Nordic probabilistic AI school

Variational Inference and Optimization

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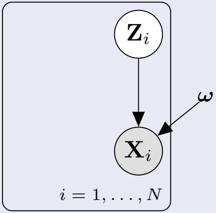
Deep Bayesian Learning – The VAE

The Variational Auto Encoder (VAE)

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**.
- **Goal:** 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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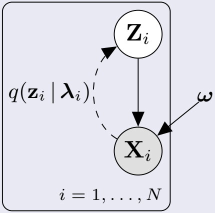

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Variational Inference

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

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

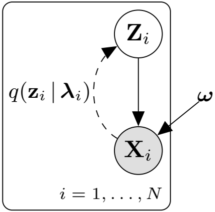
- **Initial plan:** Fit $q(\mathbf{z}_i \mid \boldsymbol{\lambda}_i)$ to $p_{\boldsymbol{\omega}}(\mathbf{z}_i \mid \mathbf{x}_i)$ using variational inference.

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.



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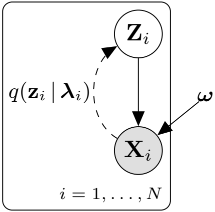

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A better plan

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

  $\rightsquigarrow$ $\boldsymbol{\lambda}_i$ and $\boldsymbol{\lambda}_j$ should be "close" if $\mathbf{x}_i$ and $\mathbf{x}_j$ are "close".

- **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!

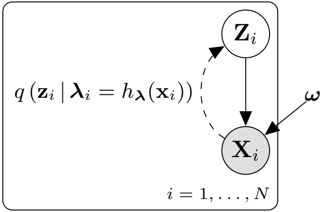
Benefits:

- 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!

VAE: Full setup

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 $\boldsymbol{\lambda}$.

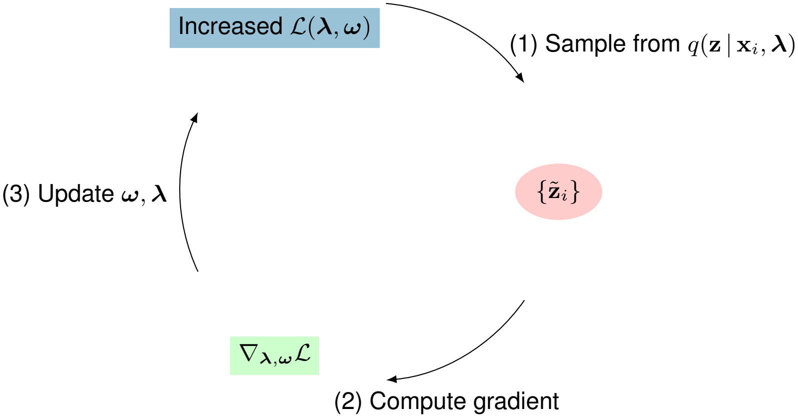


Goal:

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

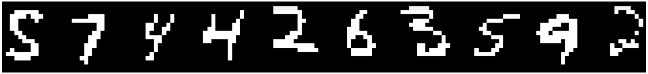
$$\mathcal{L}(\boldsymbol{\lambda}, \boldsymbol{\omega}) = -\mathbb{E}_q\left[\log \frac{q(\mathbf{z} \,|\, \mathbf{x}, \boldsymbol{\lambda})}{p_{\boldsymbol{\omega}}(\mathbf{z}, \mathbf{x} \,|\, \boldsymbol{\omega})}\right].$$

ELBO for VAEs



1. For each $\mathbf{x}_i$, sample M (typically 1) $\mathbf{z}$-values to approximate expectation in $\nabla\mathcal{L}$.
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).

- 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”).



Fun with MNIST – The model

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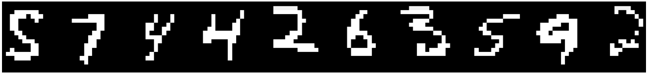

- Encoding is done in **two** dimensions. $p(\mathbf{z}_i) = \mathcal{N}(\mathbf{0}_2, \mathbf{I}_2)$.
- The **encoder network** $\mathbf{X} \rightsquigarrow \mathbf{Z}$.

$\mathbf{x}_i : 784$ dim $\xrightarrow{\text{ReLU}}$ Hidden, 256-d $\xrightarrow{\text{ReLU}}$ Hidden, 64-d

Hidden, 64-d $\xrightarrow{\text{Linear}}$ $\log \boldsymbol{\Sigma}_{\boldsymbol{\lambda}}(\mathbf{x}_i)$, 2-d

Hidden, 64-d $\xrightarrow{\text{Linear}}$ $\boldsymbol{\mu}_{\boldsymbol{\lambda}}(\mathbf{x}_i)$, 2-d

$\log \boldsymbol{\Sigma}_{\boldsymbol{\lambda}}(\mathbf{x}_i)$, $\boldsymbol{\mu}_{\boldsymbol{\lambda}}(\mathbf{x}_i)$ $\rightarrow$ $q_{\boldsymbol{\lambda}}(\mathbf{z}_i|\mathbf{x}_i, \boldsymbol{\lambda}) = \mathcal{N}(\boldsymbol{\mu}_{\boldsymbol{\lambda}}(\mathbf{x}_i), \boldsymbol{\Sigma}_{\boldsymbol{\lambda}}(\mathbf{x}_i))$, 2-d

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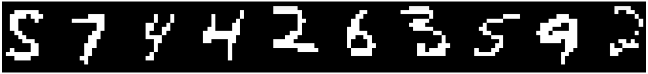

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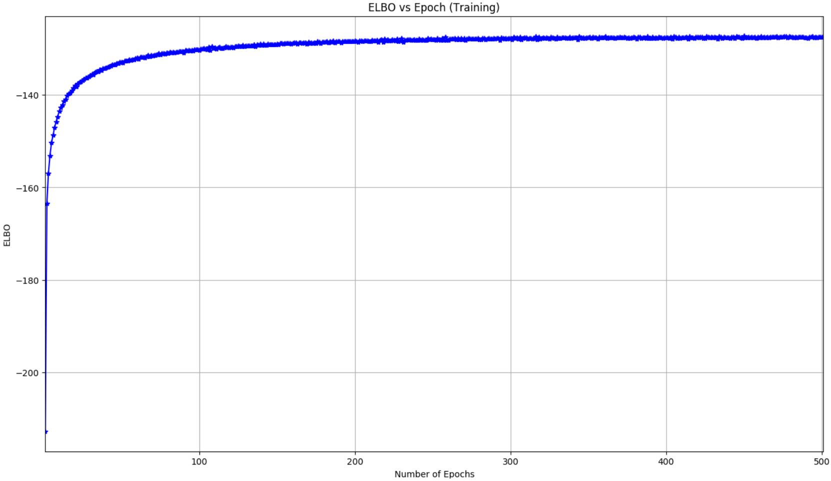
- The **encoder network** $\mathbf{X} \rightsquigarrow \mathbf{Z}$.
- The **decoder network** $\mathbf{Z} \rightsquigarrow \mathbf{X}$ is a $64 + 256$ neural net with ReLU units.

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

Learning progress; learning rate $\rho = 10^{-4}$, $M = 1$



Note! SGD algorithm uses the negative ELBO as loss.

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

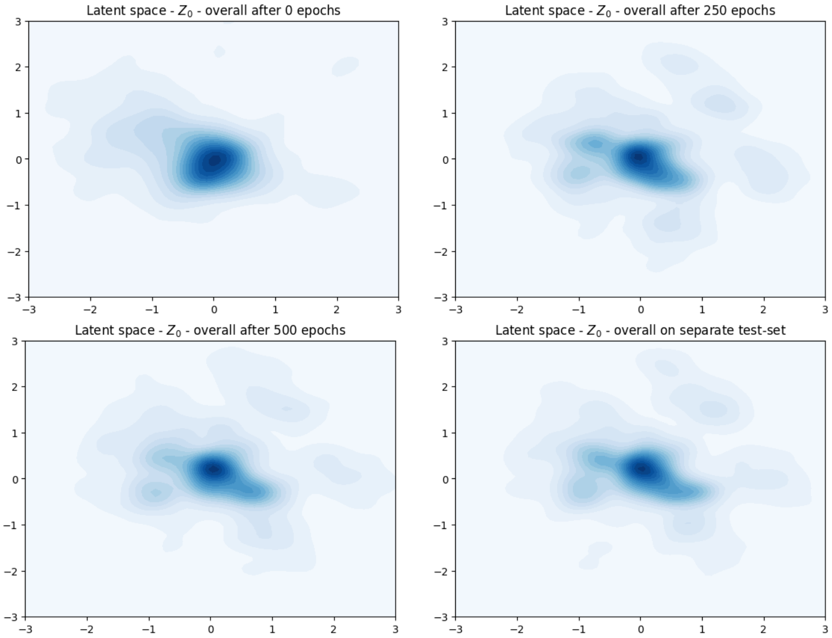
After 1 epoch

After 250 epochs

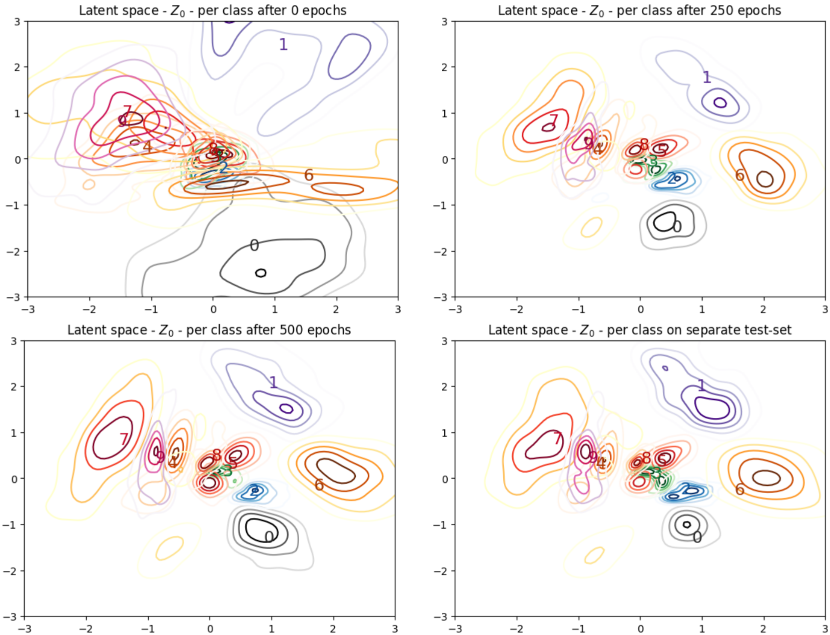
After 500 epoch

Using separate test-set

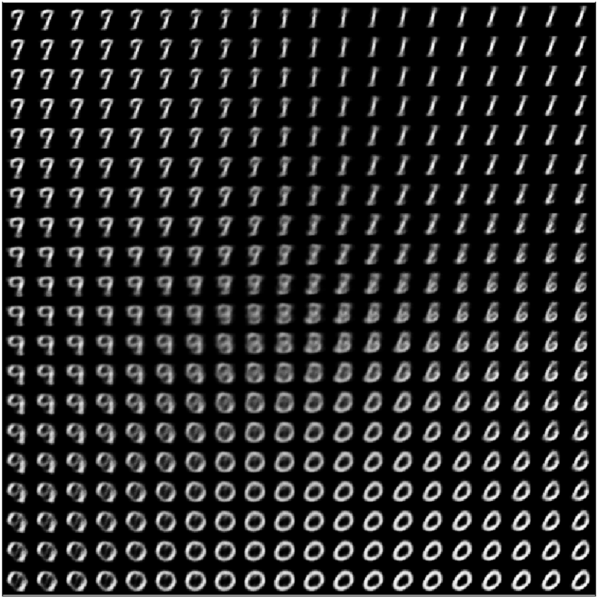
Averaged distribution over $\mathbf{Z}$



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



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



Manifold after 1 epoch

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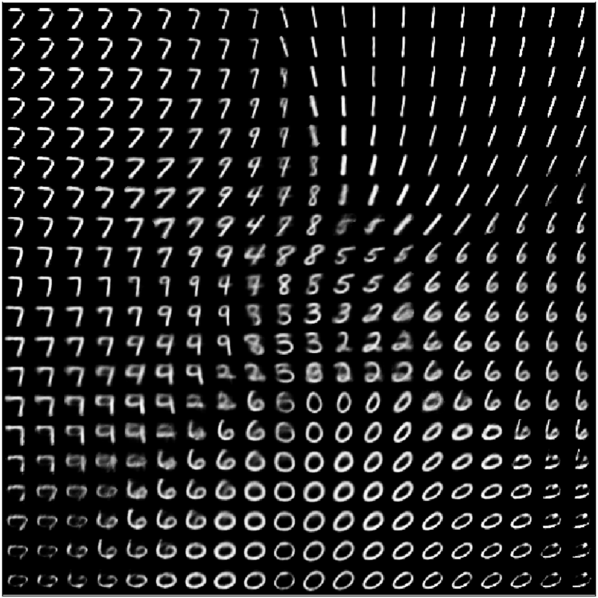
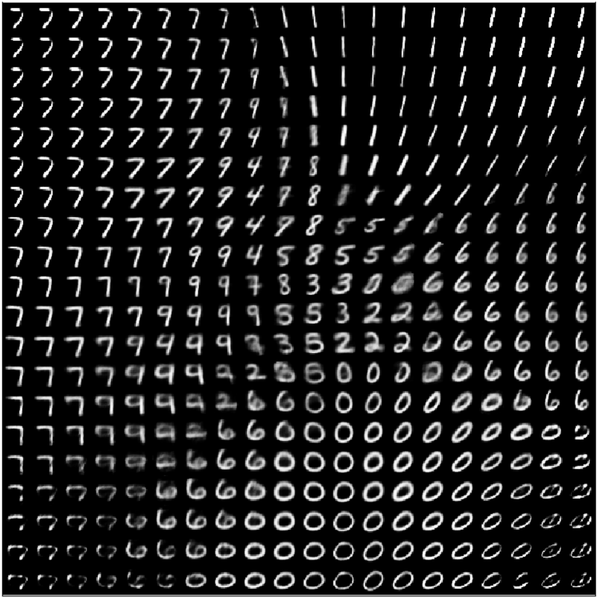


Manifold after 250 epochs

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

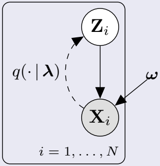


Manifold after 500 epochs

Variational Auto-Encoders in Pyro

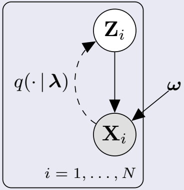
Notes

- The PYRO.MODULE call registers the parameters in the decoder network with Pyro.
- The decoder network is a subclass of NN.MODULE; the class inherits methods such as PARAMETERS() and BACKWARD for calculating gradients.



Notes

- The encoder and guide follow the same structure as the encoder and model



Code Task: VAEs in Pyro

- Learn how a VAE is coded in Pryo.
- We provide a VAE with a **linear decoder**.
- **Exercise 1: Define a Non-Linear Decoder**
  - A MLP with a hidden layer with non-linearities (e.g. Relu).
- **Exercise 2: Explore the latent space**
  - Moving from linear to non-linear decoders with different capacity.
- Notebook:

  `Day2-Evening/students_VAE.ipynb`.

Conclusions

- **Bayesian Machine Learning**
  - Represents unobserved quantities using **distributions**
  - Models **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, Infer.net, 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