Tropical Probabilistic AI school

Variational Inference and Optimization

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This material is very heavily based on what was prepared for ProbAI-23 by
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Demo: Bayesian Neural Network

Stochastic Gradient Ascent

A small side-step: Gradient Ascent

Why do we talk about this?

We want a way to optimize ELBO using gradient methods. If we can do Bayesian inference as optimization it will play well with, e.g., deep learning frameworks.

Gradient ascent algorithm for maximizing a function $f(\boldsymbol{\lambda})$:

1. Initialize $\boldsymbol{\lambda}^{(0)}$ randomly.
2. For $t = 1, \ldots$:

$$\boldsymbol{\lambda}^{(t)} \leftarrow \boldsymbol{\lambda}^{(t-1)} + \rho \cdot \nabla_{\boldsymbol{\lambda}} f\left(\boldsymbol{\lambda}^{(t-1)}\right)$$

$\boldsymbol{\lambda}^{(t)}$ converges to a (local) optimum of $f(\cdot)$ if:

- f is "sufficiently nice";
- The learning-rate ρ is "sufficiently small".

. . . and Stochastic Gradient Ascent

"Standard" gradient ascent is not enough for ELBO optimization

We won't be able to calculate $\nabla_{\boldsymbol{\lambda}} \mathcal{L}\left(q(\boldsymbol{\theta} \mid \boldsymbol{\lambda})\right)$ exactly for (at least) two reasons:

1. We may have to resolve to mini-batching (gradient from "random subset")
2. We may not be able to calculate the gradient exactly even for a mini-batch

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Stochastic gradient ascent algorithm for maximizing a function $f(\boldsymbol{\lambda})$:

If we have access to $\mathrm{g}(\boldsymbol{\lambda})$ – an **unbiased estimate** of the gradient – it still works!

1. Initialize $\boldsymbol{\lambda}^{(0)}$ randomly.
2. For $t = 1, \ldots$:

$$\boldsymbol{\lambda}^{(t)} \leftarrow \boldsymbol{\lambda}^{(t-1)} + \rho_t \cdot \mathrm{g}\left(\boldsymbol{\lambda}^{(t-1)}\right)$$

$\boldsymbol{\lambda}_t$ converges to a (local) optimum of $f(\cdot)$ if:

- f is "sufficiently nice";
- $\mathrm{g}(\boldsymbol{\lambda})$ is a random variable with $\mathbb{E}[\mathrm{g}(\boldsymbol{\lambda})] = \nabla_{\boldsymbol{\lambda}} f(\boldsymbol{\lambda})$ and $\mathrm{Var}[\mathrm{g}(\boldsymbol{\lambda})] < \infty$.
- The learning-rates $\{\rho_t\}$ is a Robbins-Monro – sequence:
  - $\sum_t \rho_t^2 < \infty$
  - $\sum_t \rho_t = \infty$

Black Box Variational Inference

Main idea: Cast inference as an optimization problem

Optimize the ELBO by stochastic gradient ascent over the parameters $\boldsymbol{\lambda}$. If that works, Bayesian inference can be **seamlessly integrated** with building-blocks from other gradient-based machine learning approaches (like deep learning).

Algorithm: Maximize $\mathcal{L}(q) = \mathbb{E}_q \left[\log \frac{p(\boldsymbol{\theta}, \mathcal{D})}{q(\boldsymbol{\theta}|\boldsymbol{\lambda})}\right]$ by gradient ascent

- Initialization:
  - $t \leftarrow 0$;
  - $\hat{\boldsymbol{\lambda}}_0 \leftarrow$ random initialization;
  - $\{\rho_t\} \leftarrow$ a Robbins-Monro sequence.
- Repeat until negligible improvement in terms of $\mathcal{L}(q)$:
  - $t \leftarrow t + 1$;
  - $\hat{\boldsymbol{\lambda}}_t \leftarrow \hat{\boldsymbol{\lambda}}_{t-1} + \rho_t \, \nabla_{\boldsymbol{\lambda}} \mathcal{L}(q)|_{\hat{\boldsymbol{\lambda}}_{t-1}}$;

Important issue:
Can we calculate $\nabla_{\boldsymbol{\lambda}} \mathcal{L}(q)$ efficiently without adding new restrictive assumptions?

BBVI - calculating the gradient

The algorithm requires that we can find

$$\nabla_{\boldsymbol{\lambda}} \mathcal{L}(q) = \nabla_{\boldsymbol{\lambda}} \mathbb{E}_{\boldsymbol{\theta} \sim q_{\boldsymbol{\lambda}}} \left[\log \frac{p(\boldsymbol{\theta}, \mathcal{D})}{q(\boldsymbol{\theta} \mid \boldsymbol{\lambda})} \right].$$

Tricky: How can we move the gradient inside the expectation?

- We would typically approximate an expectation by a sample average:

$$\mathbb{E}_{\boldsymbol{\theta} \sim q_{\boldsymbol{\lambda}}} [f(\boldsymbol{\theta}, \boldsymbol{\lambda})] \approx \frac{1}{M} \sum_{j=1}^{M} f(\boldsymbol{\theta}_j, \boldsymbol{\lambda}), \text{ with } \{\boldsymbol{\theta}_1, \ldots \boldsymbol{\theta}_M\} \text{ sampled from } q_{\boldsymbol{\lambda}}(\boldsymbol{\theta} \mid \boldsymbol{\lambda}).$$

- This doesn't work when taking a gradient related to the sampling distribution.

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Solution: Use these properties to simplify the equation:

1. $\nabla_{\boldsymbol{\lambda}} \left(f(\boldsymbol{\theta}, \boldsymbol{\lambda}) \cdot g(\boldsymbol{\theta}, \boldsymbol{\lambda}) \right) = f(\boldsymbol{\theta}, \boldsymbol{\lambda}) \cdot \nabla_{\boldsymbol{\lambda}} g(\boldsymbol{\theta}, \boldsymbol{\lambda}) + g(\boldsymbol{\theta}, \boldsymbol{\lambda}) \cdot \nabla_{\boldsymbol{\lambda}} f(\boldsymbol{\theta}, \boldsymbol{\lambda})$.
2. $\nabla_{\boldsymbol{\lambda}} f(\boldsymbol{\theta}, \boldsymbol{\lambda}) = f(\boldsymbol{\theta}, \boldsymbol{\lambda}) \cdot \nabla_{\boldsymbol{\lambda}} \log f(\boldsymbol{\theta}, \boldsymbol{\lambda})$.
3. $\mathbb{E}_q \left[\nabla_{\boldsymbol{\lambda}} \log q(\boldsymbol{\theta} \mid \boldsymbol{\lambda}) \right] = 0$ for any density function $q(\boldsymbol{\theta} \mid \boldsymbol{\lambda})$.

Now it follows that

$$\nabla_{\boldsymbol{\lambda}} \mathcal{L}(q) = \mathbb{E}_{\boldsymbol{\theta} \sim q_{\boldsymbol{\lambda}}} \left[\log \frac{p(\boldsymbol{\theta}, \mathcal{D})}{q(\boldsymbol{\theta} \mid \boldsymbol{\lambda})} \cdot \nabla_{\boldsymbol{\lambda}} \log q(\boldsymbol{\theta} \mid \boldsymbol{\lambda}) \right].$$

This is the so-called **score-function gradient**.

Calculating the gradient – Things to notice

$$\nabla_{\boldsymbol{\lambda}} \mathcal{L}\left(q\right) = \mathbb{E}_{\boldsymbol{\theta} \sim q} \left[\log \frac{p(\boldsymbol{\theta}, \mathcal{D})}{q(\boldsymbol{\theta} \mid \boldsymbol{\lambda})} \cdot \nabla_{\boldsymbol{\lambda}} \log q(\boldsymbol{\theta} \mid \boldsymbol{\lambda}) \right].$$

Calculating the gradient – Things to notice

- We still only need access to the joint distribution $p(\boldsymbol{\theta}, \mathcal{D})$ – not $p(\boldsymbol{\theta} \mid \mathcal{D})$.

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- $q(\boldsymbol{\theta} \mid \boldsymbol{\lambda})$ factorizes under MF, s.t. we can optimize per variable: $q(\theta_i \mid \boldsymbol{\lambda}_i)$.

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- We must calculate $\nabla_{\boldsymbol{\lambda}_i} \log q(\theta_i \mid \boldsymbol{\lambda}_i)$, which is also known as the "score function".

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- The expectation will be approximated using a sample $\{\boldsymbol{\theta}_1, \ldots, \boldsymbol{\theta}_M\}$ generated from $q(\boldsymbol{\theta} \mid \boldsymbol{\lambda})$. Hence we require that we can **sample from** each $q(\theta_i \mid \boldsymbol{\lambda}_i)$.

Calculating the gradient – Things to notice

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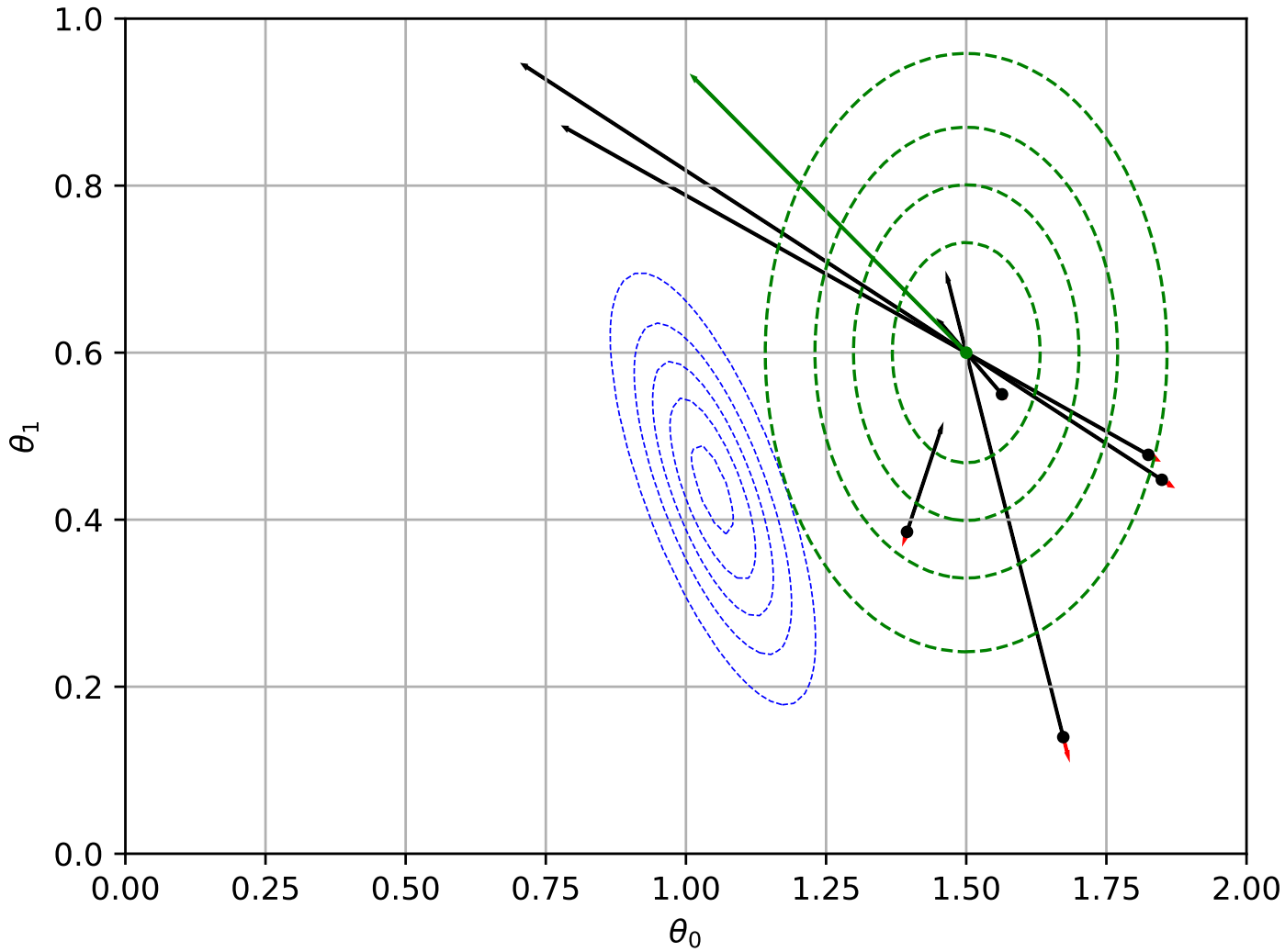
Calculating the gradient – in summary

We have observed the data $\mathcal{D}$, and our current estimate for $\boldsymbol{\lambda}$ is $\hat{\boldsymbol{\lambda}}$. Then

$$\nabla_{\boldsymbol{\lambda}} \mathcal{L}(q)|_{\boldsymbol{\lambda}=\hat{\boldsymbol{\lambda}}} \approx \frac{1}{M} \sum_{j=1}^{M} \log \frac{p(\boldsymbol{\theta}_j, \mathcal{D})}{q(\boldsymbol{\theta}_j \mid \hat{\boldsymbol{\lambda}})} \cdot \nabla_{\boldsymbol{\lambda}} \log q(\boldsymbol{\theta}_j \mid \hat{\boldsymbol{\lambda}}),$$

where $\{\boldsymbol{\theta}_1, \ldots \boldsymbol{\theta}_M\}$ are samples from $q(\cdot \mid \hat{\boldsymbol{\lambda}})$. Typically M is fairly small.

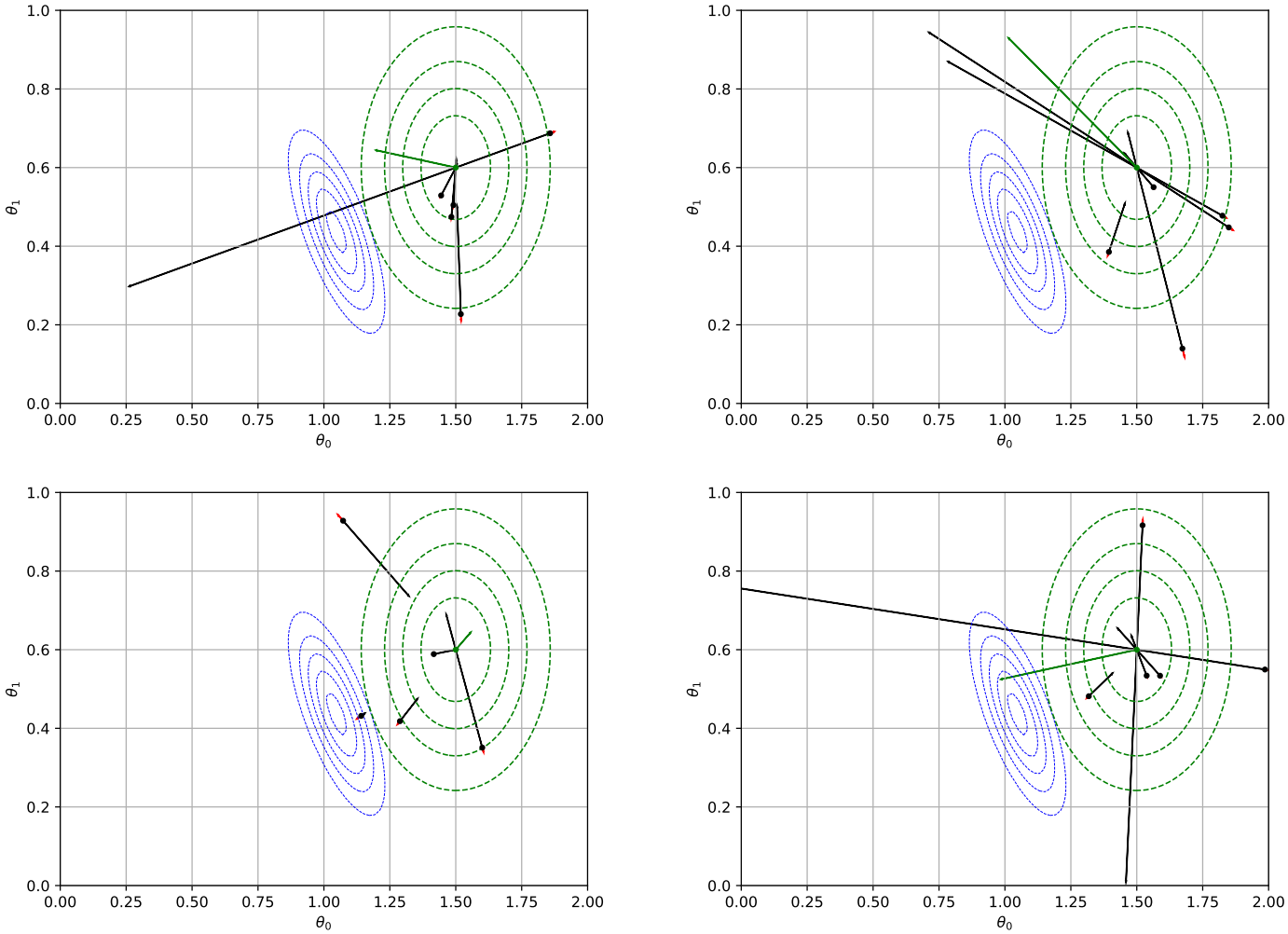
Does it work?



$\nabla_{\boldsymbol{\lambda}} \log q(\boldsymbol{\theta}_i \mid \boldsymbol{\lambda})$; $\log \frac{p(\boldsymbol{\theta}_i, \mathcal{D})}{q(\boldsymbol{\theta}_i \mid \boldsymbol{\lambda})} \cdot \nabla_{\boldsymbol{\lambda}} \log q(\boldsymbol{\theta}_i \mid \boldsymbol{\lambda})$; $\frac{1}{M} \sum_{j=1}^{M} \log \frac{p(\boldsymbol{\theta}_j, \mathcal{D})}{q(\boldsymbol{\theta}_j \mid \boldsymbol{\lambda})} \cdot \nabla_{\boldsymbol{\lambda}} \log q(\boldsymbol{\theta}_j \mid \boldsymbol{\lambda})$

Length of gradients increased for visibility. Graphics inspired by Arto Klami @ ProbAI2021.

Does it work?



Different samples, each with $M = 5$.

$$\nabla_{\boldsymbol{\lambda}} \log q(\boldsymbol{\theta}_i \mid \boldsymbol{\lambda}); \quad \log \frac{p(\boldsymbol{\theta}_i, \mathcal{D})}{q(\boldsymbol{\theta}_i \mid \boldsymbol{\lambda})} \cdot \nabla_{\boldsymbol{\lambda}} \log q(\boldsymbol{\theta}_i \mid \boldsymbol{\lambda}); \quad \frac{1}{M} \sum_{j=1}^{M} \log \frac{p(\boldsymbol{\theta}_j, \mathcal{D})}{q(\boldsymbol{\theta}_j \mid \boldsymbol{\lambda})} \cdot \nabla_{\boldsymbol{\lambda}} \log q(\boldsymbol{\theta}_j \mid \boldsymbol{\lambda})$$

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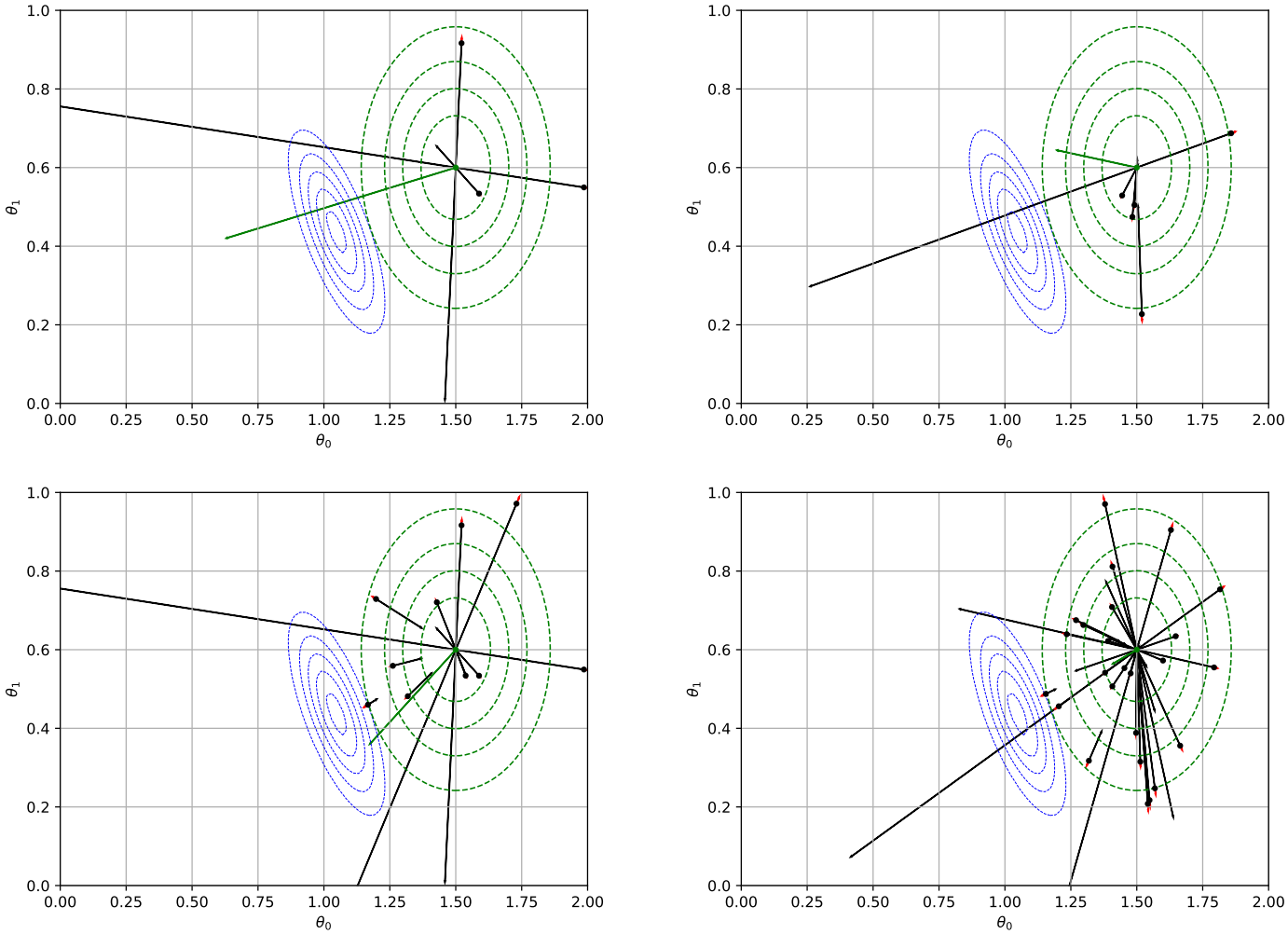

Different values of M ($M = 3$, 5, 10, and 25)

$\nabla_{\boldsymbol{\lambda}} \log q(\boldsymbol{\theta}_i \mid \boldsymbol{\lambda})$; $\log \frac{p(\boldsymbol{\theta}_i, \mathcal{D})}{q(\boldsymbol{\theta}_i \mid \boldsymbol{\lambda})} \cdot \nabla_{\boldsymbol{\lambda}} \log q(\boldsymbol{\theta}_i \mid \boldsymbol{\lambda})$; $\frac{1}{M} \sum_{j=1}^{M} \log \frac{p(\boldsymbol{\theta}_j, \mathcal{D})}{q(\boldsymbol{\theta}_j \mid \boldsymbol{\lambda})} \cdot \nabla_{\boldsymbol{\lambda}} \log q(\boldsymbol{\theta}_j \mid \boldsymbol{\lambda})$

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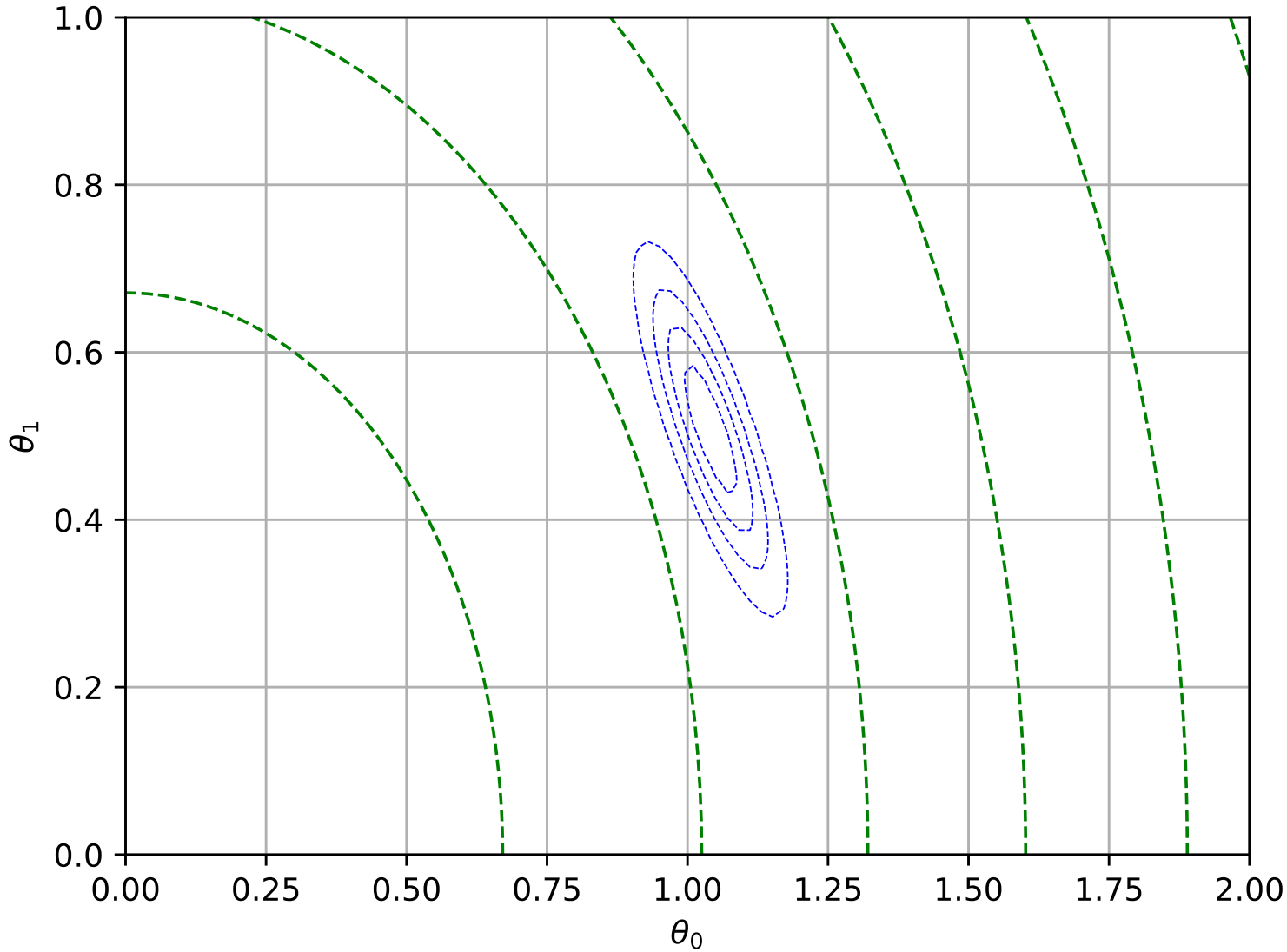
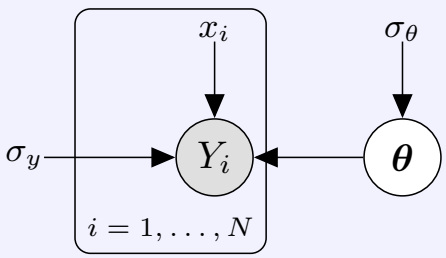
Does it work?


1.0
0.8
0.6
0.4
0.2
0.0
θ_1
0.00
0.25
0.50
0.75
1.00
1.25
1.50
1.75
2.00
θ_0

Code Task: Score-function gradient for linear regression



- $\boldsymbol{\theta} = \{w_0, w_1\}$, $\boldsymbol{\theta} \sim \mathcal{N}(\mathbf{0}, \sigma_\theta \cdot \mathbf{I}_{2\times 2})$
- $Y_i \,|\, \{\boldsymbol{\theta}, x_i, \sigma_y\} \sim \mathcal{N}(w_0 + w_1 \cdot x_i, \sigma_y^2)$
- We choose $q_j(\theta_j \,|\, \boldsymbol{\lambda}_j) = \mathcal{N}(\theta_j \,|\, \mu_j, \sigma_j^2)$, so $\boldsymbol{\lambda}_j = \{\mu_j, \sigma_j\}$

In this task you will implement the score-function gradient:

$$\nabla_{\boldsymbol{\lambda}} \mathcal{L}\,(q) = \mathbb{E}_{\boldsymbol{\theta}\sim q}\left[\log \frac{p(\boldsymbol{\theta}, \mathcal{D})}{q(\boldsymbol{\theta} \,|\, \boldsymbol{\lambda})} \cdot \nabla_{\boldsymbol{\lambda}} \log q(\boldsymbol{\theta} \,|\, \boldsymbol{\lambda})\right].$$

- Look at `Exercise 1` in the notebook `Day2/students_BBVI.ipynb`.
- Calculate $\nabla_{\boldsymbol{\lambda}} \log q(\boldsymbol{\theta} \,|\, \boldsymbol{\lambda})$, i.e., $\frac{\partial}{\partial \mu} \log \mathcal{N}(\mu, \sigma^2)$ and $\frac{\partial}{\partial \sigma} \log \mathcal{N}(\mu, \sigma^2)$ by hand.
- Implement your results in the function `score_function_gradient`.

The Reparametrization Trick

Goal: Find a more robust estimator for the gradient

$$\nabla_{\boldsymbol{\lambda}} \mathcal{L}\left(q\right) = \nabla_{\boldsymbol{\lambda}}\, \mathbb{E}_{\boldsymbol{\theta}\sim q}\left[\log \frac{p(\boldsymbol{\theta}, \mathcal{D})}{q(\boldsymbol{\theta} \mid \boldsymbol{\lambda})}\right].$$

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Assumption: $q(\boldsymbol{\theta}|\boldsymbol{\lambda})$ can be *reparametrized* as follows:

$$\begin{aligned} \boldsymbol{\epsilon} &\sim \phi(\boldsymbol{\epsilon}) \\ \boldsymbol{\theta} &= f(\boldsymbol{\epsilon}, \boldsymbol{\lambda}), \end{aligned}$$

where $\phi(\boldsymbol{\epsilon})$ is some distribution that **does not** depend on $\boldsymbol{\lambda}$ and $f(\boldsymbol{\epsilon}, \boldsymbol{\lambda})$ is a **deterministic** transformation.

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Example: The Gaussian distribution

Assume $q(\boldsymbol{\theta}|\boldsymbol{\lambda}) = \mathcal{N}(\boldsymbol{\theta} \mid \boldsymbol{\mu}, \mathbf{R}\mathbf{R}^\mathsf{T})$, so $\boldsymbol{\lambda} = \{\boldsymbol{\mu}, \mathbf{R}\}$. $q(\boldsymbol{\theta}|\boldsymbol{\lambda})$ can be reparametrized using

$$\begin{aligned} \boldsymbol{\epsilon} \sim \phi(\boldsymbol{\epsilon}) \quad &= \mathcal{N}(\mathbf{0}, \mathbf{I}) \\ \boldsymbol{\theta} = f(\boldsymbol{\epsilon}, \boldsymbol{\lambda}) &= \boldsymbol{\mu} + \mathbf{R}\,\boldsymbol{\epsilon} \sim \mathcal{N}(\boldsymbol{\mu}, \mathbf{R}\mathbf{R}^\mathsf{T}). \end{aligned}$$

Univariate case: $q(\theta|\boldsymbol{\lambda}) = \mathcal{N}(\mu, \sigma^2)$ gives $\epsilon \sim \mathcal{N}(0, 1)$ and $\theta = f(\epsilon, \boldsymbol{\lambda}) = \mu + \sigma\,\epsilon$.

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Consequences for how we can calculate the gradient:

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(See Slide 6, Point 3)

Monte-Carlo Estimation:

$$\nabla_{\boldsymbol{\lambda}} \mathcal{L}\left(q\right) \quad = \quad \mathbb{E}_{\boldsymbol{\epsilon} \sim \phi} \left[\nabla_{\boldsymbol{\theta}} \log \frac{p(\boldsymbol{\theta}, \mathcal{D})}{q(\boldsymbol{\theta} \mid \boldsymbol{\lambda})} \nabla_{\boldsymbol{\lambda}} f(\boldsymbol{\epsilon}, \boldsymbol{\lambda}) \right]$$

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$$\approx \frac{1}{M} \sum_{j=1}^{M} \left[\nabla_{\boldsymbol{\theta}} \log \frac{p(\boldsymbol{\theta}_j, \mathcal{D})}{q(\boldsymbol{\theta}_j \mid \boldsymbol{\lambda})} \nabla_{\boldsymbol{\lambda}} f(\boldsymbol{\epsilon}_j, \boldsymbol{\lambda}) \right] \quad : \boldsymbol{\epsilon}_j \sim \phi(\boldsymbol{\epsilon}),\ \boldsymbol{\theta}_j \leftarrow f(\boldsymbol{\epsilon}_j, \boldsymbol{\lambda})$$

Monte-Carlo Estimation:

$$
\begin{aligned}
\nabla_{\boldsymbol{\lambda}} \mathcal{L}(q) &= \mathbb{E}_{\boldsymbol{\epsilon} \sim \phi} \left[\nabla_{\boldsymbol{\theta}} \log \frac{p(\boldsymbol{\theta}, \mathcal{D})}{q(\boldsymbol{\theta} \mid \boldsymbol{\lambda})} \nabla_{\boldsymbol{\lambda}} f(\boldsymbol{\epsilon}, \boldsymbol{\lambda}) \right] \\
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&= \frac{1}{M} \sum_{j=1}^{M} \Big(\underbrace{\nabla_{\boldsymbol{\theta}} \log p(\boldsymbol{\theta}_j, \mathcal{D})}_{\text{Model's gradient}} - \underbrace{\nabla_{\boldsymbol{\theta}} \log q(\boldsymbol{\theta}_j \mid \boldsymbol{\lambda})}_{\text{Approximation's gradient}} \Big) \cdot \nabla_{\boldsymbol{\lambda}} f(\boldsymbol{\epsilon}_j, \boldsymbol{\lambda})
\end{aligned}
$$

Monte-Carlo Estimation:

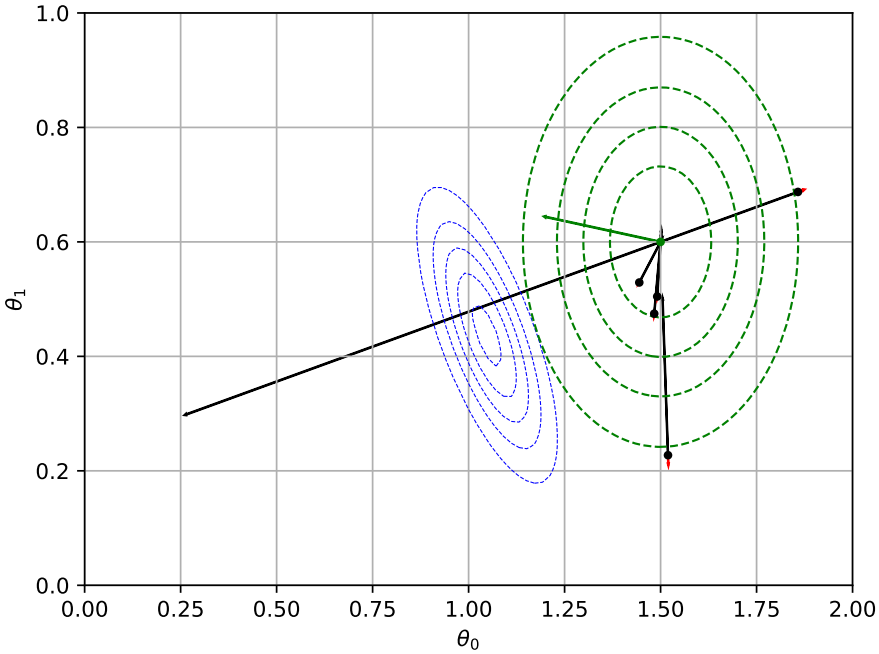
$$
\begin{aligned}
\nabla_{\boldsymbol{\lambda}} \mathcal{L}(q) &= \mathbb{E}_{\boldsymbol{\epsilon} \sim \phi}\left[\nabla_{\boldsymbol{\theta}} \log \frac{p(\boldsymbol{\theta}, \mathcal{D})}{q(\boldsymbol{\theta} \mid \boldsymbol{\lambda})} \nabla_{\boldsymbol{\lambda}} f(\boldsymbol{\epsilon}, \boldsymbol{\lambda})\right] \\
&\approx \frac{1}{M} \sum_{j=1}^{M}\left[\nabla_{\boldsymbol{\theta}} \log \frac{p(\boldsymbol{\theta}_j, \mathcal{D})}{q(\boldsymbol{\theta}_j \mid \boldsymbol{\lambda})} \nabla_{\boldsymbol{\lambda}} f(\boldsymbol{\epsilon}_j, \boldsymbol{\lambda})\right] \quad : \boldsymbol{\epsilon}_j \sim \phi(\boldsymbol{\epsilon}),\ \boldsymbol{\theta}_j \leftarrow f(\boldsymbol{\epsilon}_j, \boldsymbol{\lambda}) \\
&= \frac{1}{M} \sum_{j=1}^{M}\Big(\underbrace{\nabla_{\boldsymbol{\theta}} \log p(\boldsymbol{\theta}_j, \mathcal{D})}_{\text{Model's gradient}} - \underbrace{\nabla_{\boldsymbol{\theta}} \log q(\boldsymbol{\theta}_j \mid \boldsymbol{\lambda})}_{\text{Approximation's gradient}}\Big) \cdot \nabla_{\boldsymbol{\lambda}} f(\boldsymbol{\epsilon}_j, \boldsymbol{\lambda})
\end{aligned}
$$

This gradient estimator...

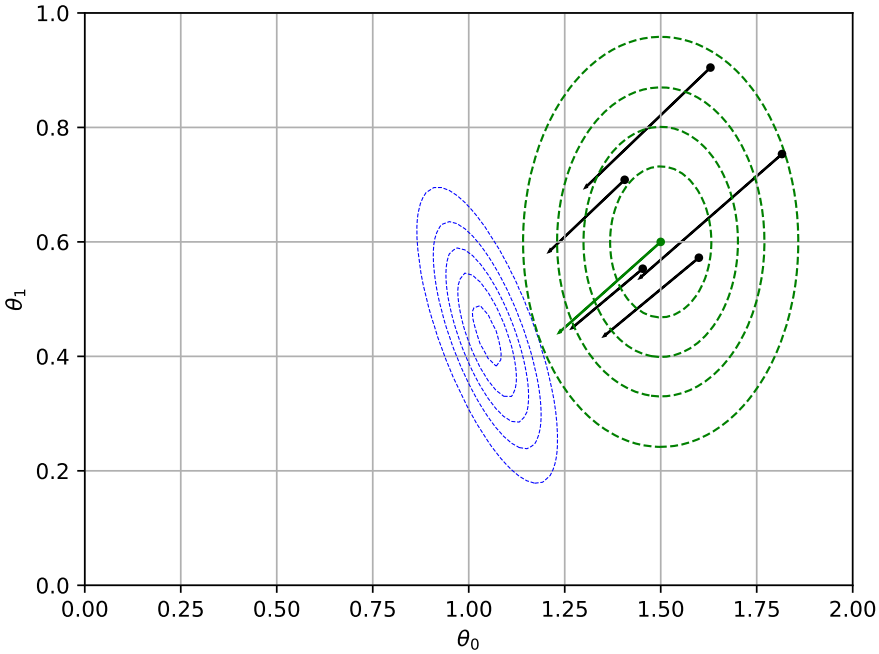
- Uses the *model's* gradients (not so for the score-function gradient).
- Requires $q(\boldsymbol{\theta}|\boldsymbol{\lambda})$ to be *reparametrizable* and *differentiable*.
- Requires $\log p(\boldsymbol{\theta}, \mathcal{D})$ to be differentiable wrt. $\boldsymbol{\theta}$.

Does it work?

Score-function gradient



Reparameterized gradient



Length of gradients increased for visibility. Graphics inspired by Arto Klami @ ProbAI2021.

Notice the direction of each sample's gradient:

- **Score-function gradient:** Towards the mode of q
- **Reparameterization-gradient:** (Approximately) towards high density region of the exact posterior $p(\boldsymbol{\theta}|\mathcal{D})$.

Score function gradients:

- Gradients point towards the mode of $q(\boldsymbol{\theta}|\boldsymbol{\lambda})$, $p(\mathcal{D}, \boldsymbol{\theta})$ only affects the *weights*.
  We need a *"large" number of samples*, typically in the order of tens to a hundred.
- **Requires** $\ln q(\boldsymbol{\theta}|\boldsymbol{\lambda})$ to be *differentiable wrt.* $\boldsymbol{\lambda}$.
- **Requires** $\ln p(\mathcal{D}, \boldsymbol{\theta})$ to be *computable*.

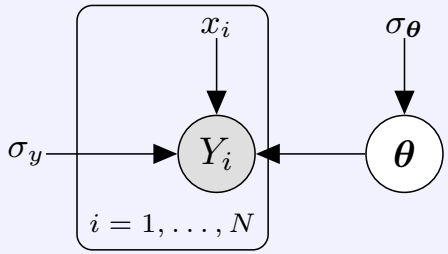
Reparametrization gradients:

- Gradients utilize the model definition via the term $\nabla_{\boldsymbol{\theta}} \ln p(\mathcal{D}, \boldsymbol{\theta})$.
  Fairly robust, so we only need a *few samples*, typically only a single one!
- **Requires** $q(\boldsymbol{\theta}|\boldsymbol{\lambda})$ to be *reparametrizable*.
- **Requires** $\ln q(\boldsymbol{\theta}|\boldsymbol{\lambda})$ to be *differentiable wrt.* $\boldsymbol{\theta}$.
- **Requires** $\ln p(\mathcal{D}, \boldsymbol{\theta})$ to be *differentiable wrt.* $\boldsymbol{\theta}$.

Conclusion

The "Score function" approach is more general, but "Reparametrization" will usually provide better results quicker when applicable.

Code Task: Reparameterization-gradient for linear regression



- $\boldsymbol{\theta} = \{w_0, w_1\}$, $\boldsymbol{\theta} \sim \mathcal{N}(\mathbf{0}, \sigma_{\boldsymbol{\theta}} \cdot \mathbf{I}_{2\times 2})$
- $Y_i \,|\, \{\boldsymbol{\theta}, x_i, \sigma_y\} \sim \mathcal{N}(w_0 + w_1 \cdot x_i, \sigma_y^2)$

In this task you will implement the score-function gradient:

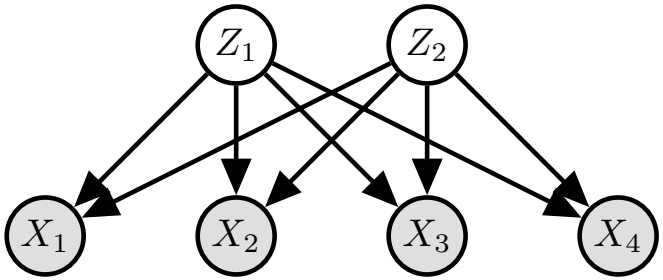
$$\nabla_{\boldsymbol{\lambda}} \mathcal{L}(q) = \mathop{\mathbb{E}}_{\epsilon \sim \phi} \left[\left(\nabla_{\boldsymbol{\theta}} \log p(\boldsymbol{\theta}, \mathcal{D}) - \nabla_{\boldsymbol{\theta}} \log q(\boldsymbol{\theta} \,|\, \boldsymbol{\lambda}) \right) \nabla_{\boldsymbol{\lambda}} f(\boldsymbol{\epsilon}, \boldsymbol{\lambda}) \right]$$

- We provide $\nabla_{\boldsymbol{\theta}} \log p(\boldsymbol{\theta}, \mathcal{D})$, $\nabla_{\boldsymbol{\theta}} \log q(\boldsymbol{\theta} \,|\, \boldsymbol{\lambda})$ and $\nabla_{\boldsymbol{\lambda}} f(\boldsymbol{\epsilon}, \boldsymbol{\lambda})$ for this model.
- Go to `Exercise 2` in

  `Day2/students_BBVI.ipynb`.
- Experiment with the number of Monte-Carlo samples M per iteration, the learning-rate, and the number of iterations. Compare with the output of the Score Function Gradient.

Deep Bayesian Learning – VAE

Starting-point: The factor analysis model, and an extension



$$\mathbf{Z} \sim \mathcal{N}(\mathbf{0}, \mathbf{I})$$

$$\mathbf{X} \,|\, \mathbf{z} \sim \mathcal{N}(\boldsymbol{\mu} + \mathbf{W}^\mathsf{T}\mathbf{z}, \boldsymbol{\Sigma})$$

- The FA model posits that the data $\mathbf{X}$ can be generated from **independent factors** $\mathbf{Z}$ pluss some sensor-noise: $\mathbf{X} \,|\, \mathbf{z} = \boldsymbol{\mu} + \mathbf{W}^\mathsf{T}\mathbf{z} + \boldsymbol{\epsilon}; \boldsymbol{\epsilon} \sim \mathcal{N}(\mathbf{0}, \boldsymbol{\Sigma})$.
- **Simple algorithms** to find estimators $\hat{\boldsymbol{\mu}}$, $\hat{\mathbf{W}}$, and $\hat{\boldsymbol{\Sigma}}$, and closed form expression for $p(\mathbf{z} \,|\, \mathbf{x})$ (which is still a Gaussian).
- The idea is that the factors can be **interpreted** and used for **downstream tasks**. Typically a sparse $\mathbf{W}$ eases the interpretation.

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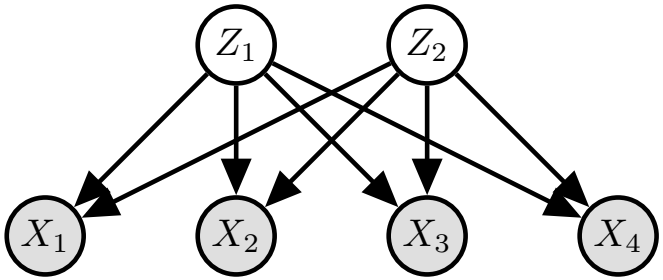

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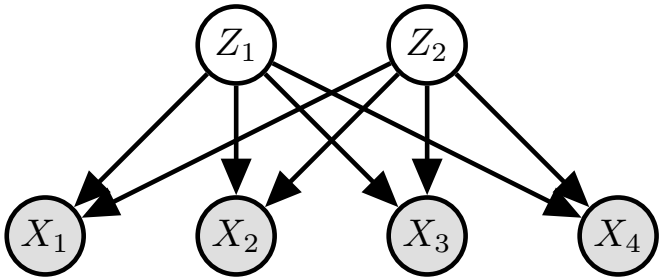
Example: Grades

We observe $\mathbf{x} = \{\texttt{Math}, \texttt{English}, \texttt{Computer Science}, \texttt{German}\}$ for N students, and will examine the data with an FA. Say the model gives us

$$\mathbb{E}[\mathbf{Z} \,|\, \mathbf{x}] = \begin{bmatrix} .25 & .25 & .25 & .25 \\ .50 & 0 & .35 & .15 \end{bmatrix} \cdot \begin{bmatrix} \texttt{Math} \\ \texttt{English} \\ \texttt{Computer Science} \\ \texttt{German} \end{bmatrix}$$

Possible interpretation: $Z_1 \approx$ “Eagerness to learn” and $Z_2 \approx$ “Logical thinking”.

Starting-point: The factor analysis model, and an extension



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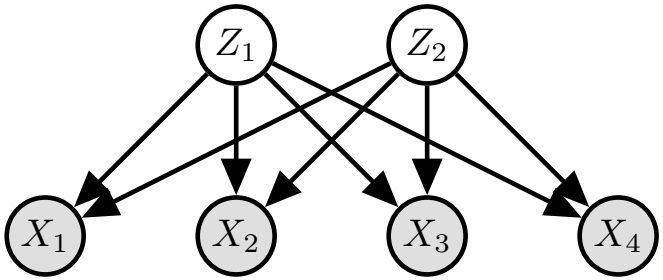
How do we feel about the FA model?

The good: Data is compressed into a (hopefully) interpretable low-dimensional representation.

The bad: The model is restrictive: Assumes everything is Gaussian, and that the relationship from $\mathbf{Z}$ to $\mathbf{X}$ has to be linear.

Starting-point: The factor analysis model, and an extension



VAE: $\mathbf{Z} \sim$ "Whatever", typically still $\mathcal{N}(\mathbf{0}, \mathbf{I})$

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From Factor Analysis to Variational Auto Encoders

VAEs allow the distribution $p(\mathbf{x} \mid \mathbf{z})$ to be **arbitrarily complex** – represented by a DNN. We no longer have analytic estimators for model parameters, cannot easily calculate $p(\mathbf{z} \mid \mathbf{x})$, and it is therefore harder to interpret the factors $\mathbf{Z}$.

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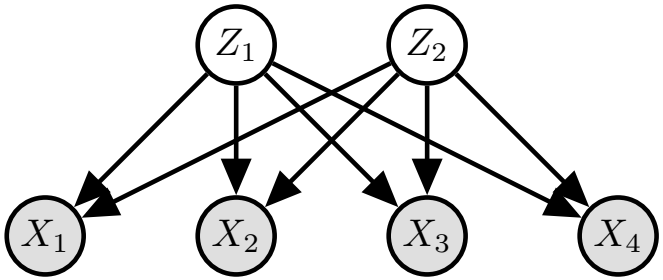

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Why that name?

VAEs are called **auto-encoders** because we can train them by "re-creating" inputs via the process $\mathbf{x} \overset{p(\mathbf{z} \mid \mathbf{x})}{\rightsquigarrow} \mathbf{z} \overset{p(\mathbf{x} \mid \mathbf{z})}{\rightsquigarrow} \hat{\mathbf{x}}$ (and expect to see $\mathbf{x} \approx \hat{\mathbf{x}}$).

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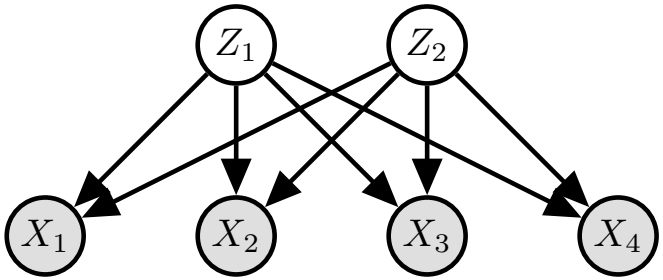

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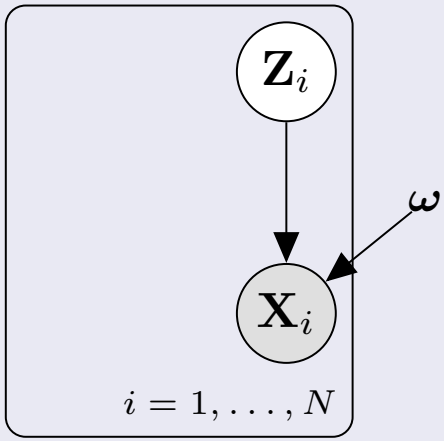
It is a **variational** auto-encoder since we use the variational objective while learning.

Model of interest



- $p(\mathbf{z}_i)$ is (usually) an isotropic Gaussian distribution.
- $p_{\boldsymbol{\omega}}(\mathbf{x}_i \mid g_{\boldsymbol{\omega}}(\mathbf{z}_i))$, where g is a deep neural network.

$$p_{\boldsymbol{\omega}}(\mathbf{x}_i|\mathbf{z}_i) \sim \text{Bernoulli}(\text{logits} = g_{\boldsymbol{\omega}}(\mathbf{z}_i))$$

- $g_{\boldsymbol{\omega}}(\mathbf{z}_i)$ plays the role of a **DECODER NETWORK**.
- Learn $\boldsymbol{\omega}$ to maximize the model's fit to $\mathcal{D}$.
  - We will cheat and find a **point estimate** for $\boldsymbol{\omega}$.

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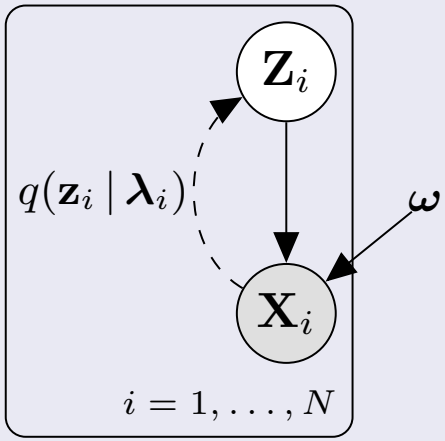

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Variational Inference

- We will need $p_{\boldsymbol{\omega}}(\mathbf{z}_i \mid \mathbf{x}_i)$ for each data-point $\mathbf{x}_i$:

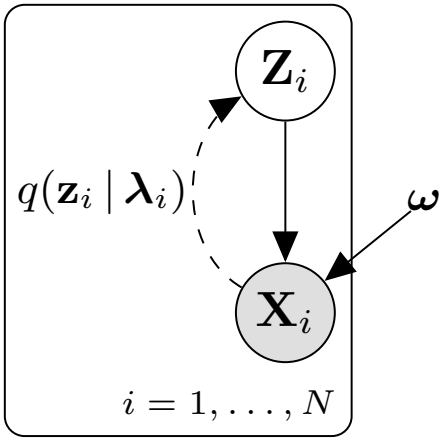
$$p_{\boldsymbol{\omega}}(\mathbf{z}_i \mid \mathbf{x}_i) = \frac{p_{\boldsymbol{\omega}}(\mathbf{z}_i) \cdot p_{\boldsymbol{\omega}}(\mathbf{x}_i \mid g_{\boldsymbol{\omega}}(\mathbf{z}_i))}{\int_{\mathbf{z}_i} p_{\boldsymbol{\omega}}(\mathbf{z}_i) \cdot p_{\boldsymbol{\omega}}(\mathbf{x}_i \mid g_{\boldsymbol{\omega}}(\mathbf{z}_i)) \, \mathrm{d}\mathbf{z}_\mathrm{i}}.$$

- **Initial plan:** Fit $q(\mathbf{z}_i \mid \boldsymbol{\lambda}_i)$ to $p_{\boldsymbol{\omega}}(\mathbf{z}_i \mid \mathbf{x}_i)$ using variational inference.

Initial plan:

- Optimize the ELBO

$$\mathcal{L}(\boldsymbol{\omega}, \boldsymbol{\lambda}_1, \ldots, \boldsymbol{\lambda}_N) = -\mathbb{E}_q \left[\log \frac{\prod_{i=1}^N q(\mathbf{z}_i \mid \boldsymbol{\lambda}_i)}{\prod_{i=1}^N p_{\boldsymbol{\omega}}(\mathbf{z}_i, \mathbf{x}_i)} \right].$$



- A natural model for $q(\mathbf{z}_i \mid \boldsymbol{\lambda}_i)$ is a Gaussian with parameters $\boldsymbol{\lambda}_i = \{\boldsymbol{\mu}_i, \boldsymbol{\Sigma}_i\}$.
- If $\mathbf{Z}_i$ is d-dim and we for simplicity assume diagonal $\boldsymbol{\Sigma}_i$, this still gives $2Nd$ variational parameters to learn.
- An $\tilde{\mathbf{x}} \notin \mathcal{D}$ at query time will be problematic.

Initial plan:

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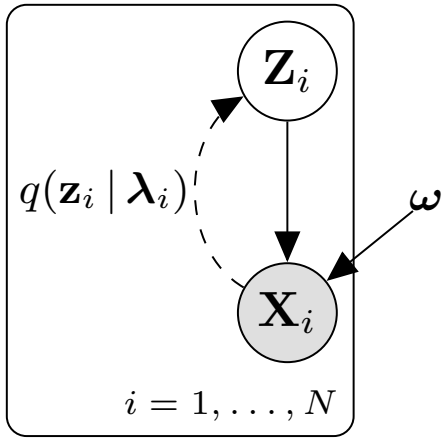

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A better plan

- Assume $g_{\boldsymbol{\omega}}(\mathbf{z})$ is smooth: $\mathbf{z}_i$ and $\mathbf{z}_j$ are "close" $\Rightarrow$ $\mathbf{x}_i$ and $\mathbf{x}_j$ are "close".

  $\rightsquigarrow$ If $\mathbf{x}_i$ and $\mathbf{x}_j$ are "close", then $\boldsymbol{\lambda}_i$ and $\boldsymbol{\lambda}_j$ should be "close", too.

- **Therefore:** Let's assume there exists a (smooth) function $h(\mathbf{x})$ so that $h(\mathbf{x}_i) = \boldsymbol{\lambda}_i$.
- $h(\cdot)$ is unavailable, so represent it using a deep neural net and learn the weights.
- $h(\mathbf{x}_i)$ plays the role of an **ENCODER NETWORK**.

Amortized inference:
To learn a model $h(\cdot)$, typically a deep neural network, so that $h(\mathbf{x}_i) = \boldsymbol{\lambda}_i$.
$h(\cdot)$ is parameterized with weights, often (abusing notation) denoted by $\boldsymbol{\lambda}$.

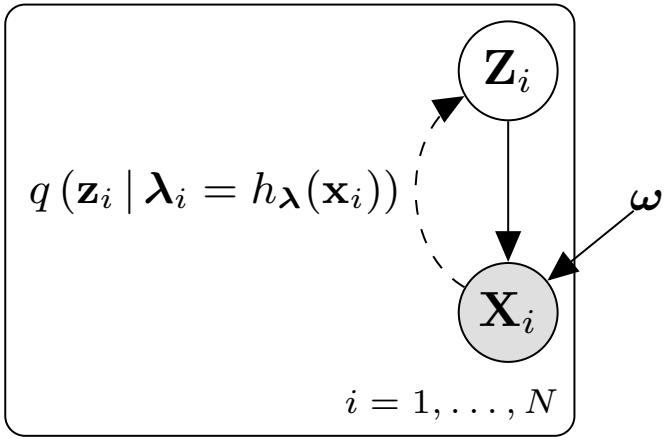
Note! Amortized inference is useful also outside VAEs!

Benefits:

- The $2Nd$ parameters $\{\boldsymbol{\lambda}_i\}_{i=1}^N$ are replaced by the fixed-sized vector $\boldsymbol{\lambda}$.
  - If N is large we may get a simpler learning problem.
- Smoothness of $h(\cdot)$ implies regularization.
- We only change the **parameterization**, not the model itself!

The full VAE approach:

- $p(\mathbf{z}_i)$ is an isotropic Gaussian distribution.
- $p_{\boldsymbol{\omega}}(\mathbf{x}_i|\mathbf{z}_i) \sim$ Bernoulli(logits $= g_{\boldsymbol{\omega}}(\mathbf{z}_i)$), where $g_{\boldsymbol{\omega}}$ is a DNN with weights $\boldsymbol{\omega}$.
- $q(\mathbf{z}_i \,|\, \mathbf{x}_i, \boldsymbol{\lambda}) \sim \mathcal{N}(\boldsymbol{\mu}_i, \boldsymbol{\Sigma}_i)$, where $\{\boldsymbol{\mu}_i, \boldsymbol{\Sigma}_i\}$ is given by $h_{\boldsymbol{\lambda}}(\mathbf{x}_i)$. $h_{\boldsymbol{\lambda}}$ is a DNN with weights $\boldsymbol{\lambda}$.

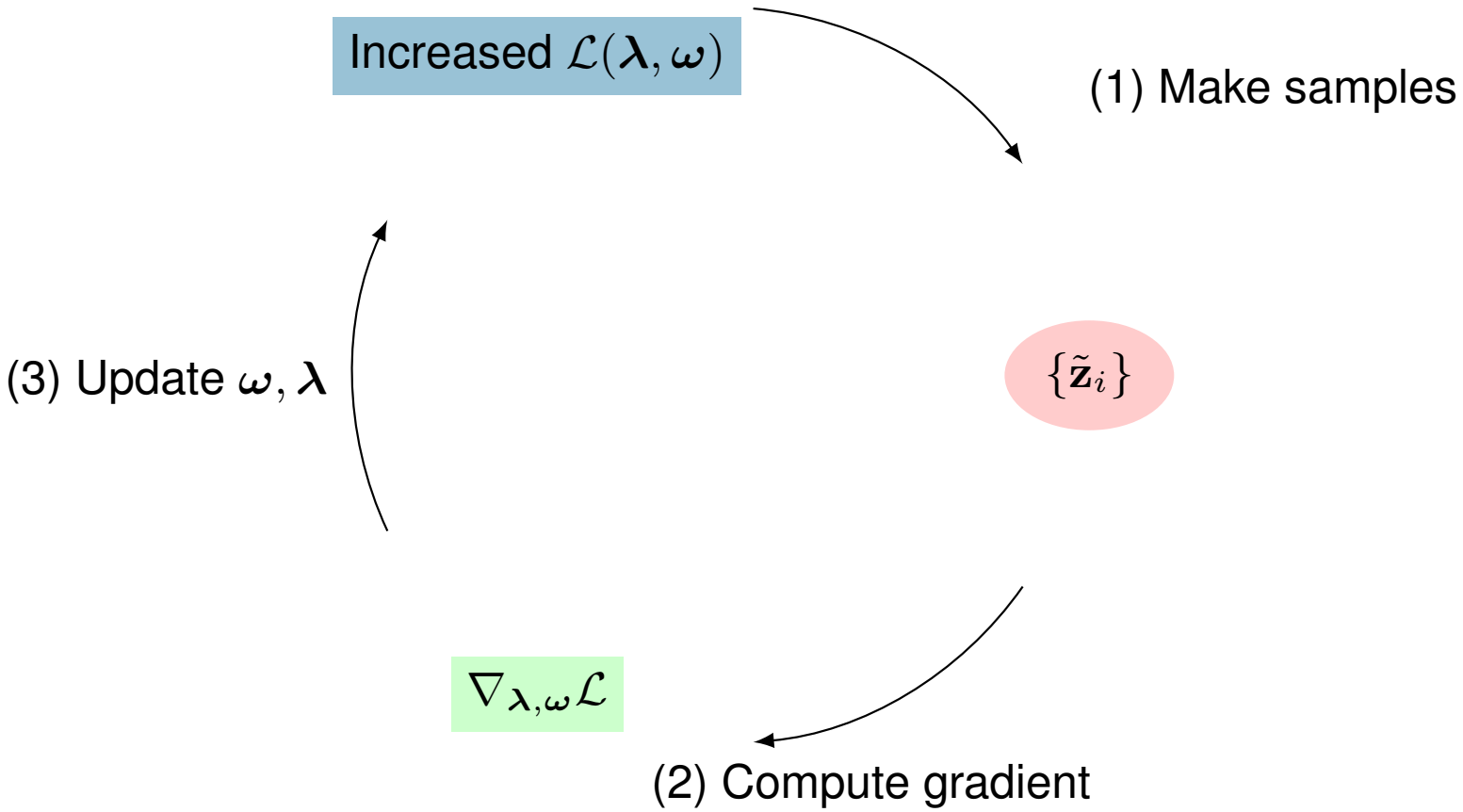


Goal:

Learn **both** $\boldsymbol{\omega}$ and $\boldsymbol{\lambda}$ by maximizing the ELBO:

$$\mathcal{L}(\boldsymbol{\lambda}, \boldsymbol{\omega}) = -\mathbb{E}_q \left[\log \frac{q(\mathbf{z} \,|\, \mathbf{x}, \boldsymbol{\lambda})}{p_{\boldsymbol{\omega}}(\mathbf{z}, \mathbf{x} \,|\, \boldsymbol{\omega})} \right].$$

ELBO for VAEs



1. For each $\mathbf{x}_i$, sample M (typically $M = 1$) $\boldsymbol{\epsilon}$-values to get $\mathbf{z}_i$ samples.
2. Calculate $\nabla_{\boldsymbol{\lambda},\boldsymbol{\omega}}\, \mathcal{L}(\boldsymbol{\lambda}, \boldsymbol{\omega})$ using the reparameterization-trick.
3. Update parameters using a standard DL optimizer (like Adam).

Sidestep: Automatic Variational Inference in PPLs

1. Manual : Define your data model $p(\mathcal{D}|\boldsymbol{\theta})$ and the prior $p(\boldsymbol{\theta})$.
2. Automatic : Define the set of variational distributions $q(\boldsymbol{\theta}|\boldsymbol{\lambda}) \in \mathcal{Q}$.
   (In *complicated* situations this step may have to be Manual).
3. Automatic : Optimize ELBO: $\boldsymbol{\lambda}_{t+1} = \boldsymbol{\lambda}_t + \rho \nabla_{\boldsymbol{\lambda}} \mathcal{L}(\boldsymbol{\lambda}_t)$ using an AutoDiff. engine.
4. Automatic : Find $q(\boldsymbol{\theta}|\boldsymbol{\lambda}^\star) = \arg\min_{q \in \mathcal{Q}} \mathrm{KL}\left(q(\boldsymbol{\theta}|\boldsymbol{\lambda}) || p(\boldsymbol{\theta}|\mathcal{D})\right)$.

Probabilistic Programming Languages and Box's loop

Modern PPLs relieve us of all the computational details!

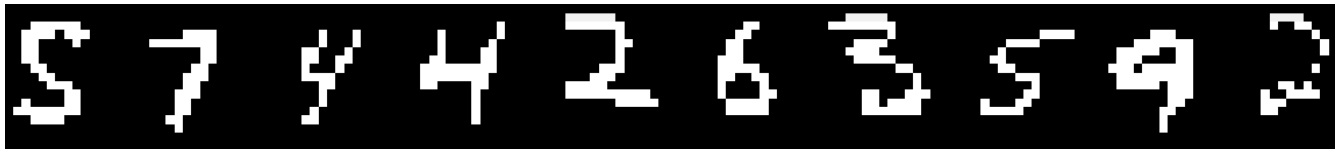
Instead we can focus on . . .

- Building models (define $p(\mathcal{D}|\boldsymbol{\theta})$ and $p(\boldsymbol{\theta})$) we believe in.
- Using computed results to validate/critique and iteratively refine the model.

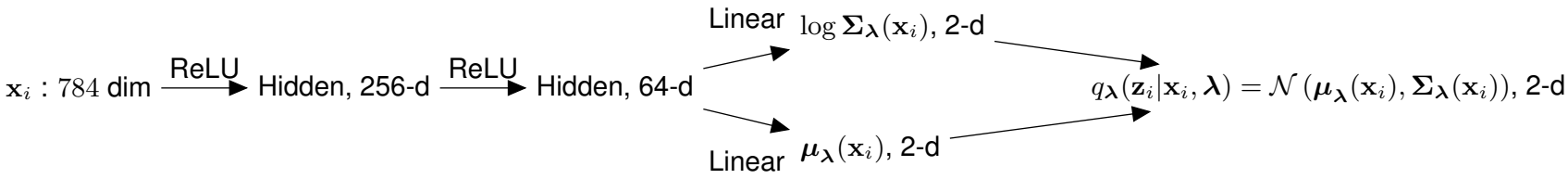
This is known as the "build – compute – critique – repeat" - cycle.

Fun with MNIST – With simple model evaluation

- The model is learned from $N = 55.000$ training examples.
- Each $\mathbf{x}_i$ is a binary vector of 784 pixel values.
- When seen as a 28×28 array, each $\mathbf{x}_i$ is a picture of a handwritten digit ("0" – "9").

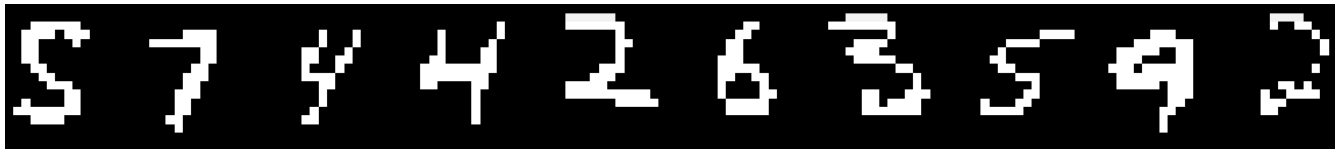


- Encoding is done in **two** dimensions. $p(\mathbf{z}_i) = \mathcal{N}(\mathbf{0}_2, \mathbf{I}_2)$.
- The **encoder network** $\mathbf{X} \rightsquigarrow \mathbf{Z}$.



Fun with MNIST – With simple model evaluation

- The model is learned from $N = 55.000$ training examples.
- Each $\mathbf{x}_i$ is a binary vector of 784 pixel values.
- When seen as a 28×28 array, each $\mathbf{x}_i$ is a picture of a handwritten digit ("0" – "9").



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- The **encoder network** $\mathbf{X} \rightsquigarrow \mathbf{Z}$.
- The **decoder network** $\mathbf{Z} \rightsquigarrow \mathbf{X}$ is a $64 + 256$ neural net with ReLU units.

$$\mathbf{z}_i : 2 \text{ dim} \xrightarrow{\text{ReLU}} \text{Hidden, 64-d} \xrightarrow{\text{ReLU}} \text{Hidden, 256-d} \xrightarrow{\text{Linear}} \text{logit}(\mathbf{p}_i), \text{ 784-d} \longrightarrow p_{\boldsymbol{\omega}}(\mathbf{x}_i \mid \mathbf{z}_i, \boldsymbol{\omega}) = \text{Bernoulli}(\mathbf{p}_i), \text{ 784-d}$$

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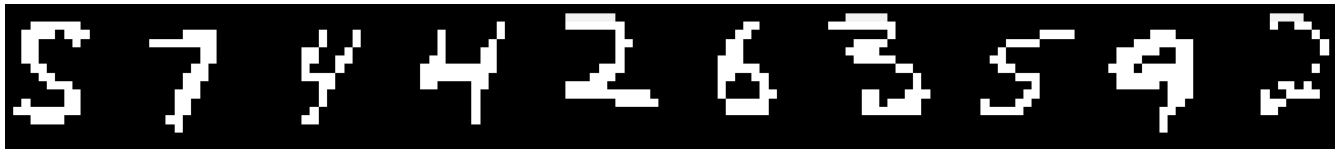

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- The **decoder network** $\mathbf{Z} \rightsquigarrow \mathbf{X}$.

Next up: Model validations – Dislaimer

The next few slides show **very simple** qualitative model critiques. These checks are by no means comprehensive, and in fact quite naïve.

See, e.g., D. Blei (2014): "*Build, Compute, Critique, Repeat: Data Analysis with Latent Variable Models*" and A. Gelman et al. (2020): "*Bayesian workflow*" for how it **should** be done.

Trying to reconstruct $\mathbf{x}$ by $\mathbb{E}_{p_\theta}[\mathbf{X} \mid \mathbf{Z} = \mathbb{E}_{q_\lambda}[\mathbf{Z} \mid \mathbf{x}]]$

An initial indication of performance:

1. For some $\mathbf{x}_0$, calculate $\mathbf{z}_0 \leftarrow \mathbb{E}_{q_\lambda}[\mathbf{Z} \mid \mathbf{X} = \mathbf{x}_0]$
2. ... and $\tilde{\mathbf{x}} \leftarrow \mathbb{E}_{p_\theta}[\mathbf{X} \mid \mathbf{Z} = \mathbf{z}_0]$.
3. Compare $\mathbf{x}_0$ and $\tilde{\mathbf{x}}$ visually.

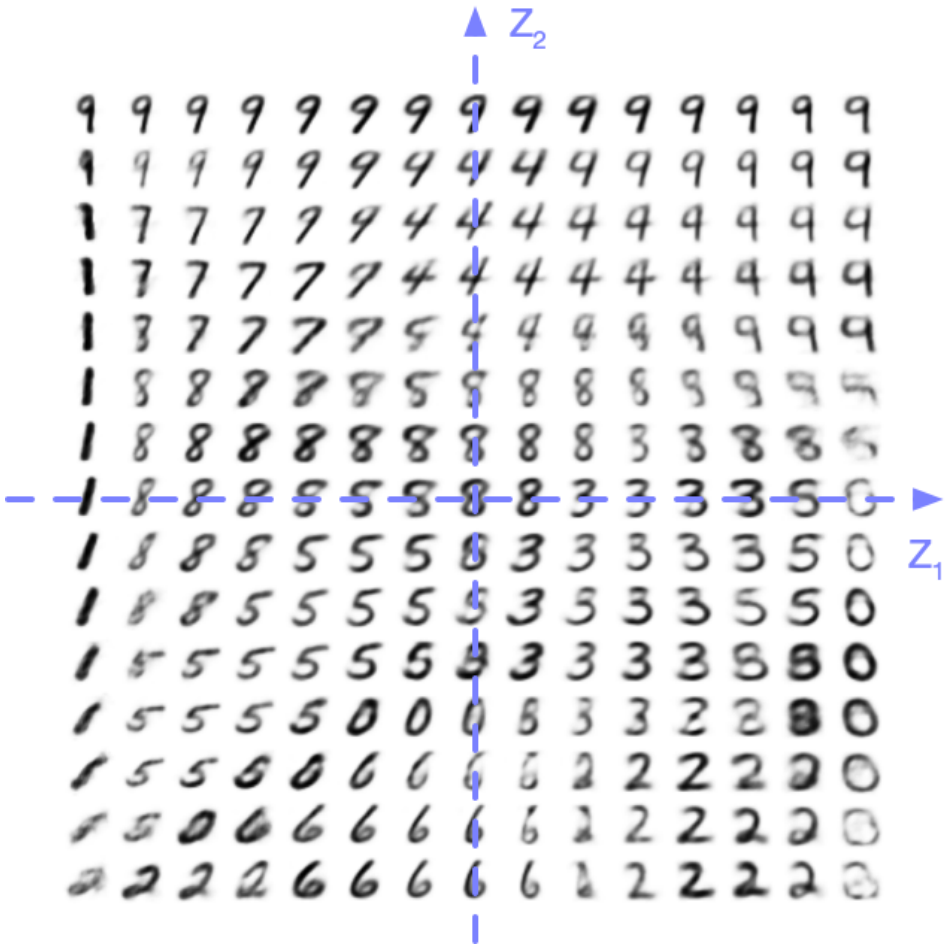
Test-set examples

Training examples (at end of training)

The picture manifold – $\mathbb{E}_{p_{\boldsymbol{\omega}}}[\mathbf{X} \mid \mathbf{z}]$ for different values of $\mathbf{z}$

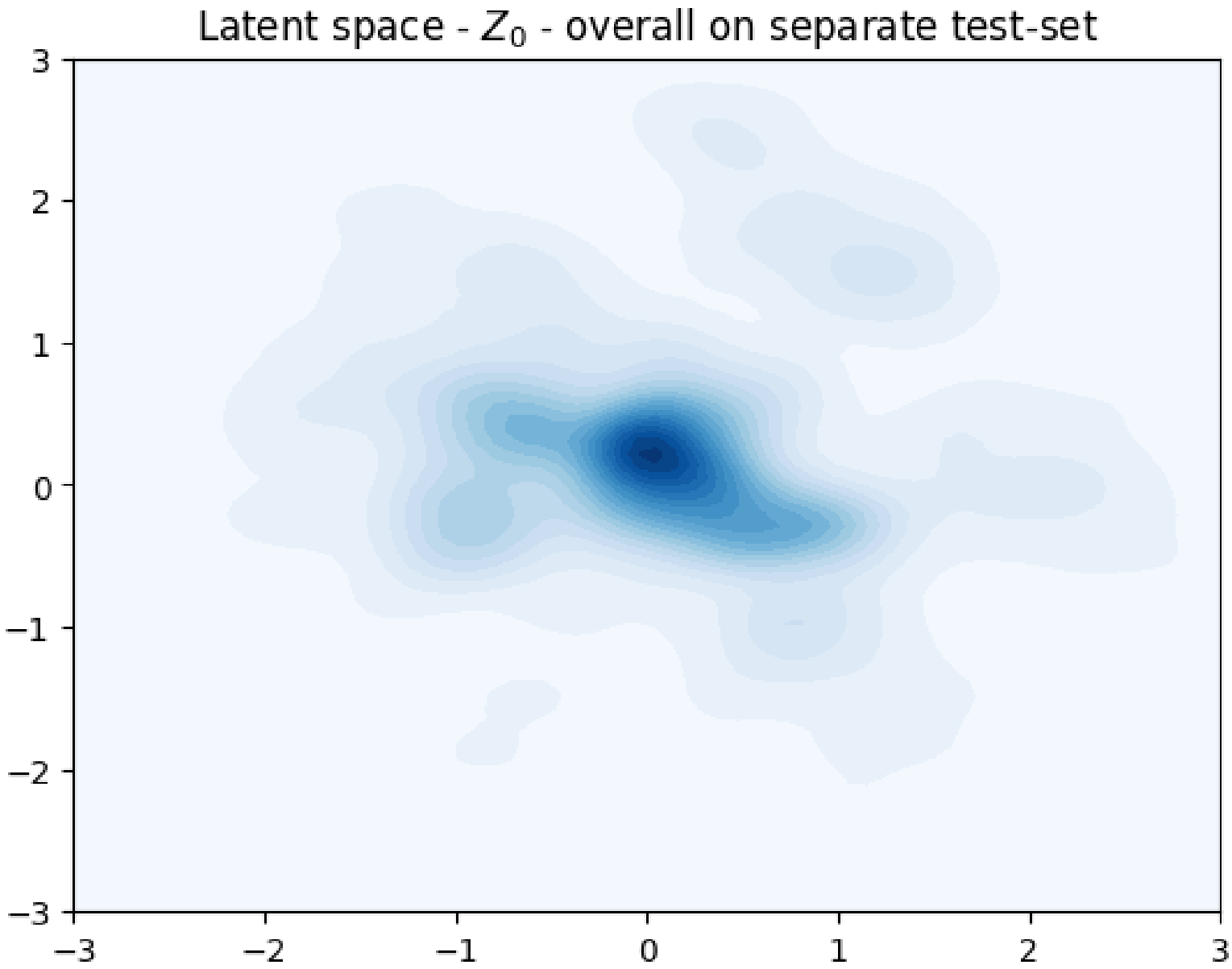
Using a VAE for generation

- The VAE is a **deep generative model** – albeit not a fancy one.
- **Process:** Sample $\mathbf{Z}_0 \sim p(\mathbf{z})$, then sample an $\mathbf{X} \sim p_{\boldsymbol{\omega}}(\mathbf{x} \mid \mathbf{z}_0)$.

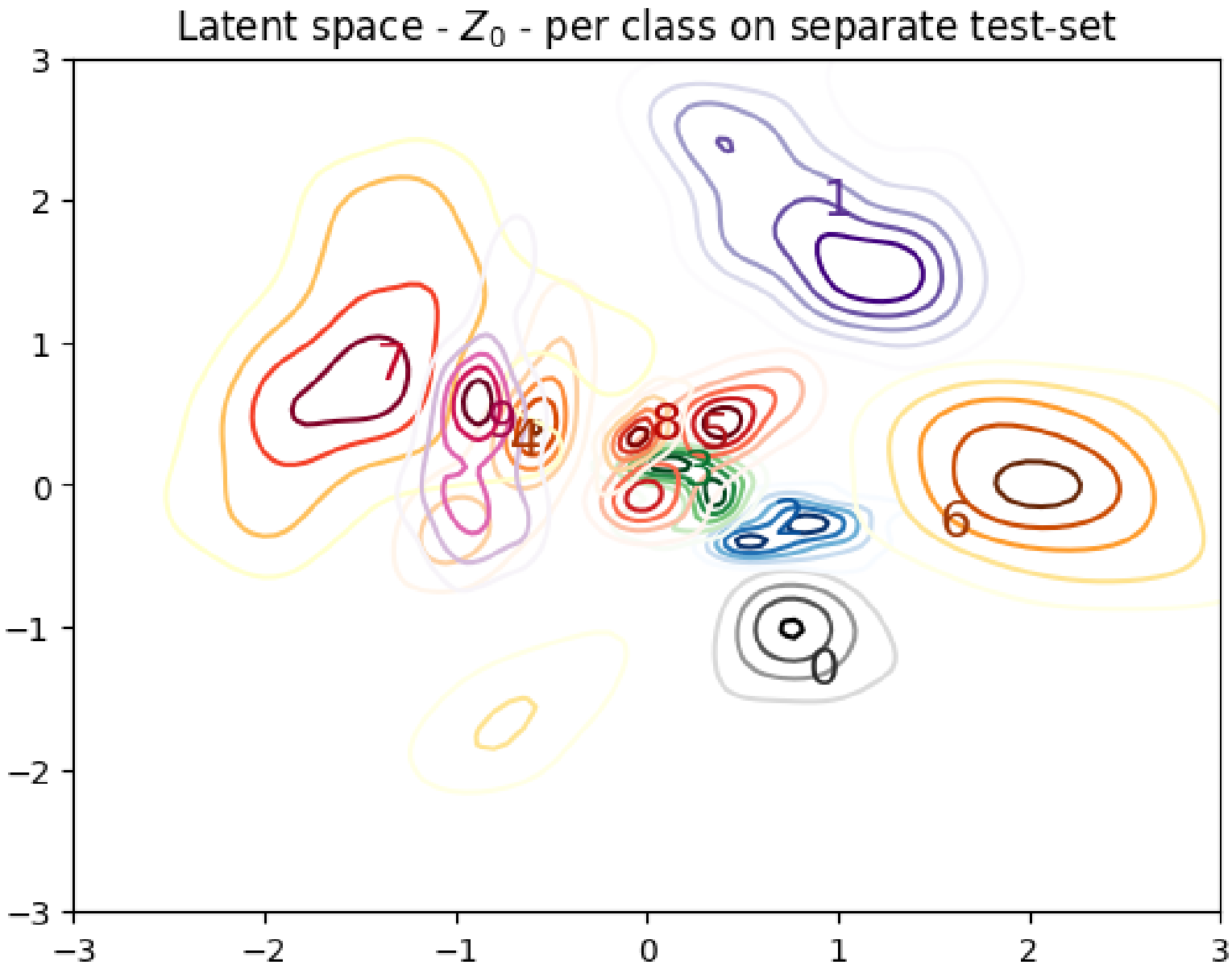


Generative ability, shown through $\mathbb{E}_{\mathbf{x} \sim p_{\boldsymbol{\omega}}}[\mathbf{X} \mid \mathbf{z}]$ for different values of $\mathbf{z}$.

Averaged distribution over $\mathbb{Z}$



Averaged distribution over $\mathbb{Z}$ – per class



Probabilistic programming: Variational inference in Pyro

Pyro

Pyro (`pyro.ai`) is a Python library for probabilistic modeling, inference, and criticism, integrated with PyTorch.

Modeling:
- Directed graphical models
- Neural networks (via `nn.Module`)
- ...

Inference:
- Variational inference – including BBVI, SVI
- Monte Carlo – including Importance sampling and Hamiltonian Monte Carlo
- ...

Criticism:
- Point-based evaluations
- Posterior predictive checks
- ...

... and there are also many other possibilities

`Tensorflow` is integrating probabilistic thinking into its core, `InferPy` is a local alternative, etc.

Simple example

$$\begin{aligned} \text{temp} &\sim \mathcal{N}(15, 2) \\ \text{sensor} &\sim \mathcal{N}(\text{temp}, 1) \end{aligned}$$

$$p(\text{sensor} = 18, \text{temp})$$

Simple example

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Pyro models:

- random variables $\Leftrightarrow$ `pyro.sample`
- observations $\Leftrightarrow$ `pyro.sample` with the `obs` argument

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Pyro models:

- random variables $\Leftrightarrow$ `pyro.sample`
- observations $\Leftrightarrow$ `pyro.sample` with the `obs` argument

```
#The observatons
obs = {'sensor': torch.tensor(18.0)}

def model(obs):
    temp = pyro.sample('temp', dist.Normal(15.0, 2.0))
    sensor = pyro.sample('sensor', dist.Normal(temp, 1.0), obs=obs['sensor'])
```

Inference Problem

$$p(\text{temp}|\text{sensor} = 18)$$

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Variational Solution

$$\min_{q} \mathrm{KL}\left(q(\text{temp})||p(\text{temp}|\text{sensor} = 18)\right)$$

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Pyro Guides:

- Define the q **distributions** in variational settings.

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$$p(\text{temp}|\text{sensor} = 18)$$

Variational Solution

$$\min_{q} \mathrm{KL}\left(q(\text{temp})||p(\text{temp}|\text{sensor} = 18)\right)$$

Pyro Guides:

- Define the q **distributions** in variational settings.
- Build **proposal distributions** in importance sampling, MCMC.
- ...

Pyro Guides:

- Guides are **arbitrary stochastic functions**.
- Guides produces samples for those variables of the model which are **not observed**.

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- Guides are **arbitrary stochastic functions**.
- Guides produces samples for those variables of the model which are **not observed**.

Guide requirements

1. the guide has the same input signature as the model
2. all unobserved sample statements that appear in the model appear in the guide.

Example

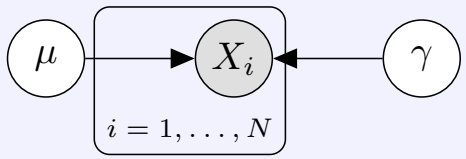
```
#The observatons
obs = {'sensor': torch.tensor(18.0)}

def model(obs):
    temp = pyro.sample('temp', dist.Normal(15.0, 2.0))
    sensor = pyro.sample('sensor', dist.Normal(temp, 1.0), obs=obs['sensor'])
```

```
#The guide
def guide(obs):
    a = pyro.param("mean", torch.tensor(0.0))
    b = pyro.param("scale", torch.tensor(1.), constraint=constraints.positive)
    temp = pyro.sample('temp', dist.Normal(a, b))
```

Exercise: Pyro implementation for a simple Gaussian model

`Day2-AfterLunch/student_simple_gaussian_model_pyro.ipynb`



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

- Implement a pyro **guide** for the graphical model above.
- Specify suitable **variational approximation** in the form of a Pyro guide.

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

- **Check** the differences with the following notebook (no Pyro implementation).

`Day2-BeforeLunch/student_simple_model.ipynb`

Code Task: Play with VAEs

- We provide a VAE with a **linear decoder** implemented in Pyro. You will extend it!
- **Exercise (summary):**
  - Define a Non-Linear Decoder, e.g., an MLP with a hidden layer and non-linearities (e.g. Relu).
  - Explore the latent space when moving from linear to non-linear decoders with different capacity.
- Notebook:

`Day2/students_VAE.ipynb`.

Conclusions

- **Bayesian Machine Learning**
  - Represents unobserved quantities using **distributions**
  - Represents **epistemic** uncertainty using $p(\boldsymbol{\theta} \mid \mathcal{D})$

- **Bayesian Machine Learning**

- **Variational inference**
  - **Provides $q(\boldsymbol{\theta} \mid \boldsymbol{\lambda})$:** A distributional approximation to $p(\boldsymbol{\theta} \mid \mathcal{D})$
  - **Objective:** $\arg\min_{\boldsymbol{\lambda}} \mathrm{KL}\left(q(\boldsymbol{\theta} \mid \boldsymbol{\lambda}) || p(\boldsymbol{\theta} \mid \mathcal{D})\right) \Leftrightarrow \arg\max_{\boldsymbol{\lambda}} \mathcal{L}\left(q(\boldsymbol{\theta} \mid \boldsymbol{\lambda})\right)$
  - **Mean-field:** Divide and conquer strategy for high-dimensional posteriors
  - **Main caveat:** $q(\boldsymbol{\theta} \mid \boldsymbol{\lambda})$ underestimates the uncertainty of $p(\boldsymbol{\theta} \mid \mathcal{D})$

Recap & Conclusions

- **Bayesian Machine Learning**
- **Variational inference**
- **Coordinate Ascent Variational Inference**
  - Analytic expressions for some models (i.e., conjugate exponential family)
  - CAVI is very **efficient and stable** if it can be used
  - In principle requires **manual derivation** of updating equations
    - There are **tools** to help (using *variational message passing*)

Recap & Conclusions

- **Bayesian Machine Learning**
- **Variational inference**
- **Coordinate Ascent Variational Inference**
- **Gradient-based Variational Inference**
  - Provides the tools for VI over **arbitrary** probabilistic models
  - Directly integrates with the tools of deep learning
    - Automatic differentiation, sampling from standard distributions, and SGD
  - Sampling to approximate expectations: **Beware of the variance!**

Recap & Conclusions

- **Bayesian Machine Learning**
- **Variational inference**
- **Coordinate Ascent Variational Inference**
- **Gradient-based Variational Inference**
- **Probabilistic programming languages**
  - PPLs fuel the “build – compute – critique – repeat” - cycle through
    - ease and flexibility of modelling
    - powerful inference engines
    - efficient model evaluations
  - Many available tools (Pyro, TF Probability, Turing.jl, . . .)

Recap & Conclusions

- **Bayesian Machine Learning**
- **Variational inference**
- **Coordinate Ascent Variational Inference**
- **Gradient-based Variational Inference**
- **Probabilistic programming languages**
- **What's next?**
  - The "VI toolbox" is reaching maturity
    - From *only* a research area to almost a *prerequisite* for Probabilistic AI
    - ... yet there are still things to explore further!
  - Today's material should suffice to read (and write!) Prob-AI papers