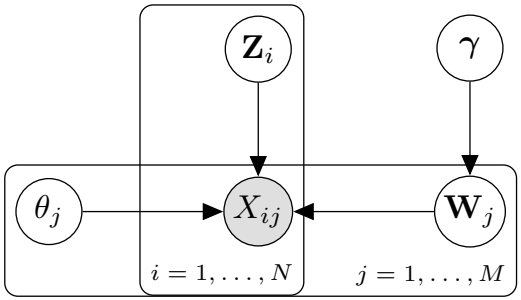
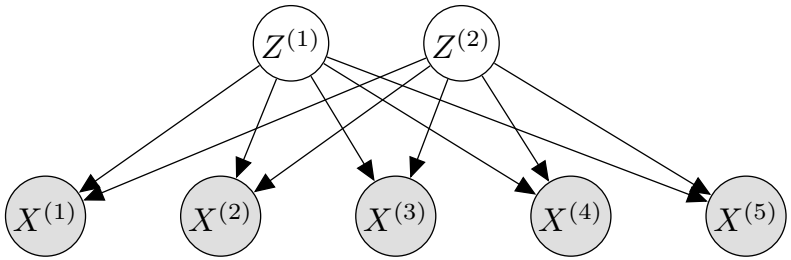
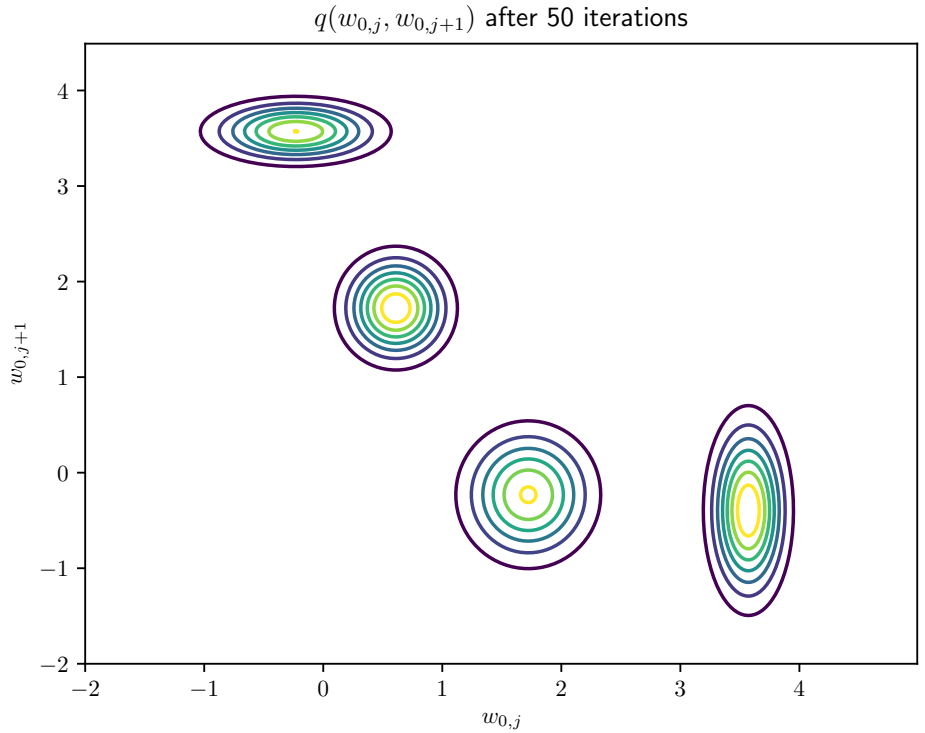
Global model



Local model



Variational posteriors



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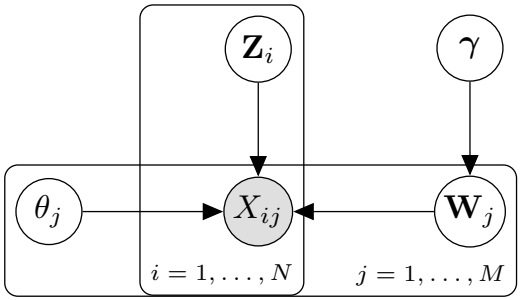
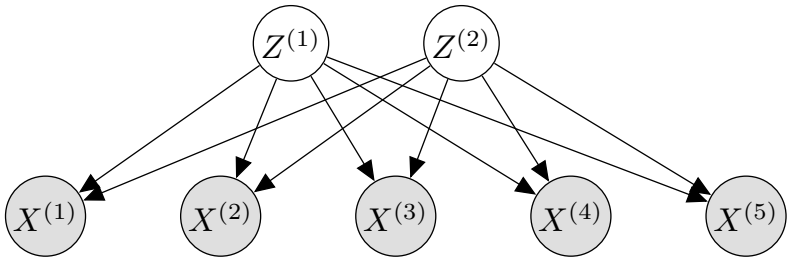
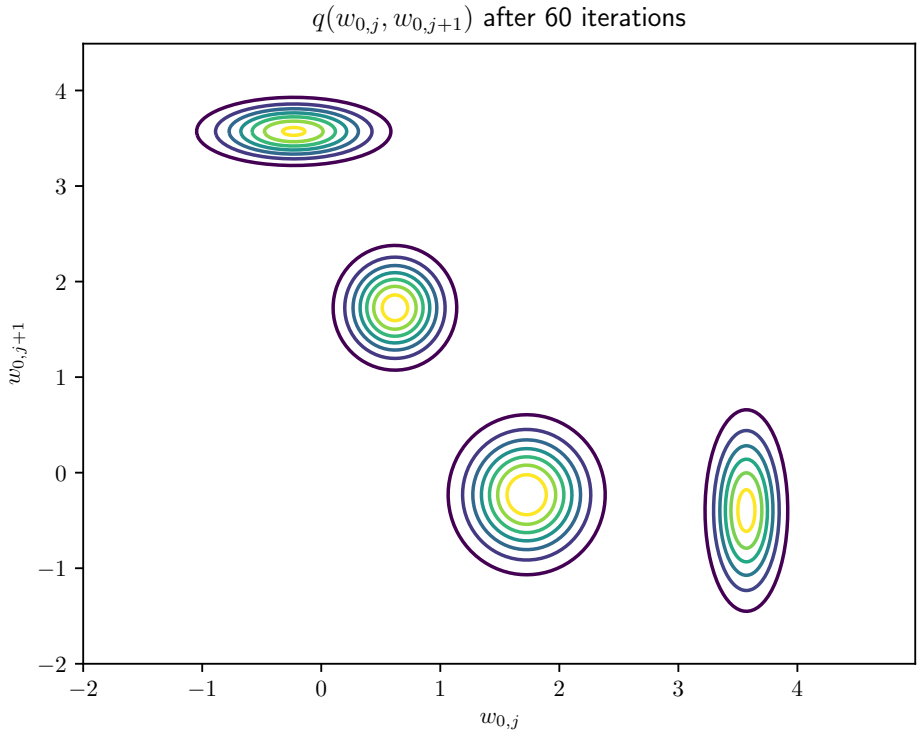


Local model



Variational posteriors



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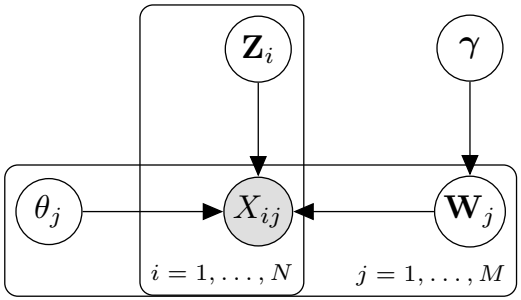
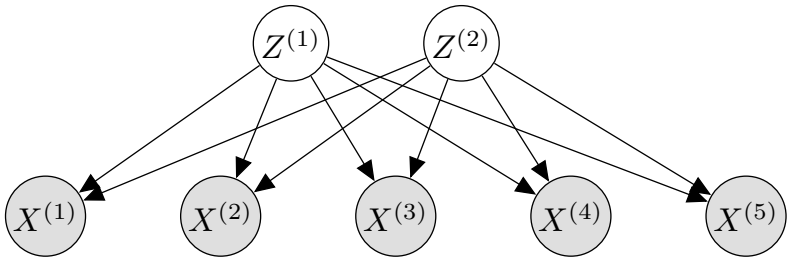
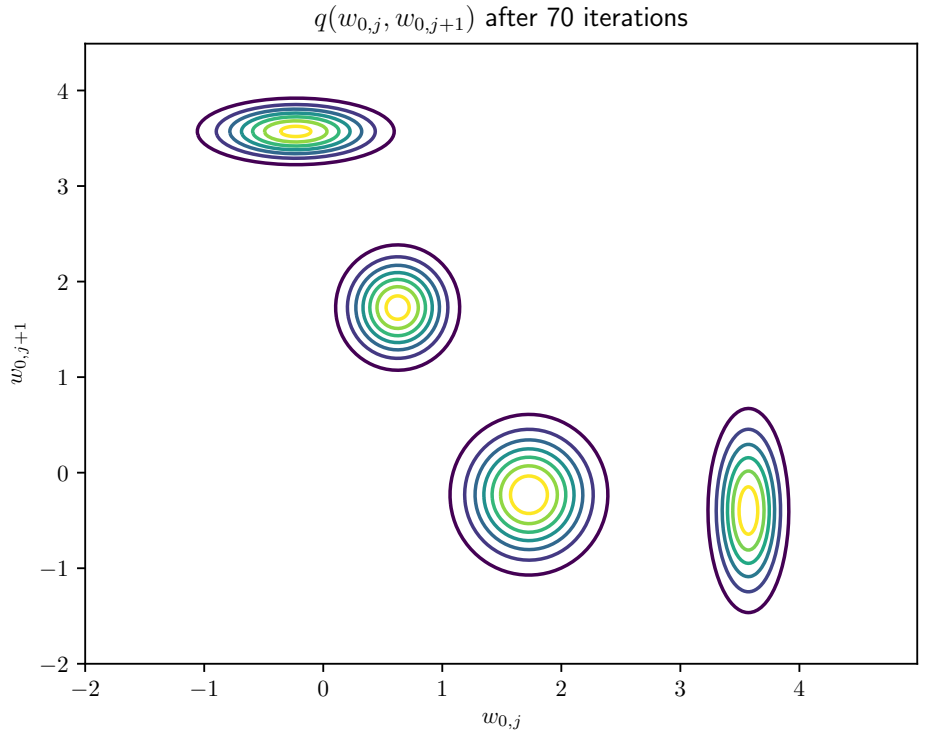
Global model



Local model



Variational posteriors



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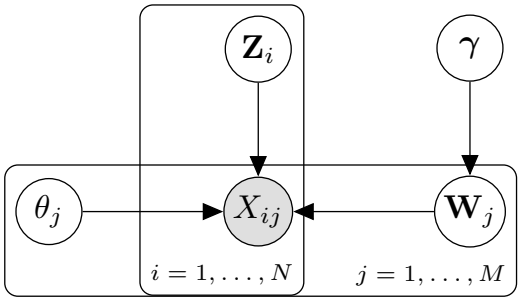
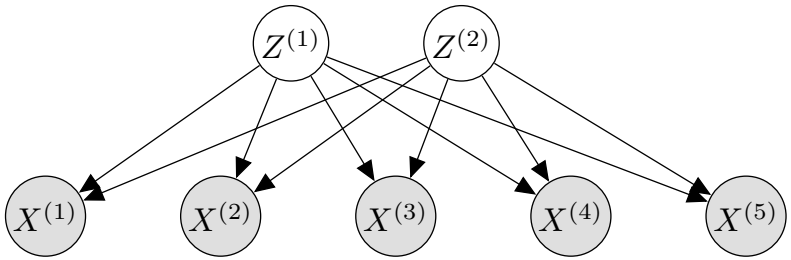
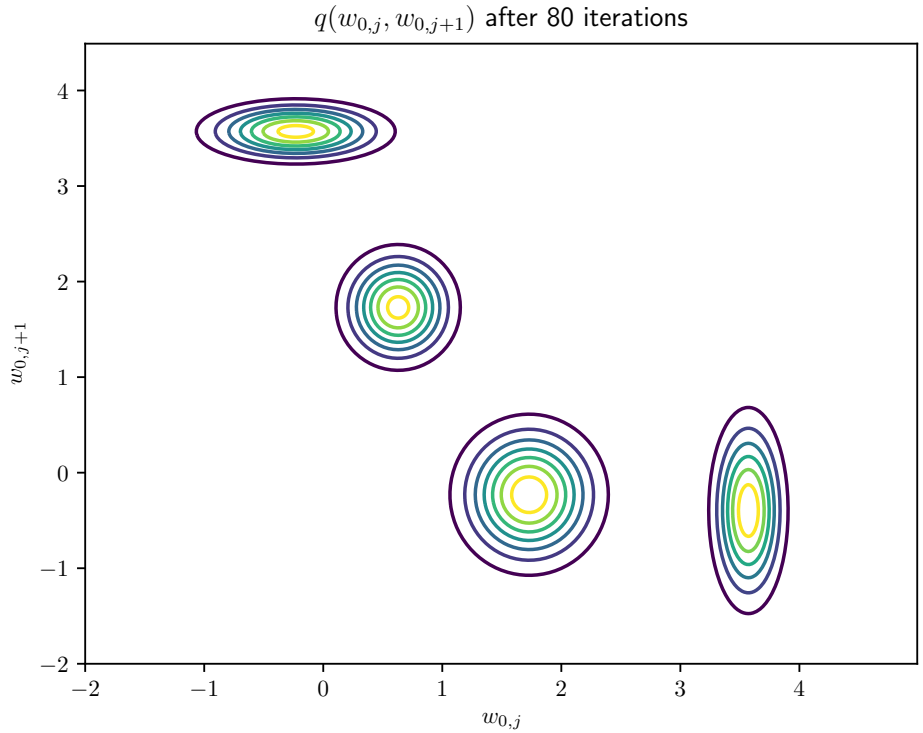


Local model



Variational posteriors



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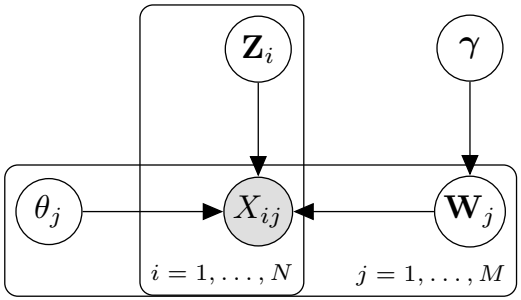
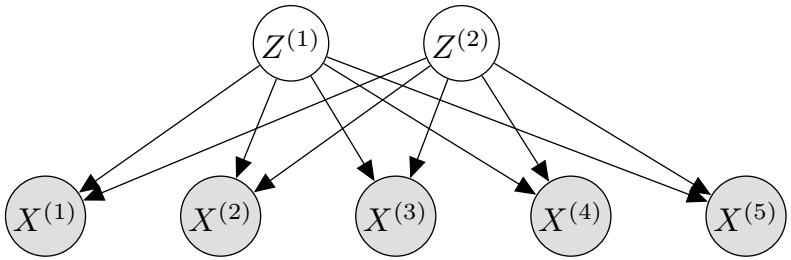
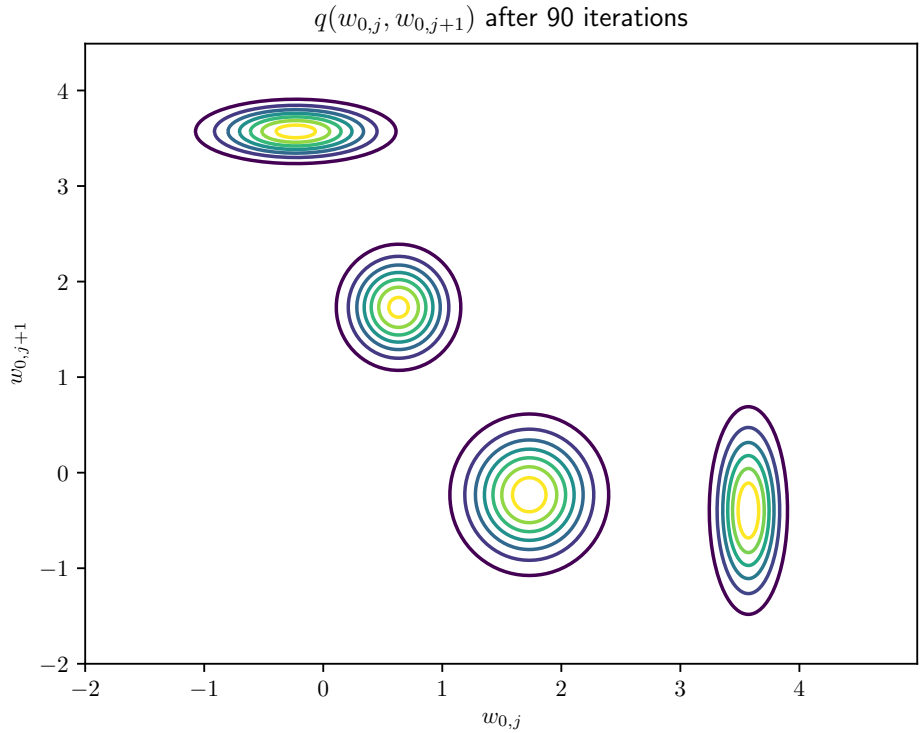


Local model



Variational posteriors



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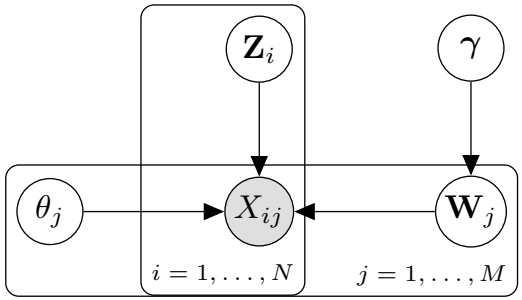
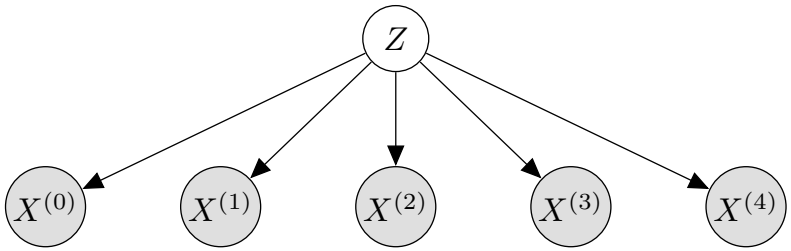
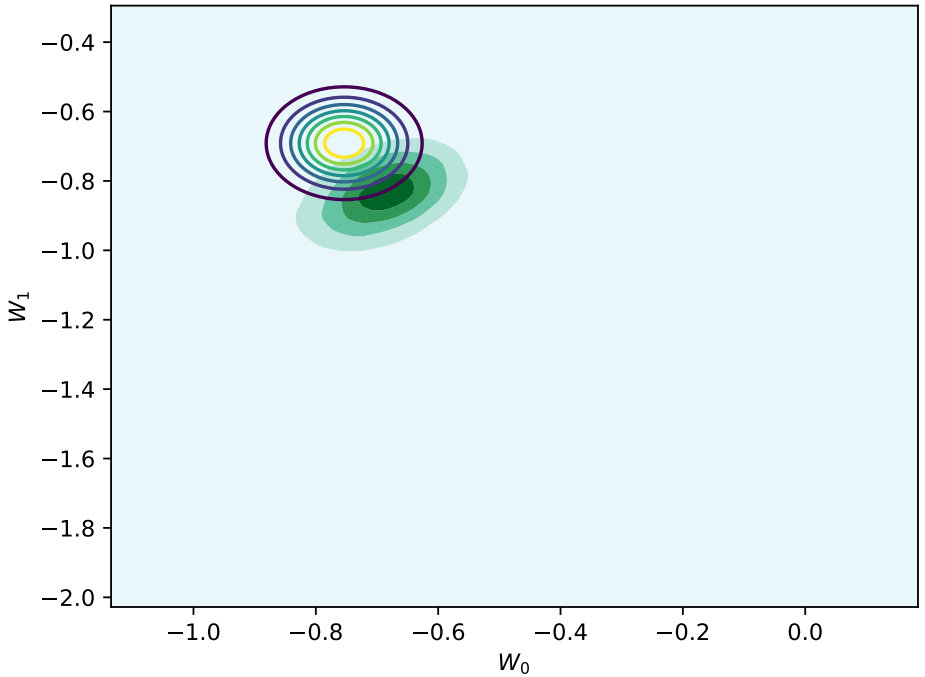


Local model



Comparison with Gibbs sampling



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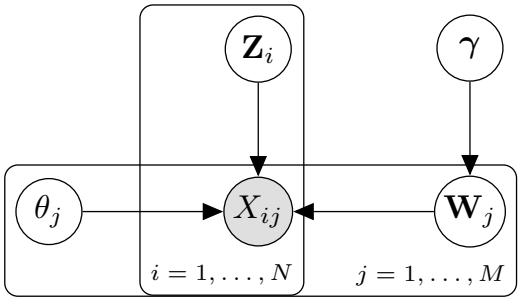
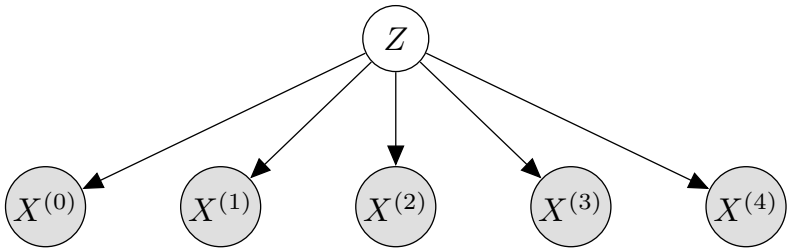
Global model



Local model



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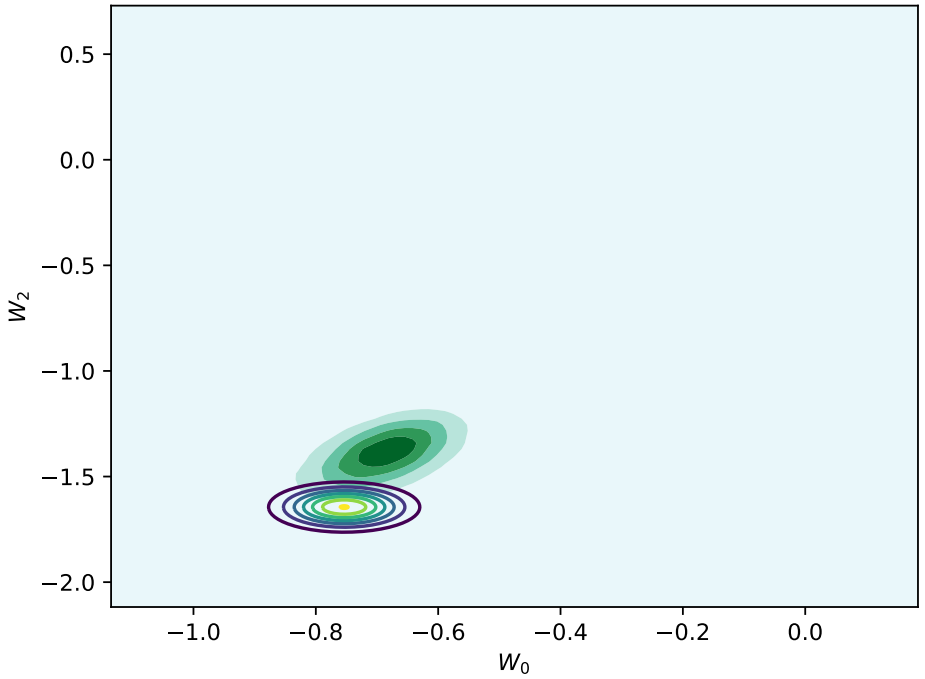

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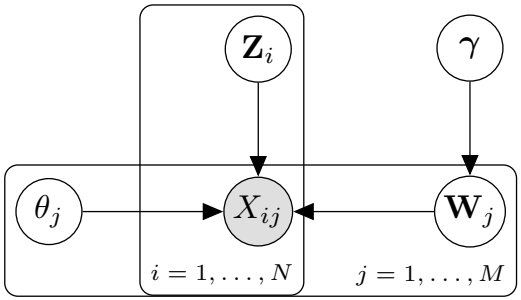
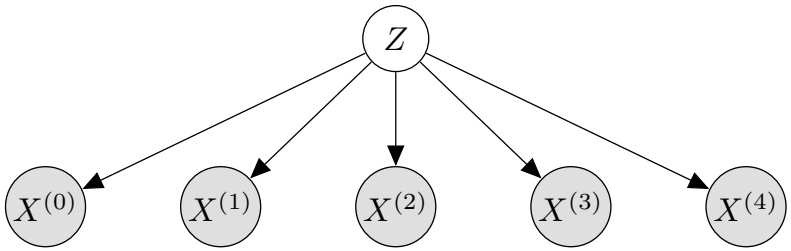


Local model



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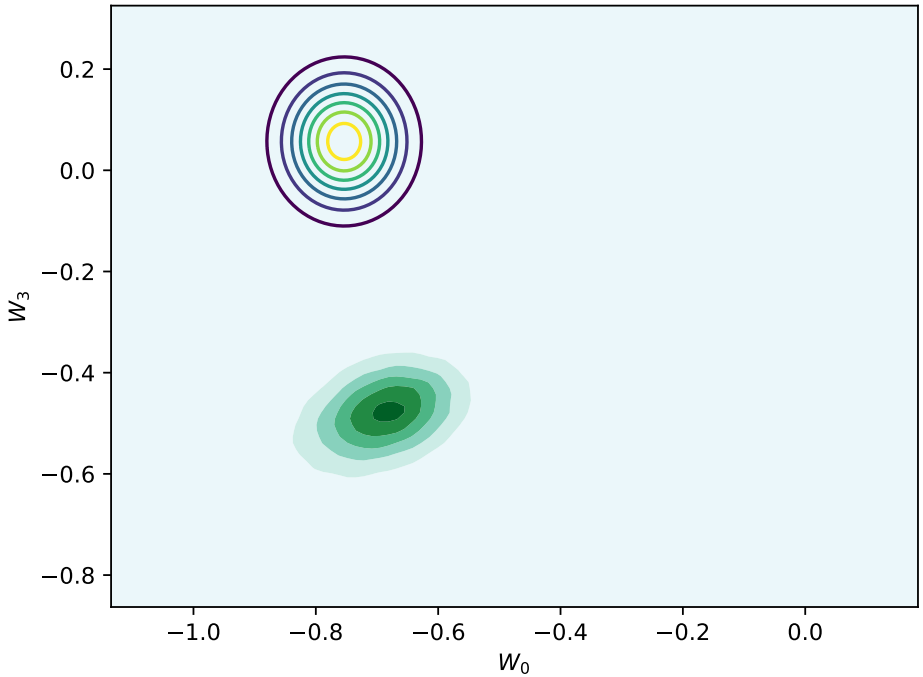

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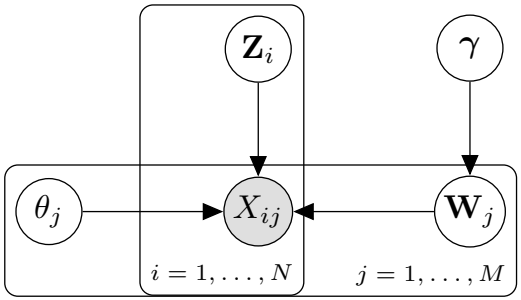
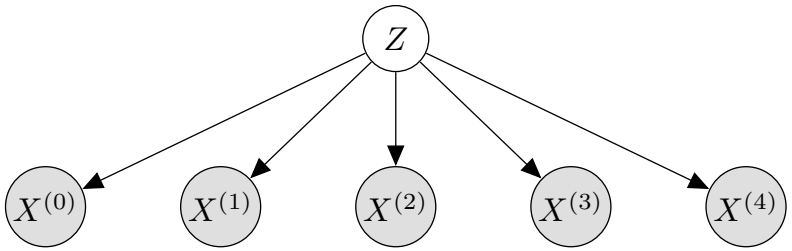
Global model



Local model



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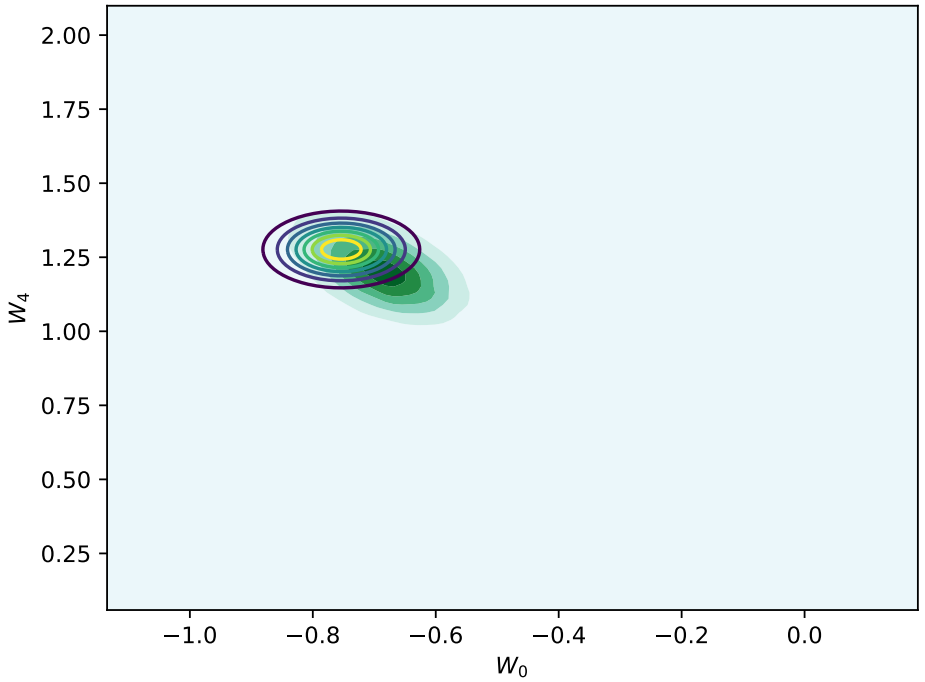

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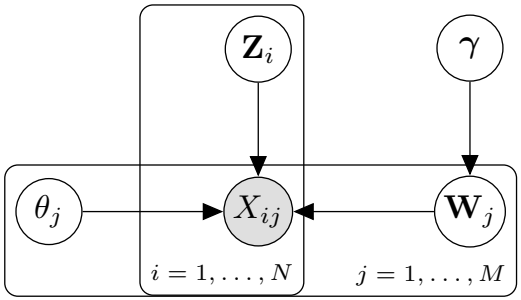

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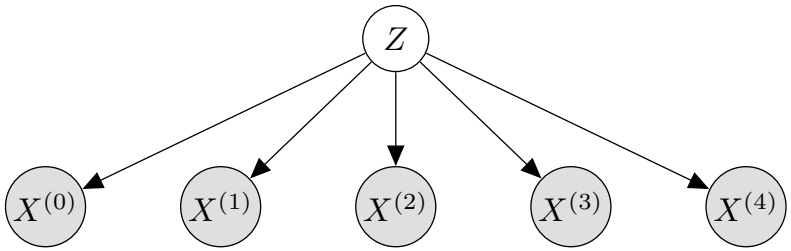

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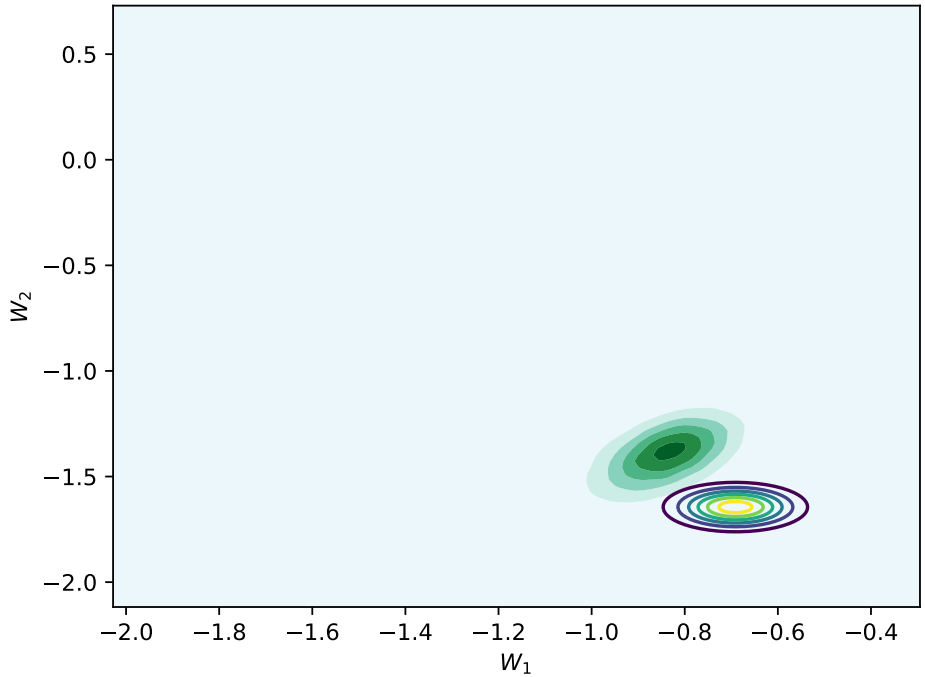

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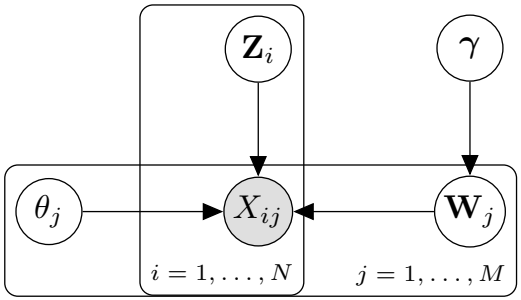

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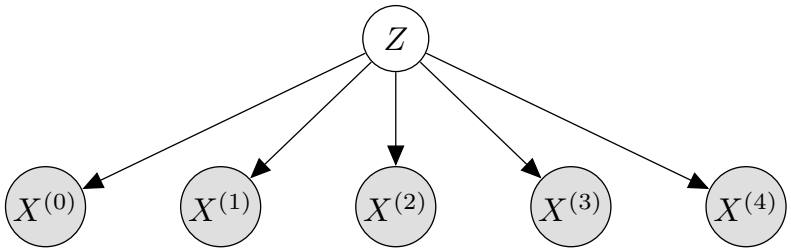

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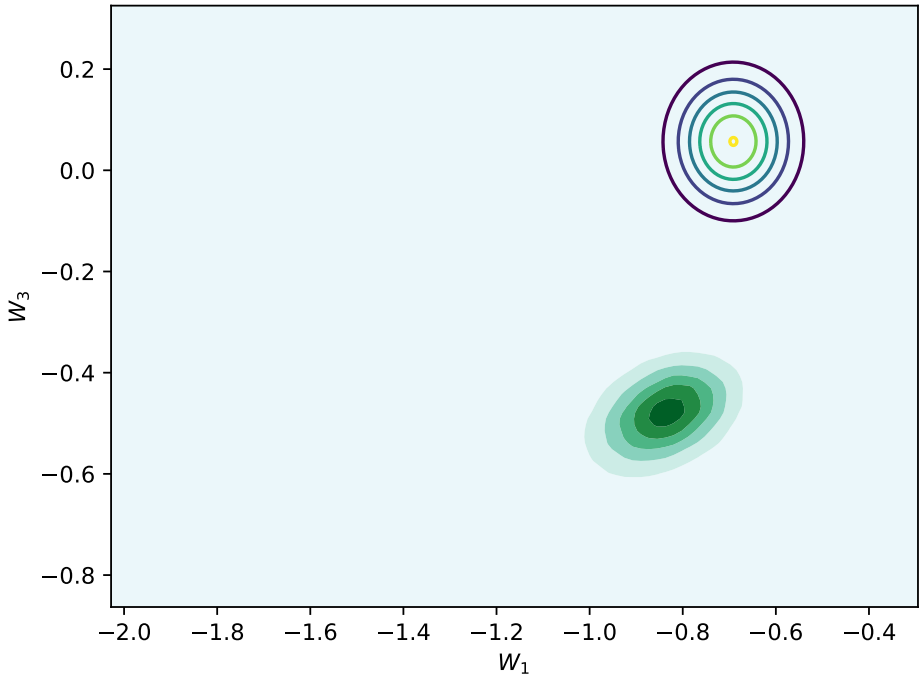

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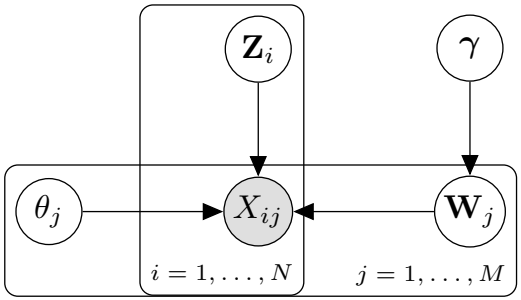

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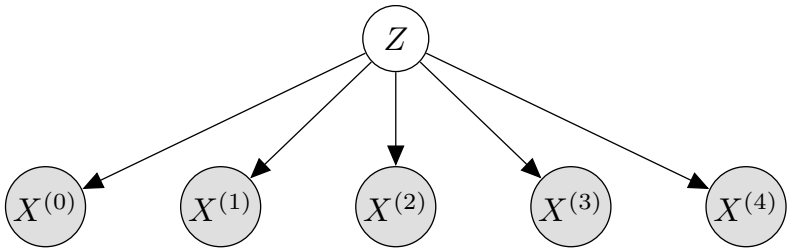

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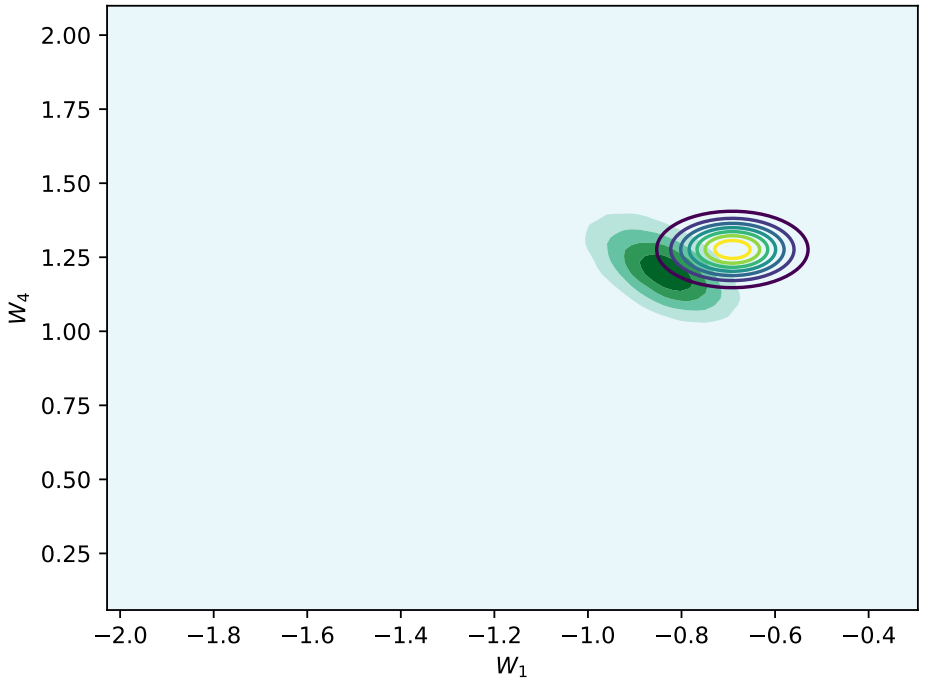

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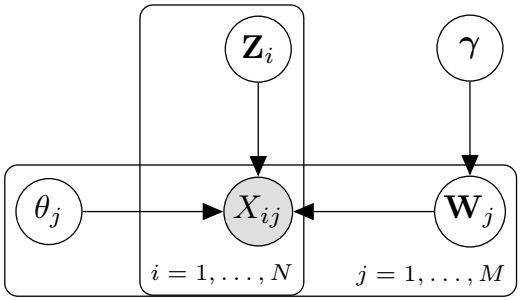

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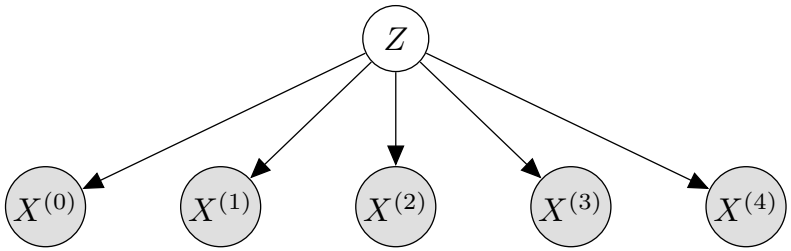

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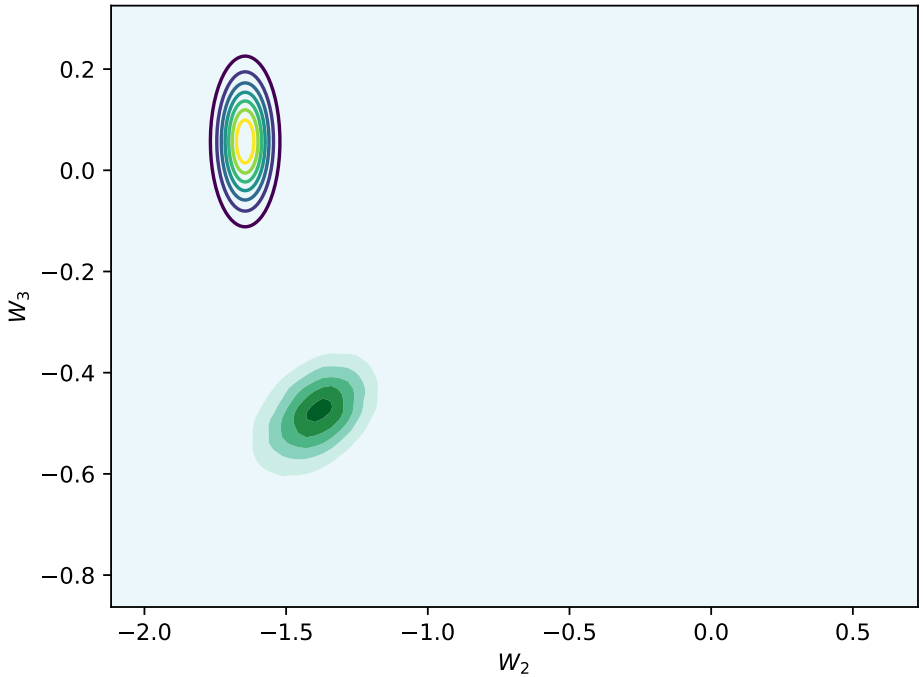

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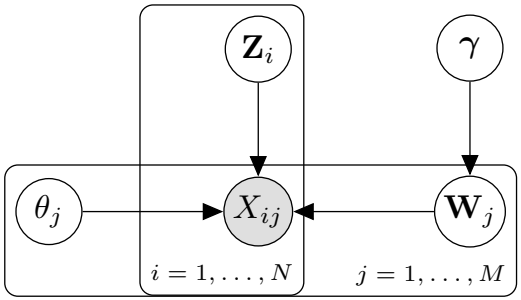

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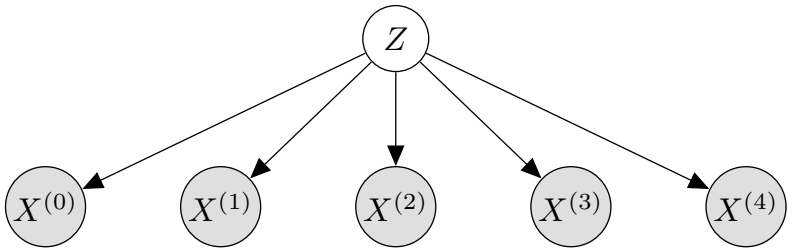

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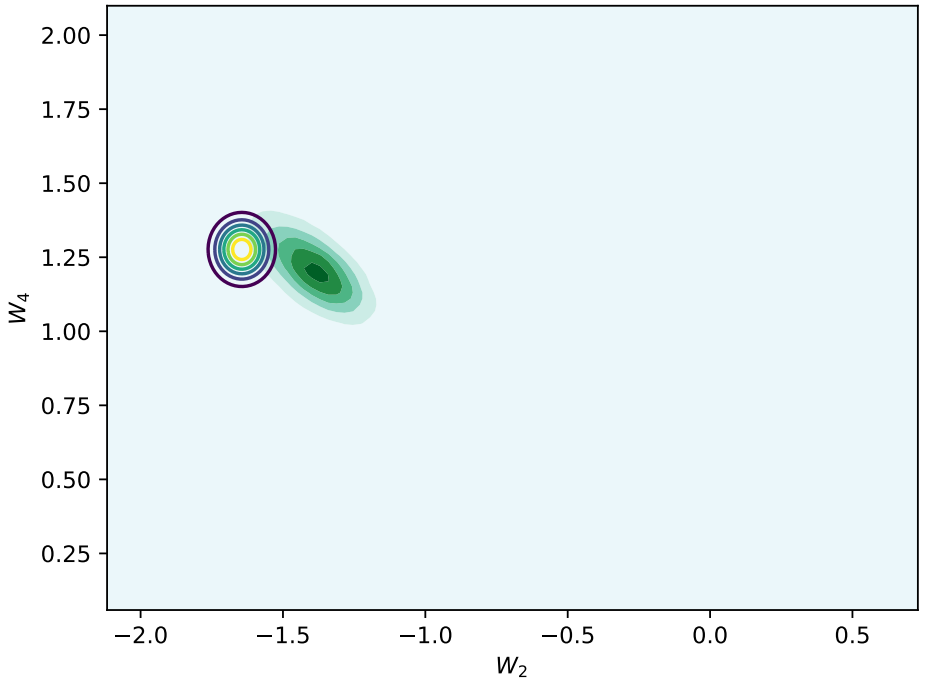

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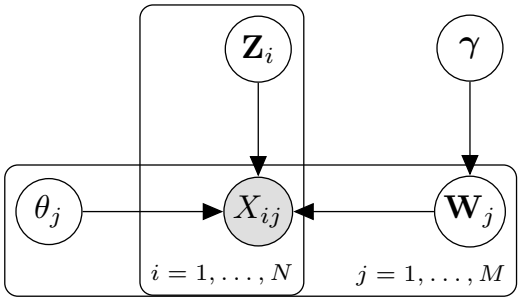

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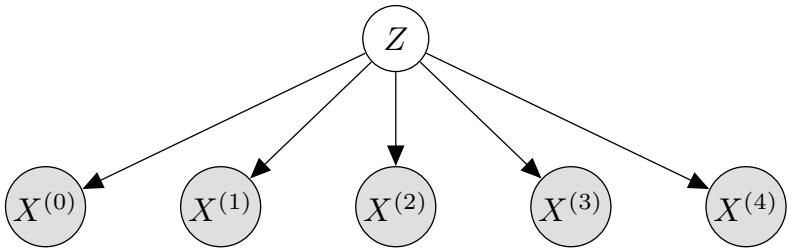

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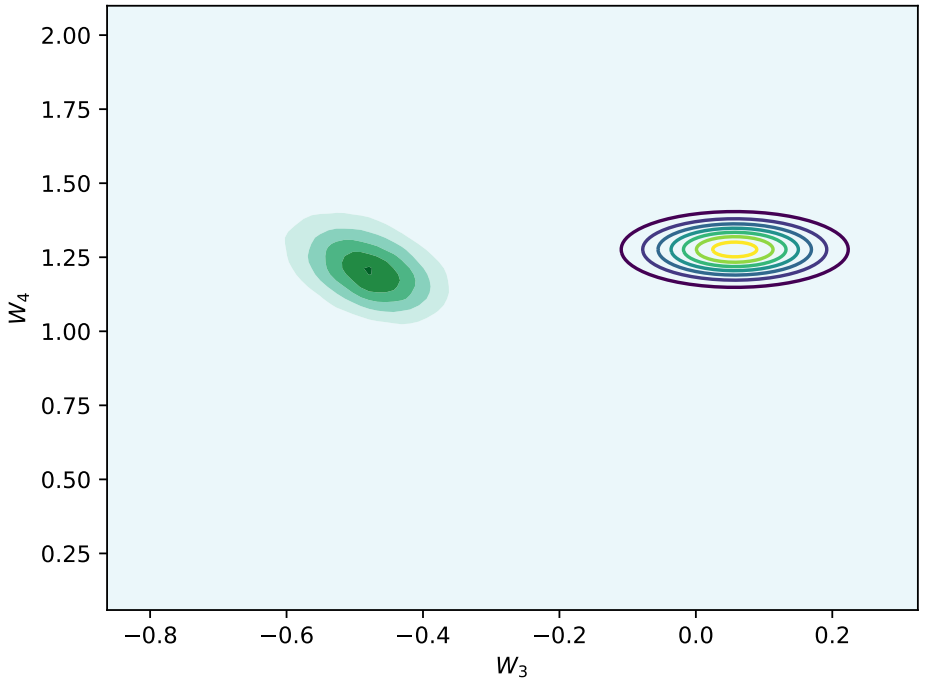

Not seen from the plot, **but** the results strongly dependent on the VI initialization.

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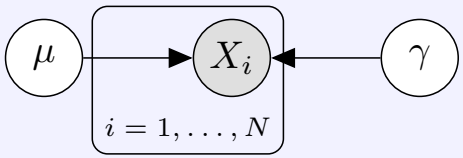
As we just realized, calculations of $\mathbb{E}_{q_{\neg j}}\left[\log p(\mathbf{z}, \mathbf{x})\right]$ and $\mathcal{L}(q)$ are quite tedious – and apparently must be done separately for each model we make.

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

Code Task: VB for the 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 $q(\mu, \gamma) = q(\mu) \cdot q(\tau)$ that best approximates $p(\mu, \tau \mid x_1, \ldots, x_N)$ wrt. the VB measure $\mathrm{KL}\,(q||p)$.

- Calculate the update rules for $q(\mu)$ and $q(\gamma)$.
  - Hint: $q(\mu)$ is Gaussian with mean ν^* and precision τ^*; $q(\gamma)$ is Gamma-distributed with parameters α^* and β^*.
- Implement the update rules you find in the notebook

  `students_simple_model.ipynb`

It may be useful to recall the definition of pdfs:

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

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, . . .

* Under certain regularity conditions. . .

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.

Definition – univariate exponential family model

Consider a univariate distribution $f_X(x \mid \boldsymbol{\theta})$, 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
- $\boldsymbol{\eta}(\boldsymbol{\theta})$: the natural parameters
- $\mathbf{t}(x)$: the sufficient statistics
- $A(\boldsymbol{\theta})$: the log partition function

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Members:

- Bernoulli (and Multinomial)

Example:

- $h(x) = 0$
- $\boldsymbol{\eta}(p) = \log(p/1-p)$
- $\mathbf{t}(x) = x$
- $A(p) = -\log(1-p)$

$$\begin{aligned} f_X(x \mid \boldsymbol{\theta}) &= \exp\left(h(x) + \boldsymbol{\eta}(\boldsymbol{\theta})^\mathsf{T}\mathbf{t}(x) - A(\boldsymbol{\theta})\right) \\ &= \exp\left\{\log\left[p/(1-p)\right] \cdot x + \log(1-p)\right\} \\ &= \left[p/(1-p)\right]^x \cdot (1-p) \\ &= p^x\,(1-p)^{1-x} \end{aligned}$$

The Bernoulli is in the exponential family

Definition – univariate exponential family model

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Members:

- Bernoulli (and Multinomial)
- Gaussians

Example:

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

$$\begin{aligned} f_X(x \mid \boldsymbol{\theta}) &= \exp\left\{\left[\tau\mu, -\frac{\tau}{2}\right]\begin{bmatrix} x \\ x^2 \end{bmatrix} \right. \\ &\qquad \left. -\frac{1}{2}\log(2\pi) - (\tau\mu^2/2 - \frac{1}{2}\log\tau)\right\} \\ &= \sqrt{\frac{\tau}{2\pi}} \cdot \exp\left(-\tau(x-\mu)^2/2\right) \end{aligned}$$

The Gaussian is in the exponential family

Definition – univariate exponential family model

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

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Members:

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

Example:

- $h(x) = 0$
- $\boldsymbol{\eta}(\alpha, \beta) = [-\beta, (\alpha - 1)]^\mathsf{T}$
- $\mathbf{t}(x) = [x, \log(x)]^\mathsf{T}$
- $A(\boldsymbol{\theta}) = \log(\Gamma(\alpha)) - \alpha \log(\beta)$

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

The Gamma is in the exponential family

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.

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

Define

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

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:

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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 $\boldsymbol{\eta}$ take the role of the parameters $\boldsymbol{\theta}$, and – for the model we consider – a one-to-one mapping between $\boldsymbol{\eta}$ and $\boldsymbol{\theta}$.

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

$$\boldsymbol{\theta} = [\boldsymbol{\mu}, \boldsymbol{\Sigma}]^{\mathsf{T}} = \left[-\frac{1}{2}\boldsymbol{\eta}_2^{-1}\boldsymbol{\eta}_1, -\frac{1}{2}\boldsymbol{\eta}_2^{-1}\right]^{\mathsf{T}}.$$

Given that $\boldsymbol{\theta}$ and $\boldsymbol{\eta}$ are interchangable, we will simplify notation, and use this form:

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

Some nice features

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:

$\nabla^k A(\boldsymbol{\eta})$ 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:

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

Some nice features

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:

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

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

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

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.