

Nordic probabilistic AI school

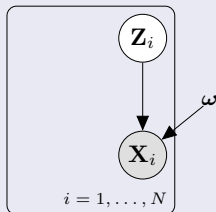
Variational Inference and Optimization

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Deep Bayesian Learning – VAE

Model of interest

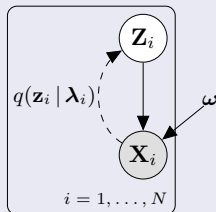


- $p(\mathbf{z}_i)$ is (usually) an isotropic Gaussian distribution.
- $p_{\omega}(\mathbf{x}_i | g_{\omega}(\mathbf{z}_i))$, where g is a deep neural network.

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

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

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Variational Inference

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

$$p_\omega(\mathbf{z}_i | \mathbf{x}_i) = \frac{p_\omega(\mathbf{z}_i) \cdot p_\omega(\mathbf{x}_i | g_\omega(\mathbf{z}_i))}{\int_{\mathbf{z}_i} p_\omega(\mathbf{z}_i) \cdot p_\omega(\mathbf{x}_i | g_\omega(\mathbf{z}_i)) d\mathbf{z}_i}.$$

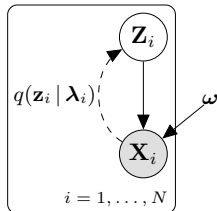
- **Initial plan:** Fit $q(\mathbf{z}_i | \lambda_i)$ to $p_\omega(\mathbf{z}_i | \mathbf{x}_i)$ using variational inference.

Initial plan:

- Optimize the ELBO

$$\mathcal{L}(\omega, \lambda_1, \dots, \lambda_N) = -\mathbb{E}_q \left[\log \frac{\prod_{i=1}^N q(\mathbf{z}_i | \lambda_i)}{\prod_{i=1}^N p_{\omega}(\mathbf{z}_i, \mathbf{x}_i)} \right].$$

- A natural model for $q(\mathbf{z}_i | \lambda_i)$ is a Gaussian with parameters $\lambda_i = \{\mu_i, \Sigma_i\}$.
- If \mathbf{Z}_i is d -dim and we for simplicity assume diagonal Σ_i , this still gives **$2Nd$ variational parameters** to learn.

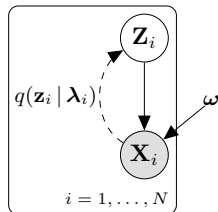


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A better plan

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

$\rightsquigarrow \lambda_i$ and λ_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 $h(\mathbf{x}_i) = \lambda_i$.
- $h(\cdot)$ 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 $\boldsymbol{\lambda}$.

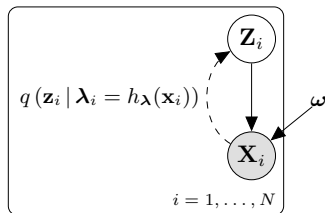
Note! Amortized inference is useful also outside VAEs!

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:

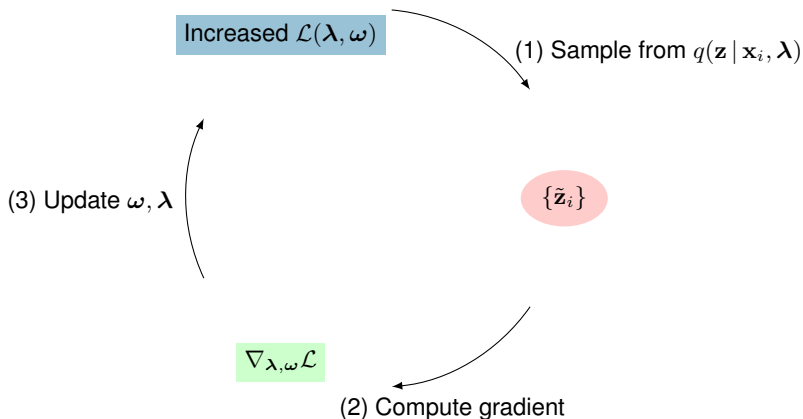
- $p(\mathbf{z}_i)$ is an isotropic Gaussian distribution.
- $p_{\omega}(\mathbf{x}_i | \mathbf{z}_i) \sim \text{Bernoulli}(\text{logits} = g_{\omega}(\mathbf{z}_i))$,
where g_{ω} is a DNN with weights ω .
- $q(\mathbf{z}_i | \mathbf{x}_i, \lambda) \sim \mathcal{N}(\mu_i, \Sigma_i)$,
where $\{\mu_i,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



Goal:

Learn **both** ω and λ by maximizing the ELBO:

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



- ➊ For each \mathbf{x}_i , sample M (typically 1) \mathbf{z} -values to approximate expectation in $\nabla \mathcal{L}$.
- ➋ Calculate $\nabla_{\lambda, \omega} \mathcal{L}(\lambda, \omega)$ using the reparameterization-trick.
- ➌ 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”).

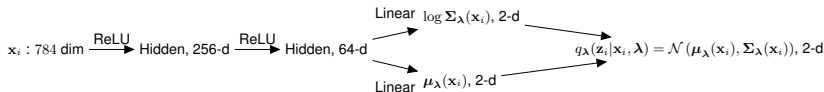


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- Encoding is done in **two** dimensions. $p(\mathbf{z}_i) = \mathcal{N}(\mathbf{0}_2, \mathbf{I}_2)$.

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

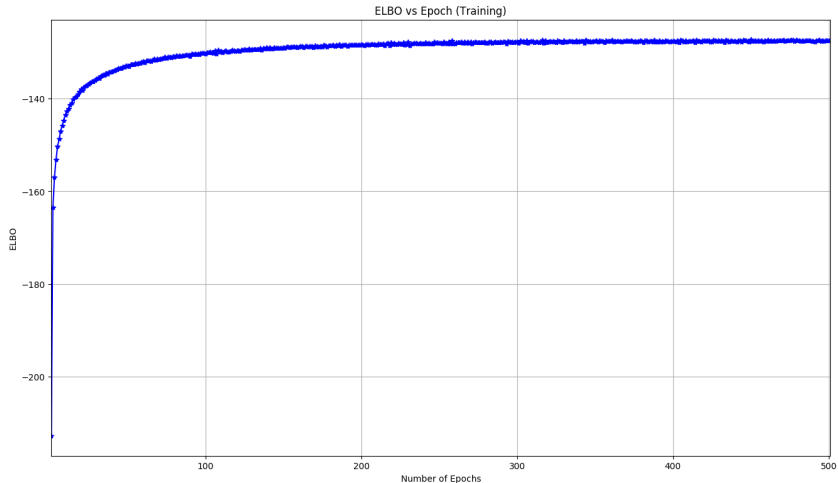


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- Encoding is done in **two** dimensions. $p(\mathbf{z}_i) = \mathcal{N}(\mathbf{0}_2, \mathbf{I}_2)$.
- The **encoder network** $\mathbf{X} \rightsquigarrow \mathbf{Z}$.
- The **decoder network** $\mathbf{Z} \rightsquigarrow \mathbf{X}$ is a $64 + 256$ neural net with ReLU units.

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



Note! SGD algorithm uses the negative ELBO as loss.



After 1 epoch



After 250 epochs

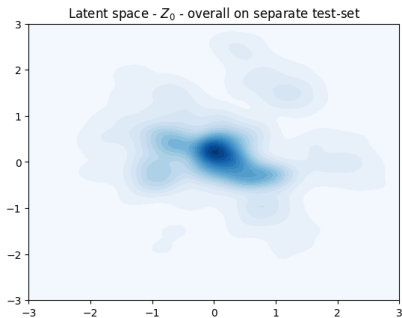
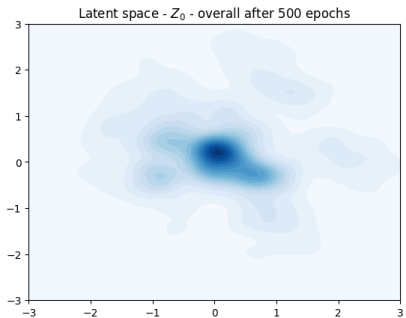
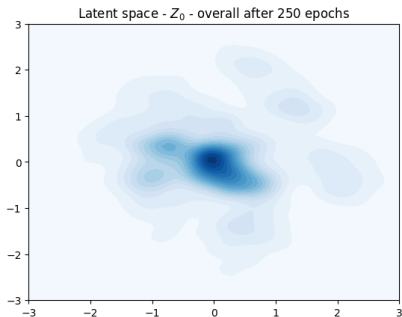
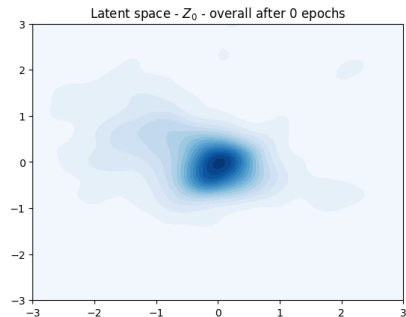


After 500 epoch

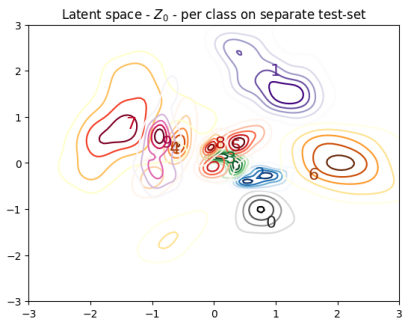
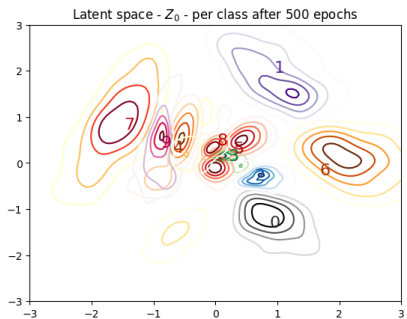
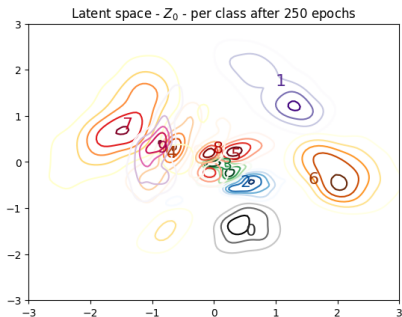
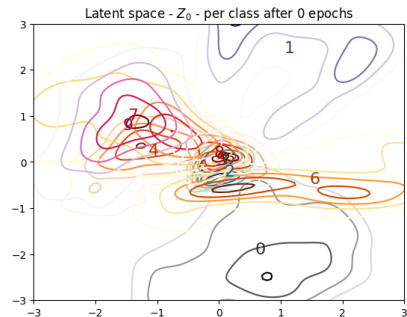


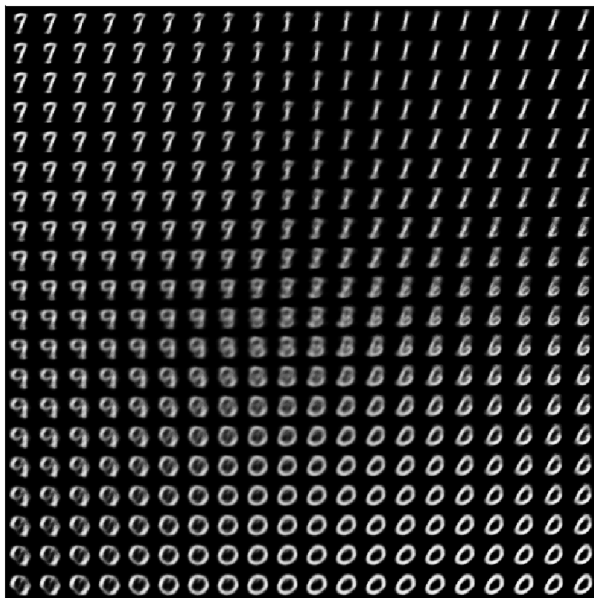
Using separate test-set

Averaged distribution over Z

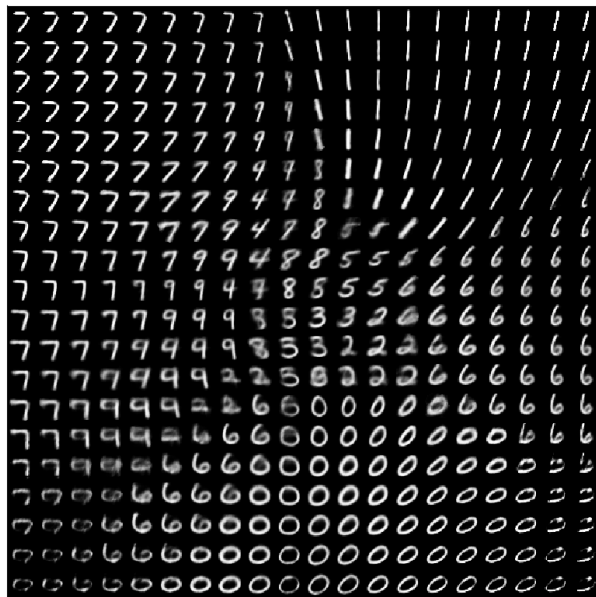


Averaged distribution over Z – per class

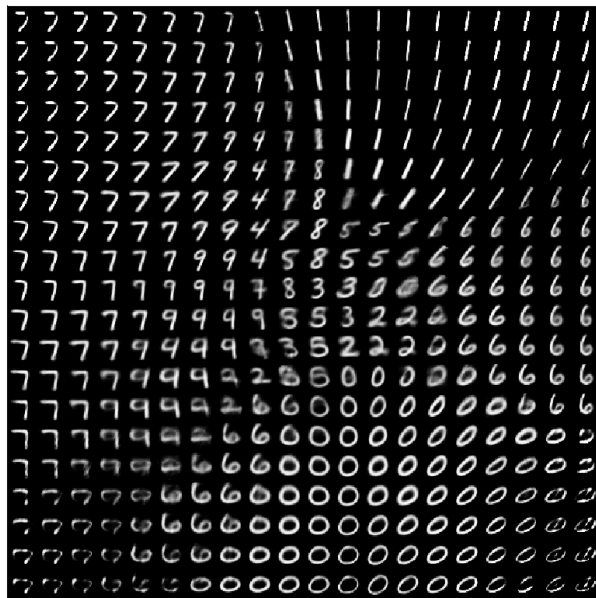




Manifold after 1 epoch



Manifold after 250 epochs

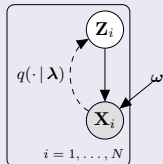


Manifold after 500 epochs

Variational Auto-Encoders in Pyro

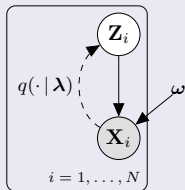
Notes

- 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 Pyro.
- 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 $p(\theta \mid \mathcal{D})$

- **Bayesian Machine Learning**

- **Variational inference**

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

- **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*)

- **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!**

- **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, ...)

- **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