

# Nordic probabilistic AI school

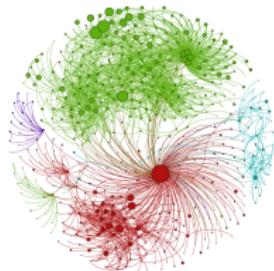
## Variational Inference and Optimization

Helge Langseth, Andrés Masegosa, and Thomas Dyhre Nielsen

June 13, 2023

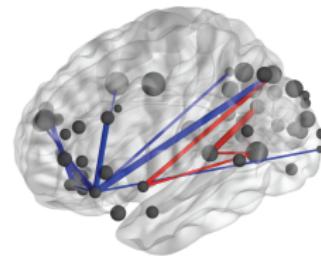
# Introduction

# Examples



Communities discovered in a 3.7M node network of U.S. Patents

[Gopalan and Blei, PNAS 2013]



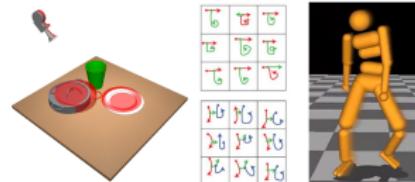
Neuroscience analysis of 220 million fMRI measurements

[Manning et al., PLOS ONE 2014]



Analysis of 1.7M taxi trajectories, in Stan

[Kucukelbir et al., 2016]

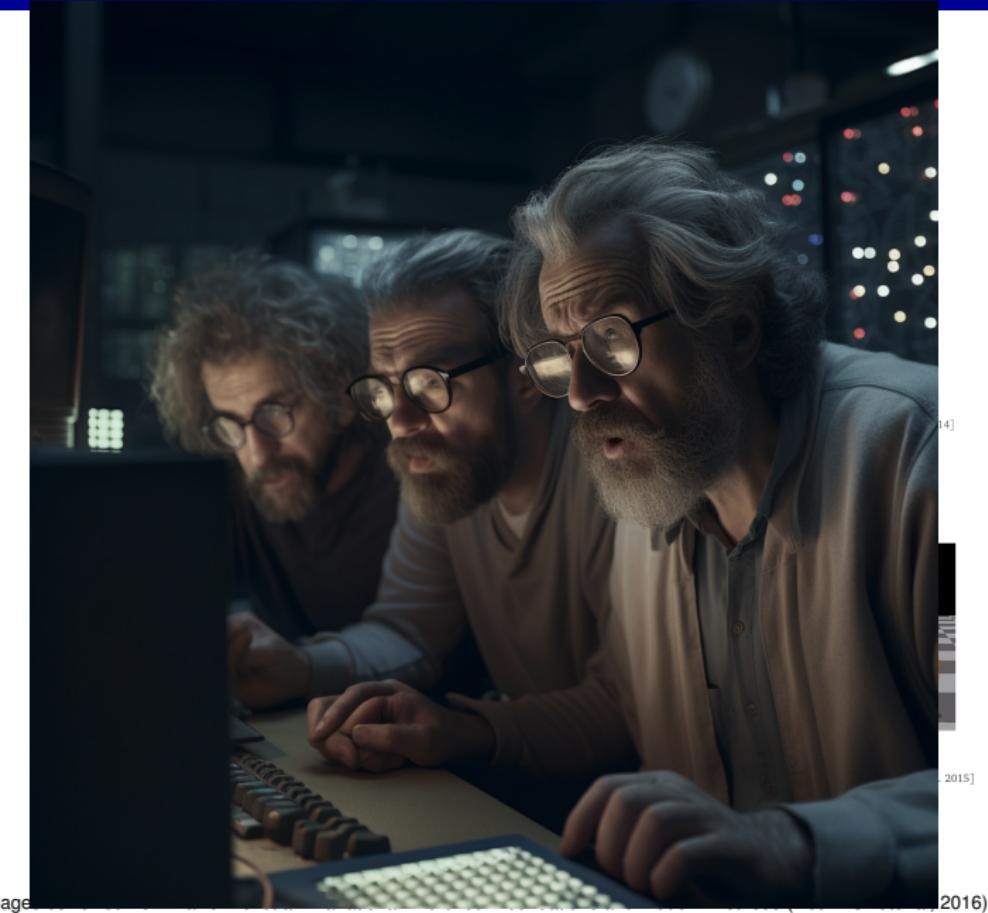


Scenes, concepts and control.

[Eslami et al., 2016, Lake et al. 2015]

Images borrowed from David Blei et al.: *Variational Inference: Foundations and Modern Methods* (NeurIPS Tutorial, 2016)

# Examples



Image

[14]

[2015]

(2016)

## Common challenges in many real-world projects:

- **Modelling:** Efficient representations, incorporate domain expert knowledge, ...
- **Data:** Missing data, erroneous data, low signal-to-noise ratio, ...
- **Scalability:** Large number of variables, large number of observations, ...
- **Robustness:** Statistical variations, concept drift, adversarial attacks, ...
- **Trustworthiness:** Uncertainty awareness, , ...
- **Regulations:** Transparency, bias, ...

## Our strategy: Probabilistic Machine Learning

- Build a **probabilistic model**.
- Apply **probabilistic inference algorithms**.

## Bayesian Machine Learning = Probabilistic model + Bayesian inference

- **Likelihood-part:** A probabilistic model typically defined by  $p(x | \theta)$ .
- **Prior:**  $p(\theta)$  reflects our *a priori* belief about the parameters  $\theta$ .

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Now we can calculate the posterior over  $\boldsymbol{\theta}$  given observations  $\mathcal{D} = \{\mathbf{x}_1, \dots, \mathbf{x}_N\}$ ,

$$p(\boldsymbol{\theta} | \mathcal{D}) = \frac{p(\boldsymbol{\theta}) p(\mathcal{D} | \boldsymbol{\theta})}{p(\mathcal{D})},$$

... and, e.g., the predictive distribution of a new observation  $\mathbf{x}'$ :

$$p(\mathbf{x}' | \mathcal{D}) = \int_{\boldsymbol{\theta}} p(\mathbf{x}' | \boldsymbol{\theta}) p(\boldsymbol{\theta} | \mathcal{D}) d\boldsymbol{\theta}.$$

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**Being Bayesian means maintaining a distribution over  $\boldsymbol{\theta}$ .**

Using a point-estimate for  $\boldsymbol{\theta}$  is **probabilistic** (but not **Bayesian**) ML.

## Example: Linear regression

A Bayesian linear regression with univariate explanatory variables:

**Likelihood –  $p(\mathcal{D} | \boldsymbol{\theta})$ :**  $p(y_i | \mathbf{w}, x_i, \sigma_y^2) = \mathcal{N}(w_0 + w_1 \cdot x_i, \sigma_y^2)$

**Note!** The observation noise,  $\sigma_y^2$  is known, so the parameter-set is simply  $\boldsymbol{\theta} = \{\mathbf{w}\}$ .

**Prior –  $p(\boldsymbol{\theta})$ :**  $p(\mathbf{w}) = \mathcal{N}(\mathbf{0}, \sigma_w^2)$

Bayesian Linear regression – Full model:

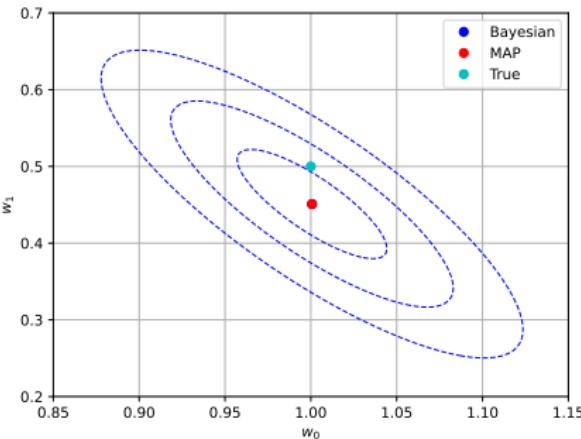
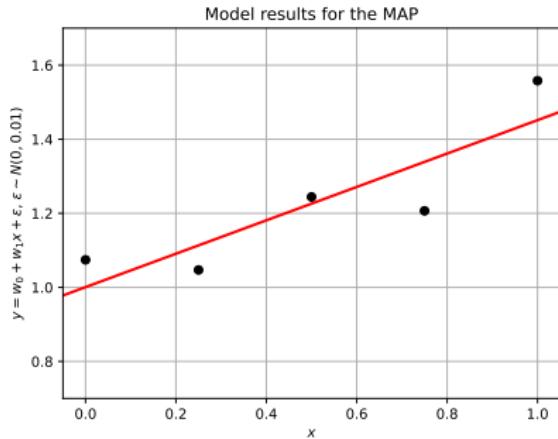
$$p(\mathcal{D}, \boldsymbol{\theta}) = p(\{y_i\}_{i=1}^n, \mathbf{w} | \{\mathbf{x}_i\}_{i=1}^n, \sigma_y^2, \sigma_w^2) = \overbrace{p(\mathbf{w} | \sigma_w^2)}^{p(\boldsymbol{\theta})} \overbrace{\prod_{i=1}^n p(y_i | \mathbf{w}, \mathbf{x}_i, \sigma_y^2)}^{p(\mathcal{D} | \boldsymbol{\theta})}$$

# Example: Linear regression – MAP vs (fully) Bayesian

## Bayes linear regression w/ some fake data:

- We have generated  $N = 5$  examples from  $y_i = 1.0 + 0.5 \cdot x_i + \epsilon_i$ ,  $\epsilon_i \sim \mathcal{N}(0, 0.1^2)$ .
- Weights unknown a priori, so here we use the vague priors  $w_j \sim \mathcal{N}(0, 100^2)$ .

## Results for the fully Bayesian model and the MAP:



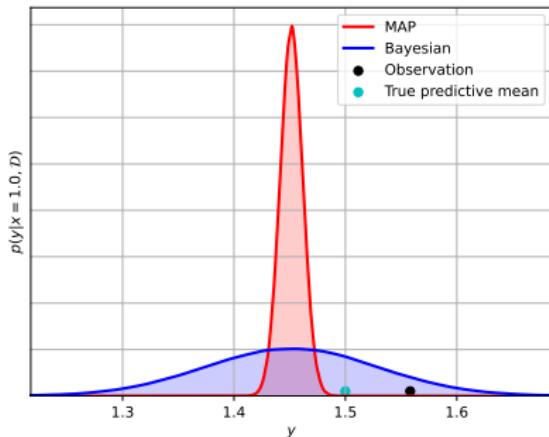
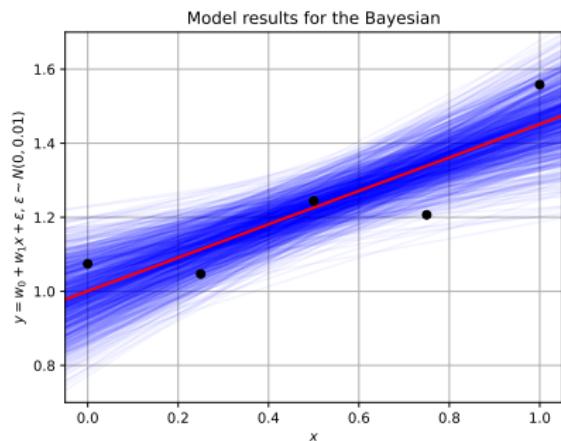
- **MAP:** Reasonable point estimate; No model uncertainty;
- **Bayes:** Model uncertainty around same MAP estimate;

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## Results for the fully Bayesian model and the MAP:



- **MAP:** Reasonable point estimate; No model uncertainty; Predictive uncertainty degenerated to observation noise: poor fit wrt. true value and observation.
- **Bayes:** Model uncertainty around same MAP estimate; Captures model uncertainty well; Predictive distribution reasonable.

**Bayesian inference** is in principle easy using Bayes' rule:

$$p(\boldsymbol{\theta} | \mathcal{D}) = \frac{p(\boldsymbol{\theta}) p(\mathcal{D} | \boldsymbol{\theta})}{p(\mathcal{D})} = \frac{p(\boldsymbol{\theta}) p(\mathcal{D} | \boldsymbol{\theta})}{\int_{\boldsymbol{\theta}} p(\boldsymbol{\theta}) p(\mathcal{D} | \boldsymbol{\theta}) d\boldsymbol{\theta}}$$

**Note!** This can only be solved analytically for **some simple models** (e.g., linear regression), but typically not for any of the really interesting models.

The big plan today: Use **optimization** to approximate  $p(\boldsymbol{\theta} | \mathcal{D})$

## What we want:

- Computationally efficient;
- Well-behaved objective;
- Easy integration with other frameworks.

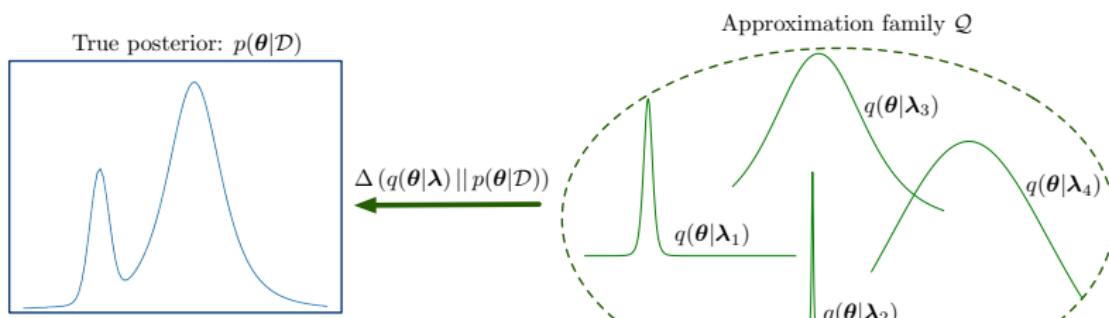
## What we don't want:

- No purely sampled-based techniques (like Gibbs sampling);
- No degenerate solutions (point estimators like MAP).

## Variational Bayes: Approximate inference by optimization

## Approximate inference through optimization – Main idea

**Variational Inference:** Approximate the true posterior distribution  $p(\theta | \mathcal{D})$  with a **variational distribution** from a tractable family of distributions  $\mathcal{Q}$ . The family is indexed by the parameters  $\lambda$ .



# Approximate inference through optimization

- **General goal:** Somehow approximate  $p(\theta | \mathcal{D})$  with a  $q(\theta | \mathcal{D})$ .
- **Note!** We use  $q(\theta)$  as a short-hand for  $q(\theta | \mathcal{D})$ .

Formalization of approximate inference through optimization:

Given a family of tractable distributions  $\mathcal{Q}$  and a distance measure between distributions  $\Delta$ , choose

$$\hat{q}(\theta) = \arg \min_{q \in \mathcal{Q}} \Delta(q(\theta) || p(\theta | \mathcal{D})).$$

Decisions to be made:

- ➊ How to define  $\Delta(\cdot || \cdot)$  so that we end up with a high-quality solution?
  - How to work with  $\Delta(q(\theta) || p(\theta | \mathcal{D}))$  when we don't know what  $p(\theta | \mathcal{D})$  is?
- ➋ How to define a family of distributions  $\mathcal{Q}$  that is both flexible enough to generate good approximations and restrictive enough to support efficient calculations?

## Desiderata

To use  $\Delta$  to measure the distance from an object  $f$  to an object  $g$  it would be relevant to require that  $\Delta$  has the following properties:

**Positivity:**  $\Delta(f \parallel g) \geq 0$  and  $\Delta(f \parallel g) = 0$  if and only if  $f = g$ .

**Symmetry:**  $\Delta(f \parallel g) = \Delta(g \parallel f)$

**Triangle:** For objects  $f$ ,  $g$ , and  $h$  we have that  $\Delta(f \parallel g) \leq \Delta(f \parallel h) + \Delta(h \parallel g)$ .

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Standard choice when working with probability distributions

The **Kullback-Leibler divergence** is the standard distance measure:

$$\text{KL}(f \parallel g) = \int_{\boldsymbol{\theta}} f(\boldsymbol{\theta}) \log \left( \frac{f(\boldsymbol{\theta})}{g(\boldsymbol{\theta})} \right) d\boldsymbol{\theta} = \mathbb{E}_{\boldsymbol{\theta} \sim f} \left[ \log \left( \frac{f(\boldsymbol{\theta})}{g(\boldsymbol{\theta})} \right) \right].$$

Notice that while  $\text{KL}(f \parallel g)$  obeys the positivity criterion, it satisfies neither symmetry nor the triangle inequality. It is thus **not a proper distance measure**.

## Information-projection

- Minimizes  $\text{KL}(q||p) = -\mathbb{E}_{\theta \sim q}[\log p(\theta)] - \mathcal{H}_q$ .
- Preference given to  $q$  that has:
  - High  $q$ -probability allocated to  $p$ -probable regions.
  - Small  $q$  in any region where  $p$  is small.  
“ $p(\theta) \approx 0 \implies q(\theta) \approx 0$ ”.
  - High entropy ( $\sim$  variance)

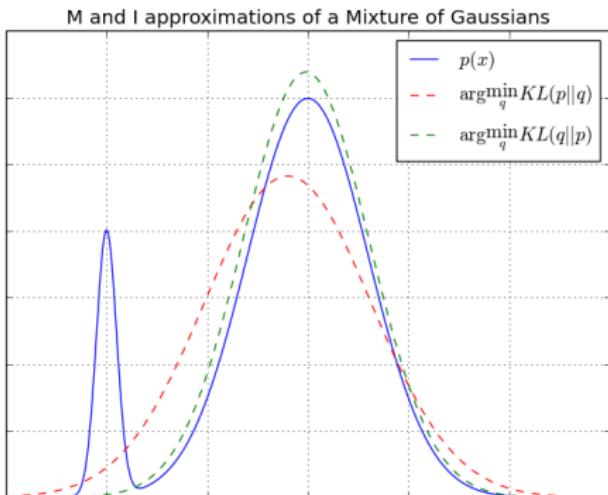
## Moment-projection

- Minimizes  $\text{KL}(p||q) = -\mathbb{E}_{\theta \sim p}[\log q(\theta)] - \mathcal{H}_p$ .
- Preference given to  $q$  that has:
  - High  $q$ -probability allocated to  $p$ -probable regions.
  - $q(\theta) > 0$  in any region where  $p$  is non-negligible.  
“ $p(\theta) > 0 \implies q(\theta) > 0$ ”
  - No explicit focus of entropy

## Cheat-sheet:

- KL-divergence:**  $\text{KL}(f||g) = \mathbb{E}_f \left[ \log \left( \frac{f(\theta)}{g(\theta)} \right) \right] = -\mathbb{E}_f [\log(g(\theta))] - \mathcal{H}_f$ .
- Entropy:**  $\mathcal{H}_f = -\int_{\theta} f(\theta) \log(f(\theta)) d\theta = -\mathbb{E}_f [\log(f(\theta))]$ .
- Intuition:** Cheat a bit (measure-zero, limit-zero-rates, etc.) and think  
“If  $g(\theta_0) \approx 0$ , then  $-\mathbb{E}_{\theta \sim f}[\log g(\theta)]$  becomes ‘huge’ unless  $f(\theta_0) \approx 0$ ”  
because  $\lim_{x \rightarrow 0^+} \log(x)$  diverges, while  $\lim_{x \rightarrow 0^+} x \cdot \log(x) = 0$ .

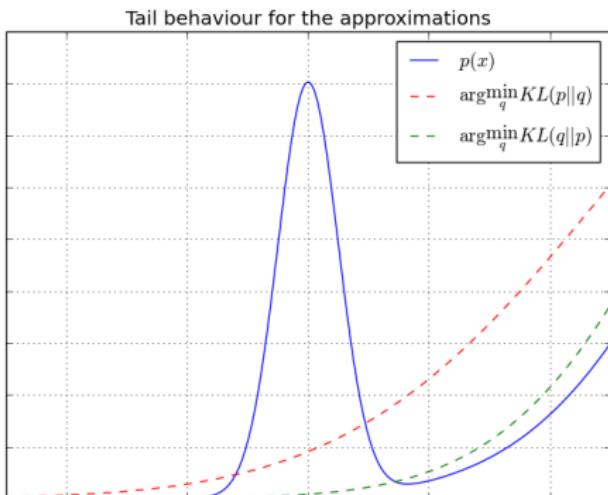
# Moment and Information projection – main difference



## Example: Approximating a Mix-of-Gaussians by a single Gaussian

- Moment projection – optimizing  $KL(p||q)$  – has slightly larger variance.
- Similar mean values, but Information projection – optimizing  $KL(q||p)$  – focuses mainly on the most prominent mode.

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## Example: Approximating a Mix-of-Gaussians by a single Gaussian

- Moment projection – optimizing  $KL(p||q)$  – has slightly larger variance.
- Similar mean values, but Information projection – optimizing  $KL(q||p)$  – focuses mainly on the most prominent mode.
- M-projection is **zero-avoiding**, while I-projection is **zero-forcing**.

VB uses information projections:

Variational Bayes relies on **information projections**, i.e., approximates  $p(\boldsymbol{\theta} \mid \mathcal{D})$  by

$$\hat{q}(\boldsymbol{\theta}) = \arg \min_{q \in \mathcal{Q}} \text{KL}(q(\boldsymbol{\theta}) \mid\mid p(\boldsymbol{\theta} \mid \mathcal{D}))$$

- **Positives:**

- Clever interpretation when used for Bayesian machine learning.
  - We will end up with an objective that lower-bounds the marginal log likelihood,  $\log p(\mathcal{D})$ .
- Very efficient when combined with cleverly chosen  $\mathcal{Q}$ .

- **Negatives:**

- May result in *zero-forcing* behaviour.
  - Typical choice of  $\mathcal{Q}$  can make this issue even more prominent.

## ELBO: Evidence Lower-BOund

Notice how we can rearrange the KL divergence as follows:

$$\text{KL}(q(\boldsymbol{\theta}) || p(\boldsymbol{\theta} | \mathcal{D})) = \mathbb{E}_{\boldsymbol{\theta} \sim q} \left[ \log \frac{q(\boldsymbol{\theta})}{p(\boldsymbol{\theta} | \mathcal{D})} \right]$$

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Evidence Lower Bound (ELBO):  $\mathcal{L}(q) = -\mathbb{E}_{\boldsymbol{\theta} \sim q} \left[ \log \frac{q(\boldsymbol{\theta})}{p(\boldsymbol{\theta}, \mathcal{D})} \right] = \mathbb{E}_{\boldsymbol{\theta} \sim q} \left[ \log \frac{p(\boldsymbol{\theta}, \mathcal{D})}{q(\boldsymbol{\theta})} \right].$

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**VB focuses on ELBO:**

$$\log p(\mathcal{D}) = \mathcal{L}(q) + \text{KL}(q(\boldsymbol{\theta})||p(\boldsymbol{\theta}|\mathcal{D}))$$

Since  $\log p(\mathcal{D})$  is constant wrt. the distribution  $q$  it follows:

- We can minimize  $\text{KL}(q(\boldsymbol{\theta})||p(\boldsymbol{\theta}|\mathcal{D}))$  by maximizing  $\mathcal{L}(q)$
- This is **computationally simpler** because it uses  $p(\boldsymbol{\theta}, \mathcal{D})$  and not  $p(\boldsymbol{\theta}|\mathcal{D})$ .
- $\mathcal{L}(q)$  is a **lower bound** of  $\log p(\mathcal{D})$  because  $\text{KL}(q(\boldsymbol{\theta})||p(\boldsymbol{\theta}|\mathcal{D})) \geq 0$ .

↔ Look for  $\hat{q}(\boldsymbol{\theta}) = \arg \max_{q \in \mathcal{Q}} \mathcal{L}(q)$ .

# ELBO: Evidence Lower-Bound

Notice how we can rearrange the KL divergence as follows:

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## Summary:

- We started out looking for  $\arg \min_{q \in \mathcal{Q}} \text{KL}(q(\boldsymbol{\theta})||p(\boldsymbol{\theta}|\mathcal{D}))$ .
- Didn't know how to calculate  $\text{KL}(q(\boldsymbol{\theta})||p(\boldsymbol{\theta}|\mathcal{D}))$  because  $p(\boldsymbol{\theta}|\mathcal{D})$  is unknown.
- Still, we can find the optimal approximation by maximizing  $\mathcal{L}(q)$ :

$$\arg \max_{q \in \mathcal{Q}} \mathcal{L}(q) = \arg \min_{q \in \mathcal{Q}} \text{KL}(q(\boldsymbol{\theta})||p(\boldsymbol{\theta}|\mathcal{D})).$$

- It all makes sense: We aim to maximize  $\mathcal{L}(q)$ , which is a lower-bound of  $\log p(\mathcal{D})$ .

## Variational Bayes w/ Mean Field

# The mean field assumption

What we have ...

We now have the first building-block of the approximation:

$$\Delta(q \parallel p) = \text{KL}(q(\boldsymbol{\theta}) \parallel p(\boldsymbol{\theta} \mid \mathcal{D})) ,$$

and avoided the issue with  $p(\boldsymbol{\theta} \mid \mathcal{D})$  by focusing on  $\mathcal{L}(q)$ .

We still need the set  $\mathcal{Q}$ :

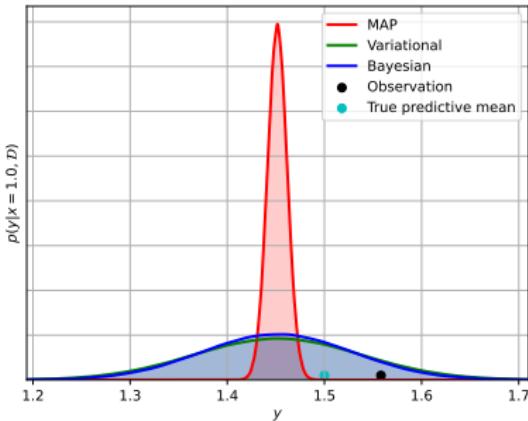
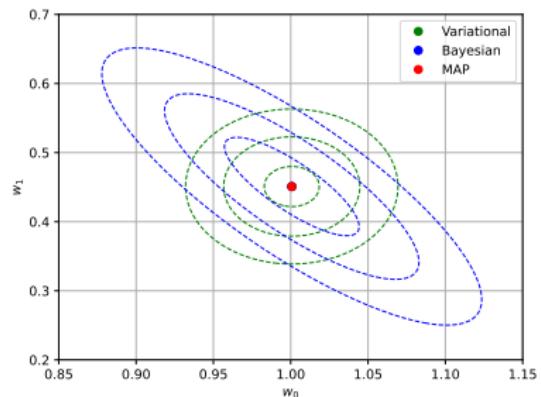
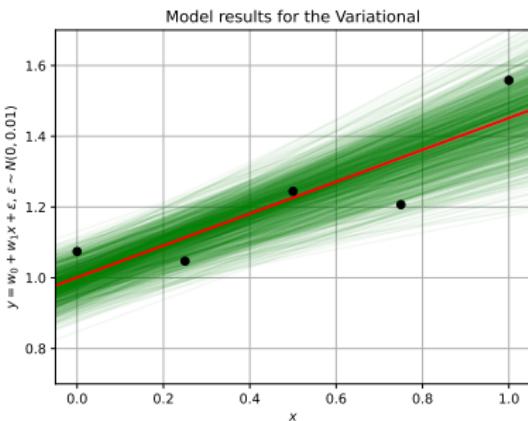
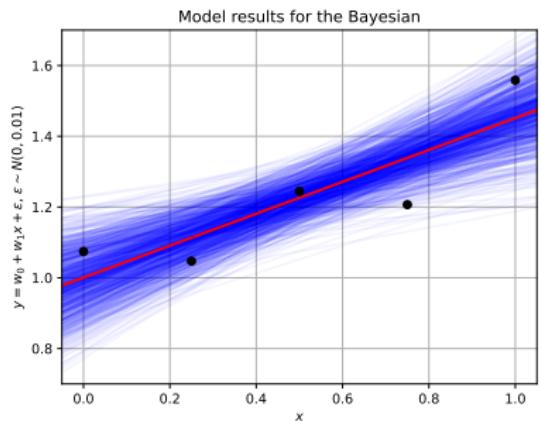
Very often you will see the **mean field assumption**, which states that  $\mathcal{Q}$  consists of distributions that **factorize** according to the equation

$$q(\boldsymbol{\theta}) = \prod_i q_i(\theta_i) .$$

This may seem like a very restricted set, but you'll get to see some tricks later ...

# VB-MF example – “sanity check”

**Bayes linear regression** with likelihood  $y_i \mid \{w_0, w_1, x_i, \sigma_y^2\} = \mathcal{N}(w_0 + w_1 x_i, \sigma_y^2)$ .



## Setup:

- We have observed  $\mathcal{D}$ , and can calculate the full joint  $p(\boldsymbol{\theta}, \mathcal{D}) = p(\boldsymbol{\theta}) \cdot p(\mathcal{D} | \boldsymbol{\theta})$ .
- We use the ELBO as our objective, and assume  $q(\boldsymbol{\theta})$  factorizes.
- We posit a *variational family* of distributions  $q_j(\cdot | \boldsymbol{\lambda}_j)$ , i.e., we choose the distributional form, while wanting to optimize the parameterization  $\boldsymbol{\lambda}_j$ .

## Algorithm:

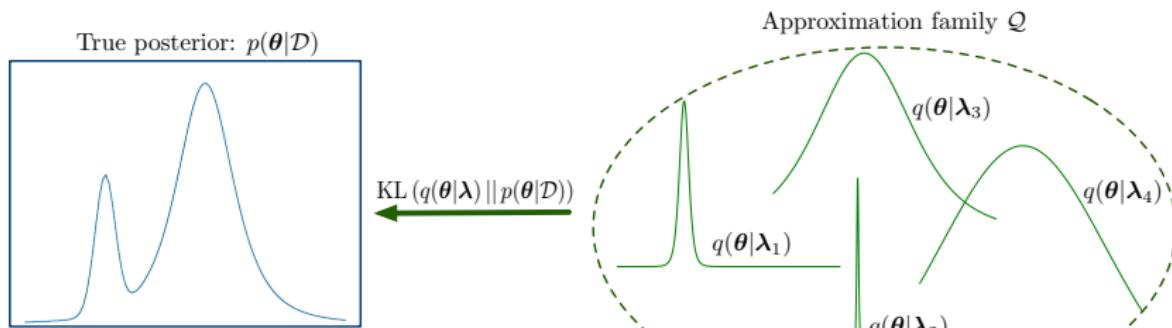
Repeat until negligible improvement in terms of  $\mathcal{L}(q)$ :

- ① For each  $j$ :
  - Somehow choose  $\boldsymbol{\lambda}_j$  to maximize  $\mathcal{L}(q)$ , based on  $\mathcal{D}$  and  $\{\boldsymbol{\lambda}_i\}_{i \neq j}$ .
- ② Calculate the new  $\mathcal{L}(q)$ .

## Solving the VB optimization

## Recap: What is variational inference?

**VI:** Approximate the true posterior distribution  $p(\theta | \mathcal{D})$  with a **variational distribution** from a tractable family of distributions  $\mathcal{Q}$ . The family is indexed by the parameters  $\lambda$ .



Our computational challenge:

Fit the variational parameters  $\hat{\lambda}$  so that the “distance”  $\text{KL}(q(\theta | \lambda) || p(\theta | \mathcal{D}))$  is minimized:

$$q(\theta | \hat{\lambda}) = \arg \min_{q \in \mathcal{Q}} \text{KL}(q(\theta) || p(\theta | \mathcal{D})) = \arg \max_{\lambda} \mathcal{L}(q(\theta | \lambda))$$

## Solving the VB equation one $\theta_j$ at the time

We will maximize  $\mathcal{L}(q) = \mathbb{E}_q \left[ \log \frac{p(\boldsymbol{\theta}, \mathcal{D})}{q(\boldsymbol{\theta})} \right]$  under the assumption that  $q(\cdot)$  factorizes.

Let us pick one  $j$ , utilize that  $q(\boldsymbol{\theta}) = q_j(\theta_j) \cdot q_{\neg j}(\boldsymbol{\theta}_{\neg j})$  under MF, and keep  $q_{\neg j}(\cdot)$  fixed.

$$\begin{aligned}\mathcal{L}(q) &= \mathbb{E}_q [\log p(\boldsymbol{\theta}, \mathcal{D})] - \mathbb{E}_q [\log q(\boldsymbol{\theta})] \\ &= \mathbb{E}_{q_j} \mathbb{E}_{q_{\neg j}} [\log p(\boldsymbol{\theta}, \mathcal{D})] - \mathbb{E}_{q_j} \mathbb{E}_{q_{\neg j}} [\log q(\boldsymbol{\theta})]\end{aligned}$$

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### Notation-trick:

For the term  $\mathbb{E}_{q_{\neg j}} [\log p(\boldsymbol{\theta}, \mathcal{D})]$  we simply define  $\tilde{f}_j(\theta_j)$  so that

$$\log \tilde{f}_j(\theta_j) := \mathbb{E}_{q_{\neg j}} [\log p(\boldsymbol{\theta}, \mathcal{D})].$$

## Solving the VB equation one $\theta_j$ at the time

We will maximize  $\mathcal{L}(q) = \mathbb{E}_q \left[ \log \frac{p(\boldsymbol{\theta}, \mathcal{D})}{q(\boldsymbol{\theta})} \right]$  under the assumption that  $q(\cdot)$  factorizes.

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$$\log \tilde{f}_j(\theta_j) := \mathbb{E}_{q_{\neg j}} [\log p(\boldsymbol{\theta}, \mathcal{D})].$$

We next define the *normalized version* by  $f_j(\theta_j) := \frac{\tilde{f}_j(\theta_j)}{\int_{\boldsymbol{\theta}} \tilde{f}_j(\theta_j) d\boldsymbol{\theta}}$ .

In all, this means that

$$\mathbb{E}_{q_{\neg j}} [\log p(\boldsymbol{\theta}, \mathcal{D})] = \log f_j(\theta_j) + c_1$$

## Solving the VB equation one $\theta_j$ at the time

We will maximize  $\mathcal{L}(q) = \mathbb{E}_q \left[ \log \frac{p(\boldsymbol{\theta}, \mathcal{D})}{q(\boldsymbol{\theta})} \right]$  under the assumption that  $q(\cdot)$  factorizes.

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## Solving the VB equation one $\theta_j$ at the time

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### Simplification:

Notice that  $\log q(\boldsymbol{\theta}) = \log q_j(\theta_j) + \log q_{\neg j}(\boldsymbol{\theta}_{\neg j})$  (under MF). Therefore

$$\begin{aligned}\boxed{\mathbb{E}_{q_j} \mathbb{E}_{q_{\neg j}} [\log q(\boldsymbol{\theta})]} &= \mathbb{E}_{q_j} \mathbb{E}_{q_{\neg j}} [\log q_j(\theta_j) + \log q_{\neg j}(\boldsymbol{\theta}_{\neg j})] \\ &= \mathbb{E}_{q_j} \mathbb{E}_{q_{\neg j}} [\log q_j(\theta_j)] + \mathbb{E}_{q_j} \mathbb{E}_{q_{\neg j}} [\log q_{\neg j}(\boldsymbol{\theta}_{\neg j})] \\ &= \mathbb{E}_{q_j} [\log q_j(\theta_j)] + \mathbb{E}_{q_{\neg j}} [\log q_{\neg j}(\boldsymbol{\theta}_{\neg j})] \\ &= \boxed{\mathbb{E}_{q_j} [\log q_j(\theta_j)] + c_2},\end{aligned}$$

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

## Solving the VB equation one $\theta_j$ at the time

We will maximize  $\mathcal{L}(q) = \mathbb{E}_q \left[ \log \frac{p(\boldsymbol{\theta}, \mathcal{D})}{q(\boldsymbol{\theta})} \right]$  under the assumption that  $q(\cdot)$  factorizes.

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## Solving the VB equation one $\theta_j$ at the time

We will maximize  $\mathcal{L}(q) = \mathbb{E}_q \left[ \log \frac{p(\boldsymbol{\theta}, \mathcal{D})}{q(\boldsymbol{\theta})} \right]$  under the assumption that  $q(\cdot)$  factorizes.

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### Almost there:

Recall that  $f_j(\theta_j)$  integrates to 1, and is per definition non-negative.

We can therefore regard it as a density function for  $\theta_j$ , and get

$$\begin{aligned}\mathbb{E}_{q_j} \log f_j(\theta_j) - \mathbb{E}_{q_j} [\log q_j(\theta_j)] &= -\mathbb{E}_{q_j} [\log q_j(\theta_j) - \log f_j(\theta_j)] \\ &= -\text{KL}(q_j(\theta_j) || f_j(\theta_j))\end{aligned}$$

## Solving the VB equation one $\theta_j$ at the time

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## Solving the VB equation one $\theta_j$ at the time

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**We get the following result:**

The ELBO is maximized wrt.  $q_j$  by choosing it equal to  $f_j(\theta_j)$ :

$$q_j(\theta_j) = \frac{1}{Z} \exp (\mathbb{E}_{q_{\neg j}} [\log p(\boldsymbol{\theta}, \mathcal{D})])$$

**... and to get there we had to make the following assumptions:**

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

## Setup

- We have observed  $\mathcal{D}$ , and can calculate the full joint  $p(\boldsymbol{\theta}, \mathcal{D})$ .
- We use the ELBO as our objective, and assume  $q(\boldsymbol{\theta})$  factorizes.
- We posit a *variational family* of distributions  $q_j(\theta_j | \boldsymbol{\lambda}_j)$ , i.e., we choose the distributional form, while wanting to optimize the parameterization  $\boldsymbol{\lambda}_j$ .

## The CAVI algorithm

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

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

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  - Calculate  $\mathbb{E}_{q_{\neg j}} [\log p(\boldsymbol{\theta}, \mathcal{D})]$  using current estimates for  $q_i(\cdot | \boldsymbol{\lambda}_i)$ ,  $i \neq j$ .
  - Choose  $\boldsymbol{\lambda}_j$  so that  $q_j(\theta_j | \boldsymbol{\lambda}_j) \propto \exp (\mathbb{E}_{q_{\neg j}} [\log p(\boldsymbol{\theta}, \mathcal{D})])$ .
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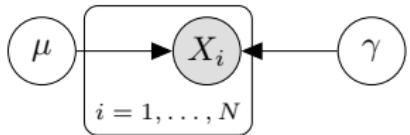
The procedure gives us the  $q(\boldsymbol{\theta} | \boldsymbol{\lambda}) \in \mathcal{Q}$  that is closest to  $p(\boldsymbol{\theta} | \mathcal{D})$ , even though we **do not know** what  $p(\boldsymbol{\theta} | \mathcal{D})$  is. Quite remarkable!

## Setup

- We have observed  $\mathcal{D}$ , and can calculate the full joint  $p(\boldsymbol{\theta}, \mathcal{D})$ .
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## A simple Gaussian model

## A Gaussian model with unknown mean and precision

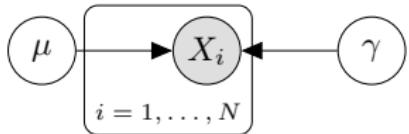


- $X_i | \{\mu, \gamma\} \sim \mathcal{N}(\mu, 1/\gamma)$
- $\mu \sim \mathcal{N}(0, \tau^{-1})$
- $\gamma \sim \text{Gamma}(\alpha, \beta)$

## The probability model

$$p(\mathcal{D}, \overbrace{\mu, \gamma}^{\theta} | \tau, \alpha, \beta) = \prod_{i=1}^N p(x_i | \mu, \gamma^{-1}) p(\mu | 0, \tau^{-1}) p(\gamma | \alpha, \beta)$$

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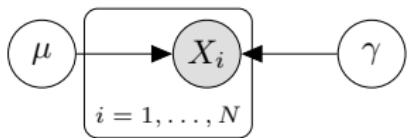
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... after taking the log

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

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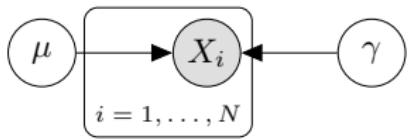
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## The variational model (full mean field)

$$q(\mu, \gamma) = q(\mu)q(\gamma), \quad \min_q \text{KL}(q(\mu)q(\gamma) || p(\mu, \gamma | \mathcal{D}))$$

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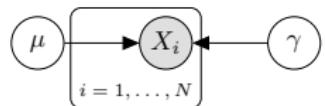
$$q(\mu, \gamma) = q(\mu)q(\gamma), \quad \min_q \text{KL}(q(\mu)q(\gamma) || p(\mu, \gamma | \mathcal{D}))$$

where

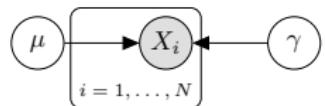
- $q(\mu) = \mathcal{N}(\nu_q, \tau_q^{-1})$
- $q(\gamma) = \text{Gamma}(\alpha_q, \beta_q)$

We choose the variational distribution so that

$$\log q(\mu | \nu_q, \tau_q^{-1}) = \mathbb{E}_{q_\gamma} [\log p(\mathcal{D}, \mu, \gamma)] + c =$$



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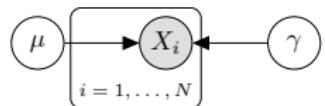


$$\log q(\mu | \nu_q, \tau_q^{-1}) = \mathbb{E}_{q_\gamma} [\log p(\mathcal{D}, \mu, \gamma)] + c =$$

Recall the normal distribution

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

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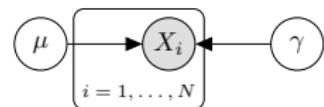


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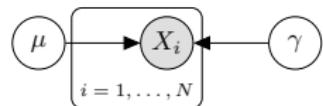


$$\begin{aligned}\log q(\mu | \nu_q, \tau_q^{-1}) &= \mathbb{E}_{q_\gamma} [\log p(\mathcal{D}, \mu, \gamma)] + c = \\ &= -\frac{1}{2} (\mathbb{E}_{q_\gamma} [\gamma] \cdot N + \tau) \mu^2 + \left( \mathbb{E}_{q_\gamma} [\gamma] \sum_{i=1}^N x_i \right) \mu + c\end{aligned}$$

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

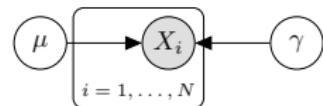
- precision  $\tau_q \leftarrow \mathbb{E}_{q_\gamma} [\gamma] \cdot N + \tau$
- mean  $\nu_q \leftarrow \tau_q^{-1} \left( \mathbb{E}_{q_\gamma} [\gamma] \sum_{i=1}^N x_i \right)$

Recall the normal distribution

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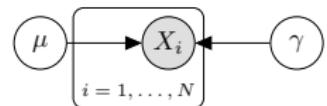
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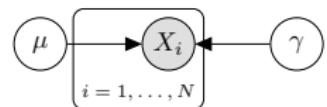


## Recall

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

We choose the variational distribution so that

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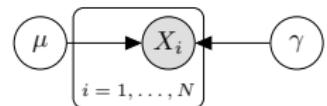


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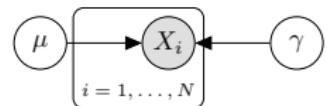


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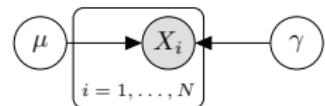
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$$\log p(\mu) = \mathcal{N}(0, \tau^{-1}) = -\frac{1}{2} \log(2\pi) + \frac{1}{2} \log(\tau) - \frac{\tau}{2} (\mu)^2$$

We choose the variational distribution so that

$$\log q(\mu) = \mathbb{E}_{q_\gamma} [\log p(\mathcal{D}, \mu, \gamma)] + c = \sum_{i=1}^N \mathbb{E}_{q_\gamma} [\log p(x_i | \mu, \gamma^{-1})] + \log p(\mu) + c$$



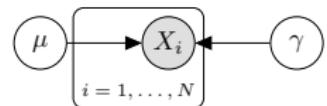
Recall

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

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We choose the variational distribution so that

$$\begin{aligned}\log q(\mu) &= \mathbb{E}_{q_\gamma} [\log p(\mathcal{D}, \mu, \gamma)] + c = \sum_{i=1}^N \mathbb{E}_{q_\gamma} [\log p(x_i | \mu, \gamma^{-1})] + \log p(\mu) + c \\ &= \sum_{i=1}^N \mathbb{E}_{q_\gamma} \left[ -\frac{\gamma}{2} (x_i - \mu)^2 \right] - \frac{\tau}{2} (\mu)^2 + c\end{aligned}$$

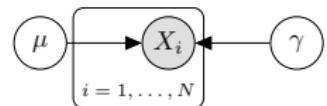


Recall

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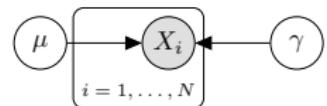
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$$\begin{aligned}
 \log q(\mu) &= \mathbb{E}_{q_\gamma} [\log p(\mathcal{D}, \mu, \gamma)] + c = \sum_{i=1}^N \mathbb{E}_{q_\gamma} [\log p(x_i | \mu, \gamma^{-1})] + \log p(\mu) + c \\
 &= \sum_{i=1}^N \mathbb{E}_{q_\gamma} \left[ -\frac{\gamma}{2} (x_i - \mu)^2 \right] - \frac{\tau}{2} (\mu)^2 + c \\
 &= -\frac{1}{2} \mathbb{E}_{q_\gamma} [\gamma] \left( \sum_{i=1}^N x_i^2 + N \cdot \mu^2 - 2\mu \sum_{i=1}^N x_i \right) - \frac{\tau}{2} (\mu)^2 + c
 \end{aligned}$$

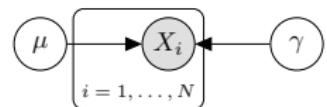
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 &= -\frac{1}{2} (\mathbb{E}_{q_\gamma} [\gamma] \cdot N + \tau) \mu^2 + \left( \mathbb{E}_{q_\gamma} [\gamma] \sum_{i=1}^N x_i \right) \mu + c
 \end{aligned}$$

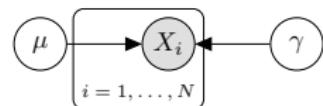
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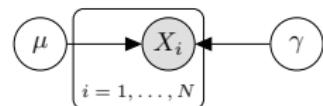
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Recall the normal distribution

$$\begin{aligned}\log q(\mu | \nu_q, \tau_q^{-1}) &= -\frac{1}{2} \log(2\pi) + \frac{1}{2} \log(\tau_q) - \frac{\tau_q}{2} (\mu - \nu_q)^2 \\ &= -\frac{1}{2} \tau_q \mu^2 + \tau_q \nu_q \mu + c\end{aligned}$$

We choose the variational distribution so that



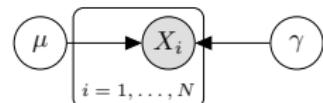
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We choose the variational distribution so that

$$\begin{aligned}\log q(\mu) &= \mathbb{E}_{q_\gamma} [\log p(\mathcal{D}, \mu, \gamma)] + c = \sum_{i=1}^N \mathbb{E}_{q_\gamma} [\log p(x_i | \mu, \gamma^{-1})] + \log p(\mu) + c \\ &= -\frac{1}{2} (\mathbb{E}_{q_\gamma} [\gamma] \cdot N + \tau) \mu^2 + \left( \mathbb{E}_{q_\gamma} [\gamma] \sum_{i=1}^N x_i \right) \mu + c\end{aligned}$$



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

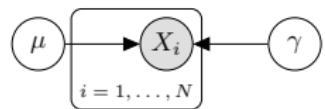
- precision  $\tau_q \leftarrow \mathbb{E}_{q_\gamma} [\gamma] \cdot N + \tau$
- mean  $\nu_q \leftarrow \tau_q^{-1} \left( \mathbb{E}_{q_\gamma} [\gamma] \sum_{i=1}^N x_i \right)$

Recall the normal distribution

$$\begin{aligned}\log q(\mu | \nu_q, \tau_q^{-1}) &= -\frac{1}{2} \log(2\pi) + \frac{1}{2} \log(\tau_q) - \frac{\tau_q}{2} (\mu - \nu_q)^2 \\ &= -\frac{1}{2} \tau_q \mu^2 + \tau_q \nu_q \mu + c\end{aligned}$$

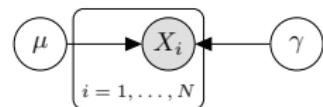
We choose the variational distribution so that

$$\log q(\gamma) = \mathbb{E}_{q_\mu} [\log p(\mathbf{x}, \mu, \gamma)] + c$$



We choose the variational distribution so that

$$\log q(\gamma) = \mathbb{E}_{q_\mu} [\log p(\mathbf{x}, \mu, \gamma)] + c$$



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

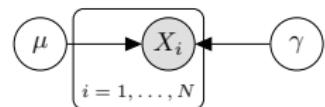
- $\alpha_q \leftarrow \frac{N}{2} + \alpha$
- $\beta_q \leftarrow \beta + \frac{1}{2} \sum_{i=1}^N \mathbb{E}_{q_\mu} [(x_i - \mu)^2]$

Note that:

- $\mathbb{E}_{q_\mu} [(x_i - \mu)^2] = x_i^2 + \mathbb{E}_{q_\mu} [\mu^2] - 2 \cdot x_i \cdot \mathbb{E}_{q_\mu} [\mu]$
- $\mathbb{E}_{q_\mu} [\mu^2] = \text{Var}(\mu) + \mathbb{E}_{q_\mu} [\mu]^2$

We choose the variational distribution so that

$$\log q(\gamma) = \mathbb{E}_{q_\mu} [\log p(\mathbf{x}, \mu, \gamma)] + c$$



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

- $\alpha_q \leftarrow \frac{N}{2} + \alpha$
- $\beta_q \leftarrow \beta + \frac{1}{2} \sum_{i=1}^N \mathbb{E}_{q_\mu} [(x_i - \mu)^2]$

Note that:

- $\mathbb{E}_{q_\mu} [(x_i - \mu)^2] = x_i^2 + \mathbb{E}_{q_\mu} [\mu^2] - 2 \cdot x_i \cdot \mathbb{E}_{q_\mu} [\mu]$
- $\mathbb{E}_{q_\mu} [\mu^2] = \text{Var}(\mu) + \mathbb{E}_{q_\mu} [\mu]^2$

Recall

$$\log q(\gamma | \alpha_q, \beta_q) = \alpha_q \cdot \log(\beta_q) + (\alpha_q - 1) \log(\gamma) - \beta_q \cdot \gamma - \log(\Gamma(\alpha_q))$$

# Monitoring the ELBO

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

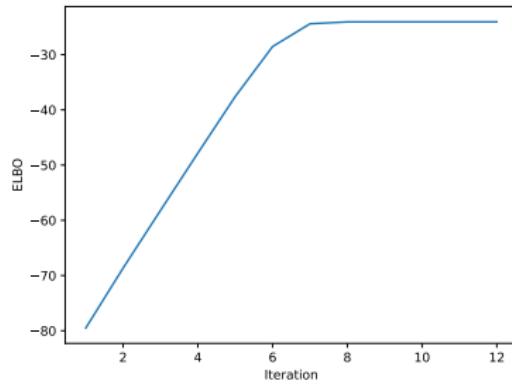
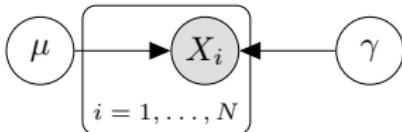
$$\mathcal{L}(q) = \mathbb{E}_q \log p(\mathbf{x}, \mu, \gamma | \tau, \alpha, \beta) - \mathbb{E}_q \log q(\mu, \gamma)$$

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

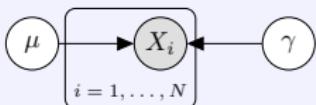
at any updating step. With some pencil pushing we arrive at a somewhat complicated but closed form expression (not shown here).

**Monitoring the ELBO** can be useful for

- Assessing convergence
- Doing debugging
- ...



## Code Task: VB for a simple Gaussian model

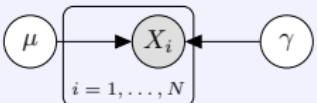


- $X_i | \{\mu, \gamma\} \sim \mathcal{N}(\mu, 1/\gamma)$
- $\mu \sim \mathcal{N}(0, \tau)$
- $\gamma \sim \text{Gamma}(\alpha, \beta)$

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

- Go though the notebook  
`students_simple_model.ipynb`  
and try to link the code to the derivations in the slides.
- Implement the update rules for  $q(\mu)$  and  $q(\gamma)$  (from the slides) in the notebook.
- Experiment with the model and the data set; try changing the prior and the data generating process.

### Code Task: VB for a simple Gaussian model



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

**Variational Updating Equation** for  $q(\mu) = \mathcal{N}(\nu_q, \tau_q^{-1})$

- precision  $\tau_q \leftarrow \mathbb{E}_{q_\gamma}[\gamma] \cdot N + \tau$
- mean  $\nu_q \leftarrow \tau_q^{-1} \left( \mathbb{E}_{q_\gamma}[\gamma] \sum_{i=1}^N x_i \right)$

**Variational Updating Equation** for  $q(\gamma) = \text{Gamma}(\alpha_q, \beta_q)$

- $\alpha_q \leftarrow \frac{N}{2} + \alpha$
- $\beta_q \leftarrow \beta + \frac{1}{2} \sum_{i=1}^N \mathbb{E}_{q_\mu}[(x_i - \mu)^2]$

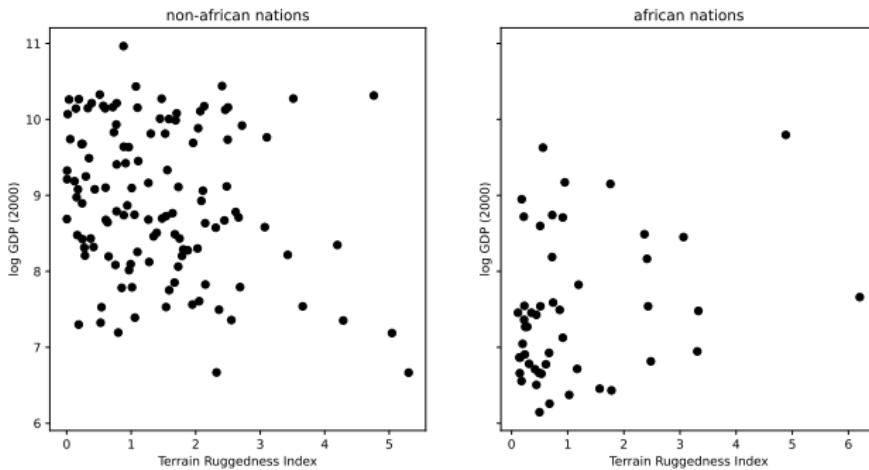
Note that:

- $\mathbb{E}_{q_\mu}[(x_i - \mu)^2] = x_i^2 + \mathbb{E}_{q_\mu}[\mu^2] - 2 \cdot x_i \cdot \mathbb{E}_{q_\mu}[\mu]$
- $\mathbb{E}_{q_\mu}[\mu^2] = \text{Var}(\mu) + \mathbb{E}_{q_\mu}[\mu]^2$
- $\mathbb{E}_{q_\gamma}[\gamma] = \frac{\alpha_q}{\beta_q}$

## Bayesian linear regression

# Real Data Example

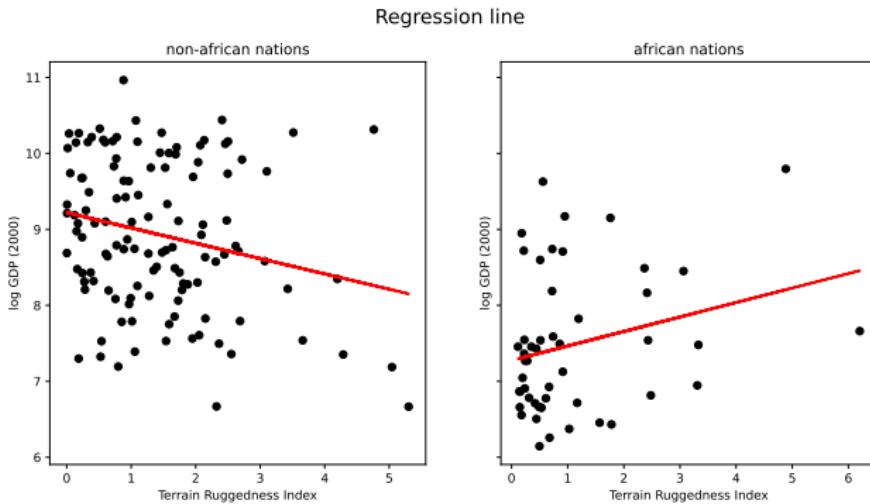
Scatter plot of data



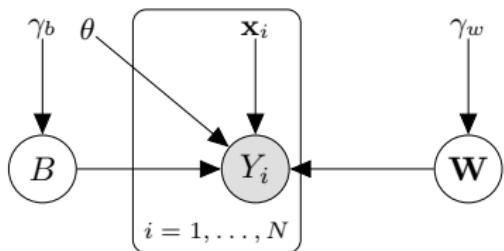
Relationship between topographic heterogeneity and GDP per capita

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

# Real Data Example

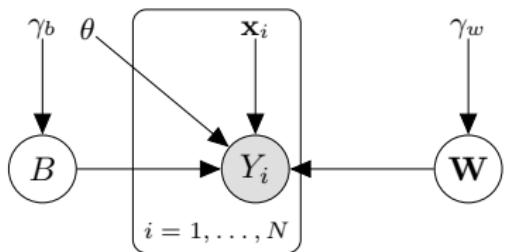


## The Bayesian linear regression model



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

## The Bayesian linear regression model

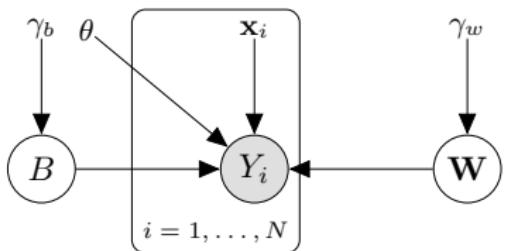


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- $\mathbf{W} \sim \mathcal{N}(\mathbf{0}, \gamma_w^{-1} \mathbf{I}_{M \times M})$
- $B \sim \mathcal{N}(0, \gamma_b^{-1})$

## The probability model

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

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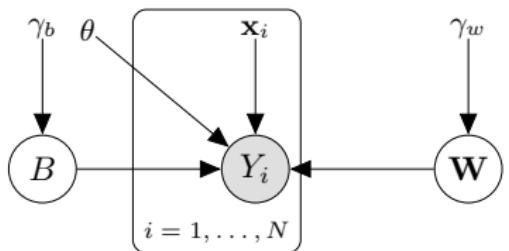
## The probability model

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

...after taking the log

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

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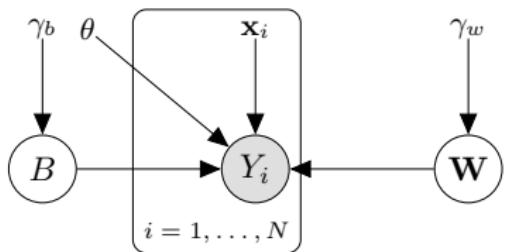
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$$p(\cdot | \mathbf{x}, \theta, \gamma_w, \gamma_b) = \prod_{i=1}^N p(y_i | \mathbf{x}_i, \mathbf{w}, b, \theta) p(\mathbf{w} | \gamma_w) p(b | \gamma_b)$$

...after taking the log

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

## The Bayesian linear regression model



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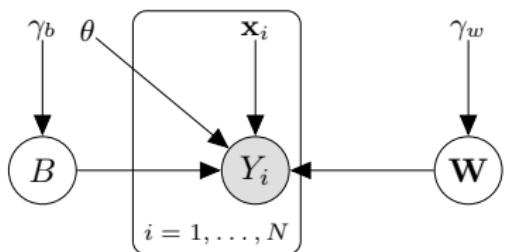
## The probability model

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

## The variational model (full mean field)

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

## The Bayesian linear regression model



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

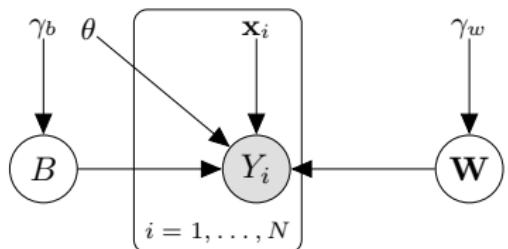
$$p(\cdot | \mathbf{x}, \theta, \gamma_w, \gamma_b) = \prod_{i=1}^N p(y_i | \mathbf{x}_i, \mathbf{w}, b, \theta) p(\mathbf{w} | \gamma_w) p(b | \gamma_b)$$

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

$q(w_j)$  is normally distributed with

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

## The Bayesian linear regression model



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

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

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

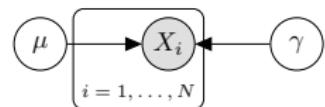
$q(b)$  is normally distributed with

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

## Supplementary

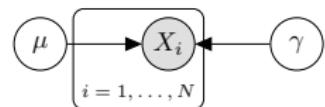
We choose the variational distribution so that

$$\log q(\gamma) = \mathbb{E}_{q_\mu} [\log p(\mathbf{x}, \mu, \gamma)] + c =$$



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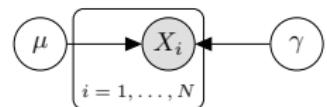


### Recall

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

We choose the variational distribution so that

$$\log q(\gamma) = \mathbb{E}_{q_\mu} [\log p(\mathbf{x}, \mu, \gamma)] + c =$$

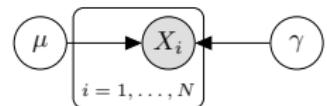


Recall

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

We choose the variational distribution so that

$$\log q(\gamma) = \mathbb{E}_{q_\mu} [\log p(\mathbf{x}, \mu, \gamma)] + c = \sum_{i=1}^N \mathbb{E}_{q_\mu} [\log p(x_i | \mu, \gamma^{-1})] + \log p(\gamma) + c$$

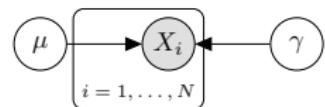


### Recall

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

We choose the variational distribution so that

$$\log q(\gamma) = \mathbb{E}_{q_\mu} [\log p(\mathbf{x}, \mu, \gamma)] + c = \sum_{i=1}^N \mathbb{E}_{q_\mu} [\log p(x_i | \mu, \gamma^{-1})] + \log p(\gamma) + c$$



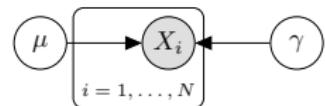
### Recall

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

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

We choose the variational distribution so that

$$\log q(\gamma) = \mathbb{E}_{q_\mu} [\log p(\mathbf{x}, \mu, \gamma)] + c = \sum_{i=1}^N \mathbb{E}_{q_\mu} [\log p(x_i | \mu, \gamma^{-1})] + \log p(\gamma) + c$$

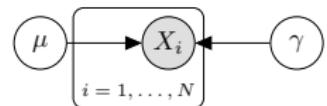


Recall

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

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

We choose the variational distribution so that



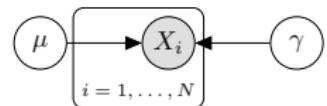
$$\begin{aligned}\log q(\gamma) &= \mathbb{E}_{q_\mu} [\log p(\mathbf{x}, \mu, \gamma)] + c = \sum_{i=1}^N \mathbb{E}_{q_\mu} [\log p(x_i | \mu, \gamma^{-1})] + \log p(\gamma) + c \\ &= \frac{N}{2} \log(\gamma) - \frac{\gamma}{2} \sum_{i=1}^N \mathbb{E}_{q_\mu} [(x_i - \mu)^2] + (\alpha - 1) \log(\gamma)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

Recall

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

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

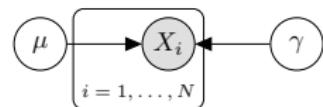
We choose the variational distribution so that



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

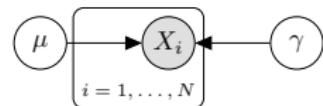
We choose the variational distribution so that

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



We choose the variational distribution so that

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

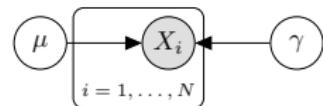


Recall

$$\log q(\gamma | \alpha_q, \beta_q) = \alpha_q \cdot \log(\beta_q) + (\alpha_q - 1) \log(\gamma) - \beta_q \cdot \gamma - \log(\Gamma(\alpha_q))$$

We choose the variational distribution so that

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

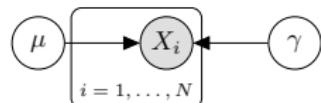


Recall

$$\log q(\gamma | \alpha_q, \beta_q) = \alpha_q \cdot \log(\beta_q) + (\alpha_q - 1) \log(\gamma) - \beta_q \cdot \gamma - \log(\Gamma(\alpha_q))$$

We choose the variational distribution so that

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



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

- $\alpha_q \leftarrow \frac{N}{2} + \alpha$
- $\beta_q \leftarrow \beta + \frac{1}{2} \sum_{i=1}^N \mathbb{E}_{q_\mu} [(x_i - \mu)^2]$

Note that:

- $\mathbb{E}_{q_\mu} [(x_i - \mu)^2] = x_i^2 + \mathbb{E}_{q_\mu} [\mu^2] - 2 \cdot x_i \cdot \mathbb{E}_{q_\mu} [\mu]$
- $\mathbb{E}_{q_\mu} [\mu^2] = \text{Var}(\mu) + \mathbb{E}_{q_\mu} [\mu]^2$

We choose the variational distribution so that

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

We choose the variational distribution so that

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

### Recall

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

We choose the variational distribution so that

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

### Recall

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

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

We choose the variational distribution so that

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

Recall

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

We choose the variational distribution so that

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

### The normal distribution

$$\log p(y_i | \mathbf{x}_i, \mathbf{w}, b, \theta) = -\frac{1}{2} \log(2\pi) + \frac{1}{2} \log(\theta) - \frac{\theta}{2} (y_i - (\mathbf{w}^\top \mathbf{x}_i + b))^2$$

$$\log p(w_j | \gamma_w) = \log \mathcal{N}(w_j | 0, \gamma_w^{-1}) = -\frac{1}{2} \log(2\pi) + \frac{1}{2} \log(\gamma_w) - \frac{\gamma_w}{2} w_j^2$$

We choose the variational distribution so that

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

### The normal distribution

$$\log p(y_i | \mathbf{x}_i, \mathbf{w}, b, \theta) = -\frac{1}{2} \log(2\pi) + \frac{1}{2} \log(\theta) - \frac{\theta}{2} (y_i - (\mathbf{w}^\top \mathbf{x}_i + b))^2$$

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We choose the variational distribution so that

$$\begin{aligned}\log q(w_j) &= \mathbb{E}_{q \sim w_j} \log p(\cdot | \mathbf{x}, \theta, \gamma_w, \gamma_b) + c = \sum_{i=1}^N \mathbb{E} \log p(y_i | \mathbf{x}_i, \mathbf{W}, B, \theta) + \log p(w_j | \gamma_w) + c \\ &= -\frac{\gamma_w}{2} w_j^2 - \frac{\theta}{2} \sum_{i=1}^N \mathbb{E}((y_i - (\mathbf{W}^\top \mathbf{x}_i + B))^2) + c\end{aligned}$$

## The normal distribution

$$\log p(y_i | \mathbf{x}_i, \mathbf{w}, b, \theta) = -\frac{1}{2} \log(2\pi) + \frac{1}{2} \log(\theta) - \frac{\theta}{2} (y_i - (\mathbf{w}^\top \mathbf{x}_i + b))^2$$

$$\log p(w_j | \gamma_w) = \log \mathcal{N}(w_j | 0, \gamma_w^{-1}) = -\frac{1}{2} \log(2\pi) + \frac{1}{2} \log(\gamma_w) - \frac{\gamma_w}{2} w_j^2$$

We choose the variational distribution so that

$$\begin{aligned}\log q(w_j) &= \mathbb{E}_{q=w_j} \log p(\cdot | \mathbf{x}, \theta, \gamma_w, \gamma_b) + c = \sum_{i=1}^N \mathbb{E} \log p(y_i | \mathbf{x}_i, \mathbf{W}, B, \theta) + \log p(w_j | \gamma_w) + c \\ &= -\frac{\gamma_w}{2} w_j^2 - \frac{\theta}{2} \sum_{i=1}^N \mathbb{E}((y_i - (\mathbf{W}^\top \mathbf{x}_i + B))^2) + c\end{aligned}$$

Expanding the square

$$(y - (\mathbf{w}^\top \mathbf{x} + b))^2 = y^2 + \mathbf{x}^\top \mathbf{w} \mathbf{w}^\top \mathbf{x} + b^2 + 2\mathbf{w}^\top \mathbf{x}b - 2y\mathbf{w}^\top \mathbf{x} - 2yb$$

$$\mathbf{x}^\top \mathbf{w} \mathbf{w}^\top \mathbf{x} = x_j^2 w_j^2 + \sum_{h, k \neq j} x_k x_h w_k w_h + 2x_j w_j \sum_{k \neq j} x_k w_k$$

We choose the variational distribution so that

$$\begin{aligned}\log q(w_j) &= \mathbb{E}_{q \sim w_j} \log p(\cdot | \mathbf{x}, \theta, \gamma_w, \gamma_b) + c = \sum_{i=1}^N \mathbb{E} \log p(y_i | \mathbf{x}_i, \mathbf{W}, B, \theta) + \log p(w_j | \gamma_w) + c \\ &= -\frac{\gamma_w}{2} w_j^2 - \frac{\theta}{2} \sum_{i=1}^N \mathbb{E}((y_i - (\mathbf{W}^\top \mathbf{x}_i + B))^2) + c\end{aligned}$$

Expanding the square

$$(y - (\mathbf{w}^\top \mathbf{x} + b))^2 = y^2 + \mathbf{x}^\top \mathbf{w} \mathbf{w}^\top \mathbf{x} + b^2 + 2\mathbf{w}^\top \mathbf{x} b - 2y\mathbf{w}^\top \mathbf{x} - 2yb$$

$$\mathbf{x}^\top \mathbf{w} \mathbf{w}^\top \mathbf{x} = \mathbf{x}_j^\top \mathbf{w}_j^2 + \sum_{h, k \neq j} x_k x_h w_k w_h + 2x_j w_j \sum_{k \neq j} x_k w_k$$

We choose the variational distribution so that

$$\begin{aligned}
 \log q(w_j) &= \mathbb{E}_{q \sim w_j} \log p(\cdot | \mathbf{x}, \theta, \gamma_w, \gamma_b) + c = \sum_{i=1}^N \mathbb{E} \log p(y_i | \mathbf{x}_i, \mathbf{W}, B, \theta) + \log p(w_j | \gamma_w) + c \\
 &= -\frac{\gamma_w}{2} w_j^2 - \frac{\theta}{2} \sum_{i=1}^N \mathbb{E}((y_i - (\mathbf{W}^\top \mathbf{x}_i + B))^2) + c \\
 &= -\frac{\gamma_w}{2} w_j^2 - \theta \sum_{i=1}^N \left( \frac{1}{2} x_{ij}^2 w_j^2 + w_j \left( \sum_{k \neq j} x_{ij} x_{ik} \mathbb{E}(W_k) + x_{ij} \mathbb{E}(B) - y x_{ij} \right) \right) + c
 \end{aligned}$$

Expanding the square

$$(y - (\mathbf{w}^\top \mathbf{x} + b))^2 = y^2 + \mathbf{x}^\top \mathbf{w} \mathbf{w}^\top \mathbf{x} + b^2 + 2\mathbf{w}^\top \mathbf{x} b - 2y\mathbf{w}^\top \mathbf{x} - 2yb$$

$$\mathbf{x}^\top \mathbf{w} \mathbf{w}^\top \mathbf{x} = x_j^2 w_j^2 + \sum_{h, k \neq j} x_k x_h w_k w_h + 2x_j w_j \sum_{k \neq j} x_k w_k$$

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

We choose the variational distribution so that

$$\begin{aligned}\log q(w_j) &= \mathbb{E}_{q \sim w_j} \log p(\cdot | \mathbf{x}, \theta, \gamma_w, \gamma_b) + c = \sum_{i=1}^N \mathbb{E} \log p(y_i | \mathbf{x}_i, \mathbf{W}, B, \theta) + \log p(w_j | \gamma_w) + c \\ &= -\frac{\gamma_w}{2} w_j^2 - \frac{\theta}{2} \sum_{i=1}^N \mathbb{E}((y_i - (\mathbf{W}^\top \mathbf{x}_i + B))^2) + c \\ &= -\frac{\gamma_w}{2} w_j^2 - \theta \sum_{i=1}^N \left( \frac{1}{2} x_{ij}^2 w_j^2 + w_j \left( \sum_{k \neq j} x_{ik} x_{ik} \mathbb{E}(W_k) + x_{ij} \mathbb{E}(B) - y x_{ij} \right) \right) + c \\ &= -\frac{1}{2} (\gamma_w + \theta \sum_{i=1}^N (x_{ij}^2) w_j^2 + w_j \theta \sum_{i=1}^N x_{ij} (y_i - (\sum_{k \neq j} x_{ik} \mathbb{E}(W_k) + \mathbb{E}(B)))) + c\end{aligned}$$

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

We choose the variational distribution so that

$$\begin{aligned}\log q(w_j) &= \mathbb{E}_{q \sim w_j} \log p(\cdot | \mathbf{x}, \theta, \gamma_w, \gamma_b) + c = \sum_{i=1}^N \mathbb{E} \log p(y_i | \mathbf{x}_i, \mathbf{W}, B, \theta) + \log p(w_j | \gamma_w) + c \\ &= -\frac{1}{2} (\gamma_w + \theta \sum_{i=1}^N (x_{ij}^2) w_j^2 + w_j \theta \sum_{i=1}^N x_{ij} (y_i - (\sum_{k \neq j} x_{ik} \mathbb{E}(W_k) + \mathbb{E}(B)))) + c\end{aligned}$$

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$$\begin{aligned}\log q(w_j) &= \mathbb{E}_{q \sim w_j} \log p(\cdot | \mathbf{x}, \theta, \gamma_w, \gamma_b) + c = \sum_{i=1}^N \mathbb{E} \log p(y_i | \mathbf{x}_i, \mathbf{W}, B, \theta) + \log p(w_j | \gamma_w) + c \\ &= -\frac{1}{2} (\gamma_w + \theta \sum_{i=1}^N (x_{ij}^2) w_j^2 + w_j \theta \sum_{i=1}^N x_{ij} (y_i - (\sum_{k \neq j} x_{ik} \mathbb{E}(W_k) + \mathbb{E}(B)))) + c\end{aligned}$$

Recall the normal distribution

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

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

We choose the variational distribution so that

$$\begin{aligned}\log q(w_j) &= \mathbb{E}_{q \sim w_j} \log p(\cdot | \mathbf{x}, \theta, \gamma_w, \gamma_b) + c = \sum_{i=1}^N \mathbb{E} \log p(y_i | \mathbf{x}_i, \mathbf{W}, B, \theta) + \log p(w_j | \gamma_w) + c \\ &= -\frac{1}{2} (\gamma_w + \theta \sum_{i=1}^N (x_{ij}^2) w_j^2 + w_j \theta \sum_{i=1}^N x_{ij} (y_i - (\sum_{k \neq j} x_{ik} \mathbb{E}(W_k) + \mathbb{E}(B)))) + c\end{aligned}$$

Recall the normal distribution

$$\begin{aligned}\log p(w | \mu, \tau) &= \log \mathcal{N}(w | \mu, \tau^{-1}) = -\frac{1}{2} \log(2\pi) + \frac{1}{2} \log(\tau) - \frac{\tau}{2} (w - \mu)^2 \\ &= -\frac{1}{2} \log(2\pi) + \frac{1}{2} \log(\tau) - \frac{1}{2} \textcolor{red}{\tau} w^2 - \frac{\tau}{2} \mu^2 + w \textcolor{green}{\tau \mu}\end{aligned}$$

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

We choose the variational distribution so that

$$\begin{aligned}\log q(w_j) &= \mathbb{E}_{q \sim w_j} \log p(\cdot | \mathbf{x}, \theta, \gamma_w, \gamma_b) + c = \sum_{i=1}^N \mathbb{E} \log p(y_i | \mathbf{x}_i, \mathbf{W}, B, \theta) + \log p(w_j | \gamma_w) + c \\ &= -\frac{1}{2} (\gamma_w + \theta \sum_{i=1}^N (x_{ij}^2) w_j^2 + w_j \theta \sum_{i=1}^N x_{ij} (y_i - (\sum_{k \neq j} x_{ik} \mathbb{E}(W_k) + \mathbb{E}(B)))) + c\end{aligned}$$

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

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

Recall the normal distribution

$$\begin{aligned}\log p(w | \mu, \tau) &= \log \mathcal{N}(w | \mu, \tau^{-1}) = -\frac{1}{2} \log(2\pi) + \frac{1}{2} \log(\tau) - \frac{\tau}{2} (w - \mu)^2 \\ &= -\frac{1}{2} \log(2\pi) + \frac{1}{2} \log(\tau) - \frac{1}{2} \textcolor{red}{\tau} w^2 - \frac{\tau}{2} \mu^2 + w \textcolor{green}{\tau \mu}\end{aligned}$$

We choose the variational distribution so that

$$\begin{aligned}\log q(b) &= \mathbb{E}_{q \sim w_j} \log p(\cdot \mid \mathbf{W}, B, \theta, \boldsymbol{\gamma}) + c = \sum_{i=1}^N \mathbb{E} \log p(y_i \mid \mathbf{x}_i, \mathbf{W}, \theta) + \log p(b \mid \gamma_b) + c \\ &= \dots \\ &= -\frac{1}{2}(\gamma_b + \theta N)b^2 + b \left( \theta \sum_{i=1}^N (y_i - \mathbb{E}(\mathbf{W})^\top \mathbf{x}_i) \right) + c\end{aligned}$$

# VB for Bayesian linear regression: updating $q(b)$

We choose the variational distribution so that

$$\begin{aligned}\log q(b) &= \underset{q \sim w_j}{\mathbb{E}} \log p(\cdot \mid \mathbf{W}, B, \theta, \gamma) + c = \sum_{i=1}^N \mathbb{E} \log p(y_i \mid \mathbf{x}_i, \mathbf{W}, \theta) + \log p(b \mid \gamma_b) + c \\ &= \dots \\ &= -\frac{1}{2} (\color{red}{\gamma_b + \theta N}) b^2 + b \left( \color{green}{\theta} \sum_{i=1}^N (y_i - \mathbb{E}(\mathbf{W})^\top \mathbf{x}_i) \right) + c\end{aligned}$$

Recall the normal distribution

$$\begin{aligned}\log p(b \mid \mu, \tau) &= \log \mathcal{N}(b \mid \mu, \tau^{-1}) = -\frac{1}{2} \log(2\pi) + \frac{1}{2} \log(\tau) - \frac{\tau}{2} (b - \mu)^2 \\ &= -\frac{1}{2} \log(2\pi) + \frac{1}{2} \log(\tau) - \frac{1}{2} \color{red}{\tau} b^2 - \frac{\tau}{2} \mu^2 + b \color{green}{\tau \mu}\end{aligned}$$

## VB for Bayesian linear regression: updating $q(b)$

We choose the variational distribution so that

$$\begin{aligned}\log q(b) &= \underset{q \sim w_j}{\mathbb{E}} \log p(\cdot \mid \mathbf{W}, B, \theta, \gamma) + c = \sum_{i=1}^N \mathbb{E} \log p(y_i \mid \mathbf{x}_i, \mathbf{W}, \theta) + \log p(b \mid \gamma_b) + c \\ &= \dots \\ &= -\frac{1}{2} (\color{red}{\gamma_b + \theta N}) b^2 + b \left( \color{green}{\theta} \sum_{i=1}^N (y_i - \mathbb{E}(\mathbf{W}^\top \mathbf{x}_i)) \right) + c\end{aligned}$$

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

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

Recall the normal distribution

$$\begin{aligned}\log p(b \mid \mu, \tau) &= \log \mathcal{N}(b \mid \mu, \tau^{-1}) = -\frac{1}{2} \log(2\pi) + \frac{1}{2} \log(\tau) - \frac{\tau}{2} (b - \mu)^2 \\ &= -\frac{1}{2} \log(2\pi) + \frac{1}{2} \log(\tau) - \frac{1}{2} \color{red}{\tau} b^2 - \frac{\tau}{2} \mu^2 + b \color{green}{\tau \mu}\end{aligned}$$

## **Temporary page!**

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