Variational inference

Partly based on material developed together with Helge Langseth

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Plan for this week

Day 1: Probabilistic programming

- Introduction to probabilistic programming
- Probabilistic programming in Pyro

Day 2: Variational inference

- Recap of variational inference (variational inference as optimization)
- Derivation and implementation of selected examples
    - Bayesian linear regression
    - Factor analysis
    - ...

Day 3: Variational inference – cont'd

- Black box variational inference
- Variational inference in Pyro
- Variational auto-encoders

Black Box Variational Inference

VI inference as optimization

We can minimize (improve the variational approximation)

$$\mathrm{KL}(q_\lambda(z), p(z \mid \mathbf{x}))$$

by maximizing the ELBO

$$\mathcal{L}(q) = \mathbb{E}_q \left[\log \frac{p(\mathbf{z}, \mathbf{x})}{q(\mathbf{z})} \right]$$

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The mean field assumption

We will often use the mean field assumption, which states that $\mathcal{Q}$ consists of all distributions that *factorizes* according to the equation

$$q(\mathbf{z}) = \prod_i q_i(z_i)$$

$\rightsquigarrow$ we can treat the variables independently.

BBVI - Vanilla version

Key requirements

We want the approach to be ...

"Black Box": Not requiring tailor-made adaptations by the modeller.

Applicable: Useful independently of the underlying model assumptions.

Efficient: Utilize modelling assumptions, including the mean field assumption, to improve computational speed.

Algorithm: Maximize $\mathcal{L}(q) = \mathbb{E}_{q_\lambda}\left[\log \frac{p_\theta(\mathbf{z},\mathbf{x})}{q_\lambda(\mathbf{z})}\right]$ by gradient ascent

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

BBVI - calculating the gradient

The algorithm requires that we can find

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

With a bit of pencil pushing it follows that

$$\nabla_\lambda \mathcal{L}\left(q\right) = \mathbb{E}_{q_\lambda}\left[\log \frac{p_\theta(\mathbf{z},\mathbf{x})}{q_\lambda(\mathbf{z})} \cdot \nabla_\lambda \log q_\lambda(\mathbf{z})\right].$$

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Properties used for derivation

1. $\nabla_\lambda \left(f(\mathbf{z}, \boldsymbol{\lambda}) \cdot g(\mathbf{z}, \boldsymbol{\lambda}) \right) = f(\mathbf{z}, \boldsymbol{\lambda}) \cdot \nabla_\lambda g(\mathbf{z}, \boldsymbol{\lambda}) + g(\mathbf{z}, \boldsymbol{\lambda}) \nabla_\lambda f(\mathbf{z}, \boldsymbol{\lambda})$
2. $\nabla_\lambda f(\mathbf{z}, \boldsymbol{\lambda}) = f(\mathbf{z}, \boldsymbol{\lambda}) \nabla_\lambda \log f(\mathbf{z}, \boldsymbol{\lambda})$
3. $\mathbb{E}_{q_\lambda} \left[\nabla_\lambda \log q_\lambda(\mathbf{z} \mid \boldsymbol{\lambda}) \right] = 0$ for a density function $q_\lambda(\mathbf{z} \mid \boldsymbol{\lambda})$

Calculating the gradient – Things to notice

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

Calculating the gradient – Things to notice

- We only need access to the un-normalized $p_\theta(\mathbf{z}, \mathbf{x})$ – not $p_\theta(\mathbf{z} \mid \mathbf{x})$.

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- We must calculate $\nabla_\lambda \log q(\mathbf{z} \mid \boldsymbol{\lambda})$, which is also known as the "score function". This depends on the distributional family of $q(\cdot)$; can be precomputed for standard distributions.

Example

If $q_{\boldsymbol{\lambda}}(z)$ follows a normal distribution ($\boldsymbol{\lambda} = (\mu, \sigma)$):

$$\frac{1}{\sqrt{2\pi\sigma^2}} \exp\left(-\frac{(z-\mu)^2}{2\sigma^2}\right),$$

then

$$\nabla_\mu \log q_{\boldsymbol{\lambda}}(z) = \frac{1}{\sigma^2}(z - \mu)$$

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- The expectation will be approximated using a sample $\{\mathbf{z}_1, \ldots, \mathbf{z}_M\}$ generated from $q(\mathbf{z} \mid \boldsymbol{\lambda})$. Hence we require that we can **sample from** $q_{\lambda_i}(\cdot)$.

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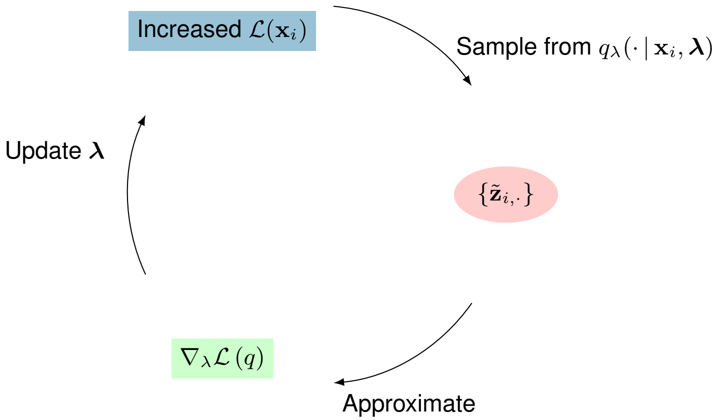
Calculating the gradient – in summary

We have observed the datapoint $\mathbf{x}$, and our current estimate for $\boldsymbol{\lambda}_i$ is $\hat{\boldsymbol{\lambda}}_i$. Then

$$\nabla_{\lambda_i} \mathcal{L}(q)|_{\lambda=\hat{\lambda}_i} \approx \frac{1}{M}\sum_{j=1}^{M} \log \frac{p(z_{i,j}, \mathbf{x})}{q(z_{i,j} \,|\, \hat{\lambda}_i)} \cdot \nabla_{\lambda_i} \log q_i(z_{i,j} \,|\, \hat{\lambda}_i).$$

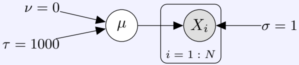
where $\{z_{i,1}, \ldots z_{i,M}\}$ are samples from $q_{\lambda_i}(\cdot \,|\, \hat{\lambda}_i)$.

ELBO optimization



Exercise: BBVI in Python

Consider the simple generative model:

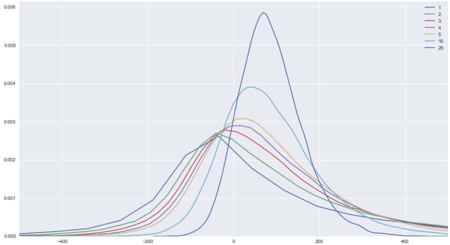


- Derive the BBVI estimate of the gradient for the variational parameters of $q(\mu) = \mathcal{N}(\lambda, 1)$.
- Implement the gradient estimate in the notebook

  `students_BBVI.ipynb`

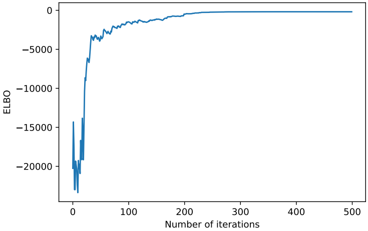
- Perform gradient ascent using your gradient implementation by running the notebook.

Density of gradient estimates



PDF for the gradient calculated at $\lambda = 9$, which is below the optimum ≈ 10. Several values for M, the sample size used to generate the estimate, are shown.

Evolution of ELBO



Based on gradient estimates using 1 sample

BBVI-full.ipynb

- Since the gradient estimate is based on a random sample, it is meaningful to evaluate the estimators' "robustness" in terms of a density function.
- We would hope to see robust estimates, also for small M, and in particular high probability for moving in the correct direction (gradient larger than 0).
- This is not the case, which has lead to a major focus on **variance reduction techniques**: while important we will **not cover them here**.

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.

Pyro models in general

- observations ⇔ `pyro.sample` with the `obs` argument
- latent random variables ⇔ `pyro.sample`
- parameters ⇔ `pyro.param`

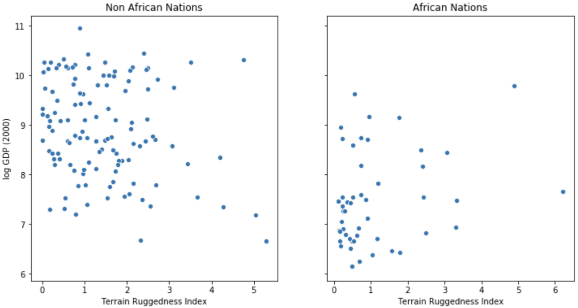
Simple example

```
#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'])
```

Bayesian linear regression

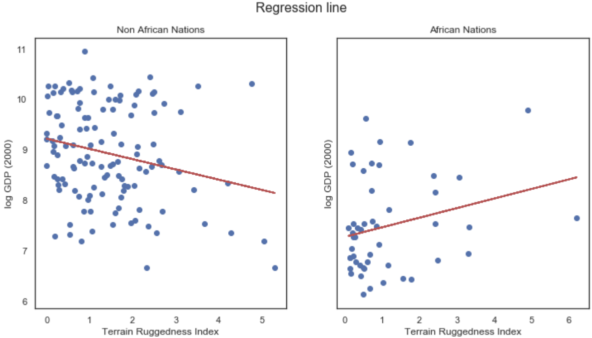
Real Data Example



Relationship between topographic heterogeneity and GDP per capita

- Terrain ruggedness or bad geography is related to poorer economic performance outside of Africa.
- Rugged terrains have had a reverse effect on income for African nations.

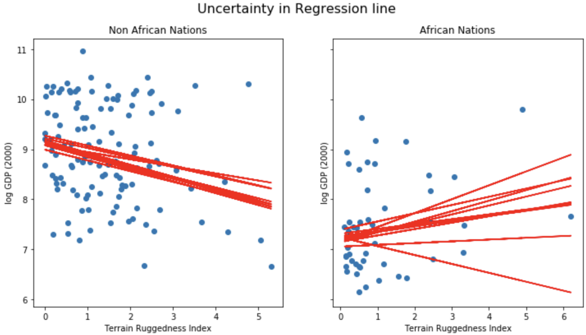
Real Data Example



Linear Regression Model

- Negative slope for Non African Nations.
- Positive slope for African Nations.

Real Data Example



Bayesian Linear Regression Model

- Modeling uncertainty about the linear coefficients (epistemic uncertainty).

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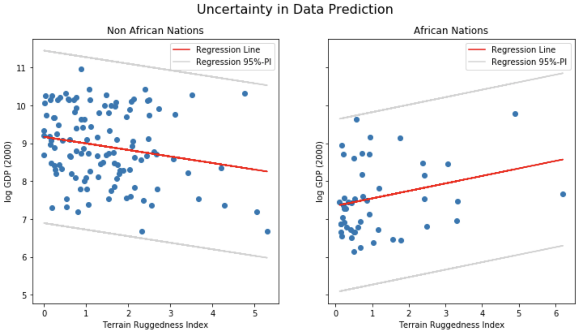

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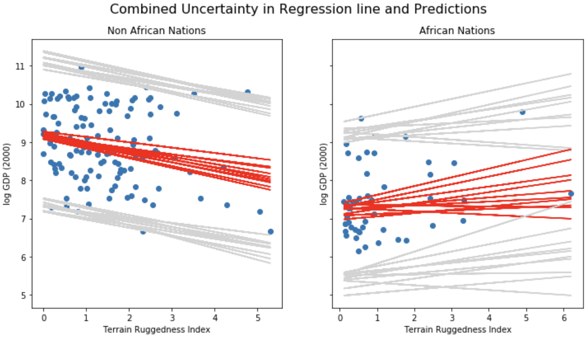

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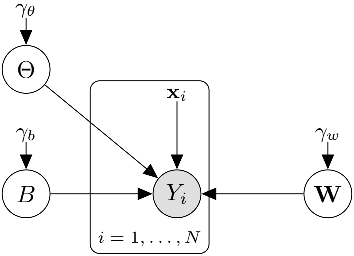
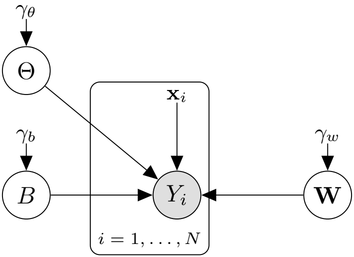
The Bayesian linear regression model



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

The Bayesian linear regression model



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The probability model

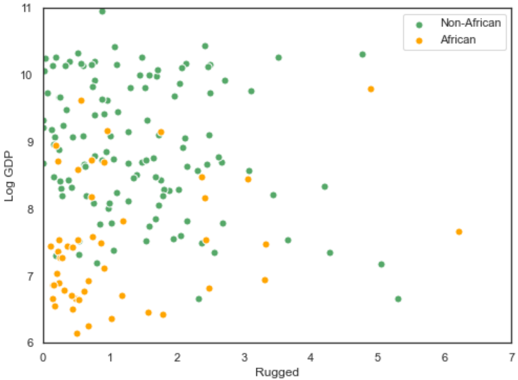
$$p(\cdot \mid \mathbf{x}, \gamma_w, \gamma_b, \gamma_\theta) = \prod_{i=1}^{N} p(y_i \mid \mathbf{x}_i, \mathbf{w}, b, \theta) p(\mathbf{w} \mid \gamma_w) p(b \mid \gamma_b) p(\theta \mid \gamma_\theta)$$

Notebook: Bayesian Linear Regression in Pyro

`Day3/bayesian_linear_regression.ipynb`

Bayesian logistic regression

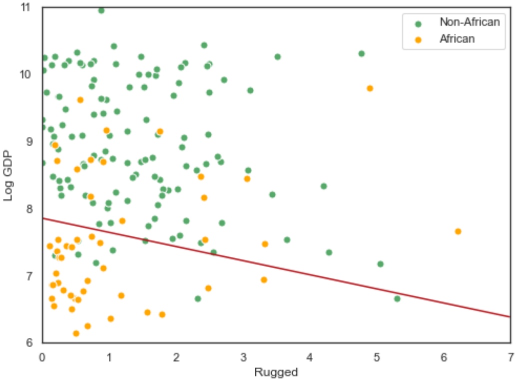
Real Data Example



Predict whether a nation is African or not as a function of:

- Terrain ruggedness or bad geography of the nation.
- (Log) GDP of the nation.

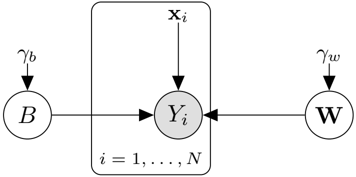
Real Data Example



Standard Logistic Regression Model

- No model uncertainty.

The Bayesian logistic regression model



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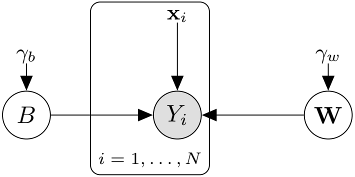
The Bayesian logistic regression model



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Exercise: Bayesian Logistic Regression in Pyro

- Play around with the first part of the notebook (Section 1)
- Complete the definition of the Bayesian Logistic Regression (Section 2.1).
- Learn the model and Play around with the evaluation (Section 2.2-2.5).

`Day3/bayesian_logistic_regression.ipynb`

Pyro's Guides

Guides

Definition:

- 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**.

Guides are used for:

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

Guide requirements

Guide functions must satisfy these two criteria to be valid approximations for a particular model:

1. all unobserved (i.e., not conditioned) sample statements that appear in the model appear in the guide.
2. the guide has the same input signature as the model (i.e., takes the same arguments)

Example

```python
#The observatons
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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'])
```
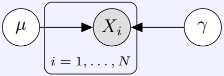

```python
#The guide
def guide(obs):
    a = pyro.param("mean", torch.tensor(0.0))
    b = pyro.param("scale", torch.tensor(1.), constraint=constraints.positive)
    temp = pyro.sample('temp', dist.Normal(a, b))
```

Code-task: VB for a simple Gaussian model

Exercise 1: Pyro implementation for a simple Gaussian model

`Day3/student_simple_gaussian_model_pyro.ipynb`



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

- Implement a pyro **model** and **guide** for the graphical model above.
- Specify appropriate **parameters** τ, α and β (e.g. try to use flat priors).
- Specify suitable **variational approximation** in the form of a Pyro guide.

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

- **Check** the differences with the notebook of Day 2.

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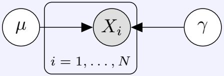

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Exercise 2: Explore Factor Analysis Model with Binomial likelihood

`Day3/FA_binomial.ipynb`

Variational Auto-Encoders

Is a *Deep Neural Network* the solution?

Limits on the scope of deep learning*

Deep learning thus far . . .

- . . . is data hungry
- . . . has no natural way to deal with hierarchical structure
- . . . is not sufficiently transparent
- . . . has not been well integrated with prior knowledge
- . . . works well as an approximation, but **its answers often cannot be fully trusted**

* Gary Marcus: *Deep Learning: A Critical Appraisal*. arXiv:1801.00631 [cs.AI]

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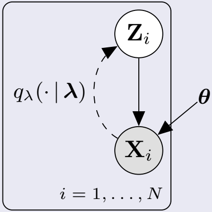
Deep Bayesian Learning

A marriage of Bayesian thinking and deep learning is a framework that ...

- ... allows explicit modelling.
- ... has a sound probabilistic foundation.
- ... balances expert knowledge and information from data.
- ... avoids restrictive assumptions about modelling families.
- ... supports efficient inference.

The Variational Auto Encoder (VAE)

Model of interest



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

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

- $g_\theta(\mathbf{z}_i)$ plays the role of a **DECODER NETWORK**.
- We want to learn $\boldsymbol{\theta}$ to maximize the model's fit to the data-set $\mathcal{D} = \{\mathbf{x}_1, \ldots, \mathbf{x}_N\}$.

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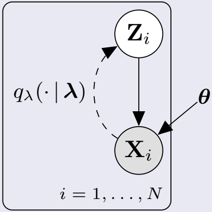

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Variational Inference:

Optimize $\mathcal{L}$ to choose $\boldsymbol{\lambda}$ and $\boldsymbol{\theta}$, where

$$\mathcal{L}(\boldsymbol{\lambda}, \boldsymbol{\theta}) = -\mathbb{E}_{q_\lambda}\left[\log \frac{q_\lambda(\mathbf{z} \mid \mathbf{x}, \boldsymbol{\lambda})}{p_\theta(\mathbf{z}, \mathbf{x} \mid \boldsymbol{\theta})}\right]$$

- The variational approximation $q_\lambda(\mathbf{z} \mid \mathbf{x}, \boldsymbol{\lambda})$ is parameterized by $\boldsymbol{\lambda}$.

$$\mathbf{z}_i|\mathbf{x}_i \sim \mathcal{N}(\mu = h_\lambda(\mathbf{x}_i)[0], \Sigma = h_\lambda(\mathbf{x}_i)[1])$$

- $h_\lambda(\mathbf{x}_i)$ is a DNN which plays the role of a **ENCODER NETWORK**.

Increased $\mathcal{L}(\boldsymbol{\lambda}, \boldsymbol{\theta})$

Sample from $q_\lambda(\mathbf{z} \mid \mathbf{x}_i, \boldsymbol{\lambda})$

$\{\tilde{\mathbf{z}}_i\}$

Compute gradient

$\nabla_{\lambda,\theta}\mathcal{L}$

Update $\boldsymbol{\theta}, \boldsymbol{\lambda}$

- 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. $p(\mathbf{z}_i) = \mathcal{N}\left(\mathbf{0}_2, \mathbf{I}_2\right)$.
- 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 $\xrightarrow{\text{Linear}}$ $\log \boldsymbol{\Sigma}_\lambda(\mathbf{x}_i)$, 2-d

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

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

Fun with MNIST – The model

- The model is learned from $N = 55.000$ training examples.
- Each $\mathbf{x}_i$ is a binary vector of 784 pixel values.
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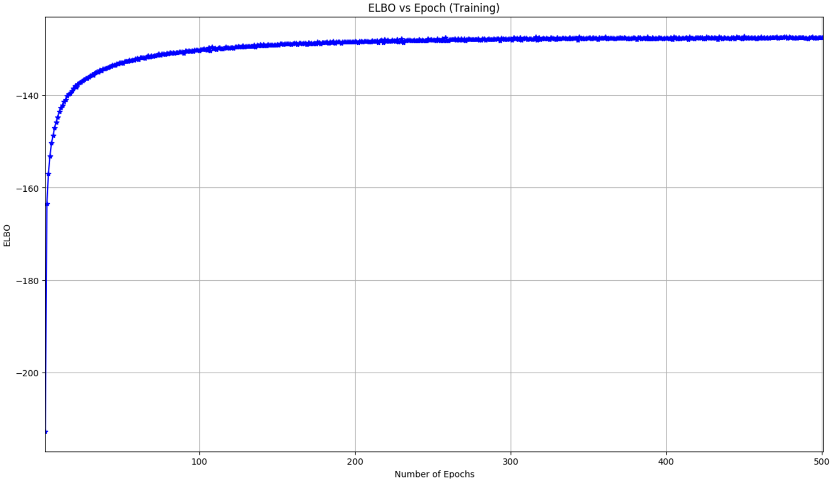
- Encoding is done in **two** dimensions. $p(\mathbf{z}_i) = \mathcal{N}(\mathbf{0}_2, \mathbf{I}_2)$.
- The **encoder network** $\mathbf{X} \rightsquigarrow \mathbf{Z}$.
- The **decoder network** $\mathbf{Z} \rightsquigarrow \mathbf{X}$ is a $64 + 256$ neural net with ReLU units.

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

Learning progress; learning rate $\mu = 10^{-4}$, mini-batch size $M = 1$



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

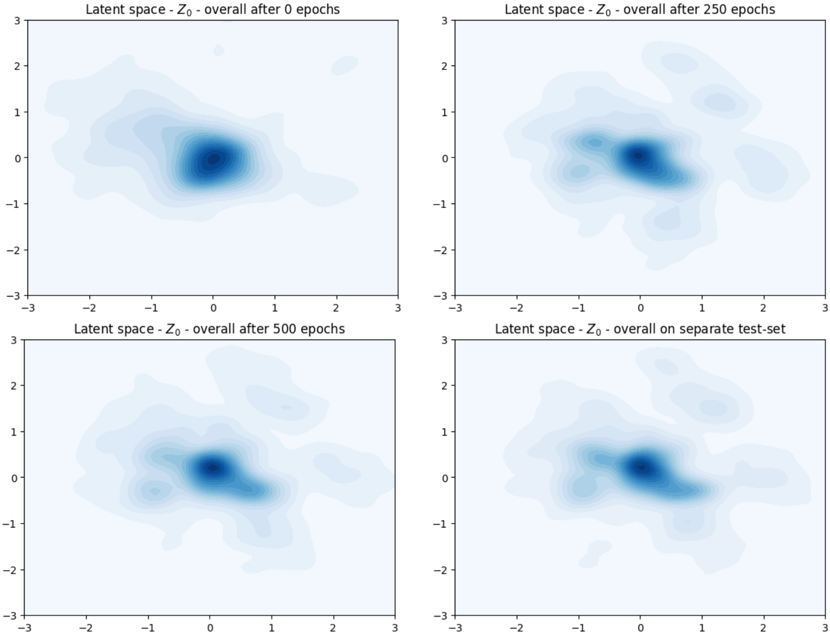
After 1 epoch

After 250 epochs

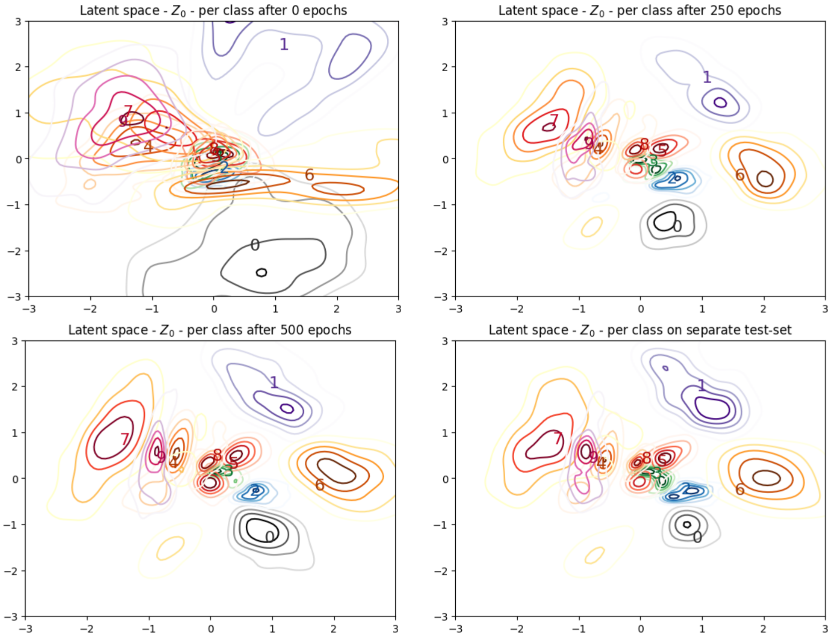
After 500 epoch

Using separate test-set

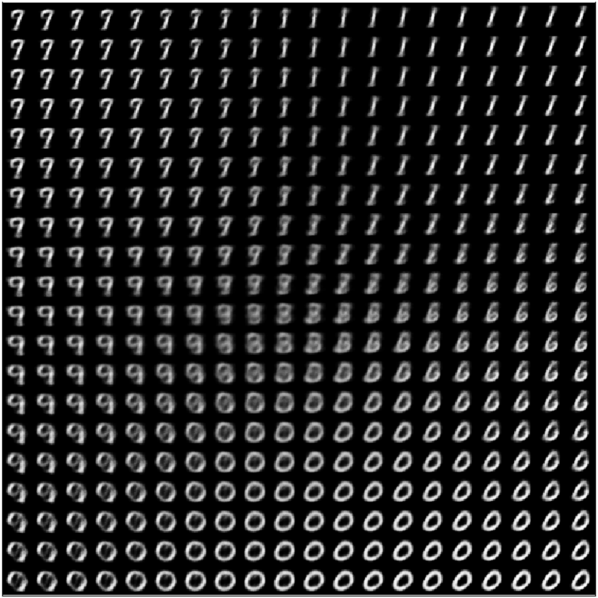
Averaged distribution over $\mathbf{Z}$



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



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



Manifold after 1 epoch

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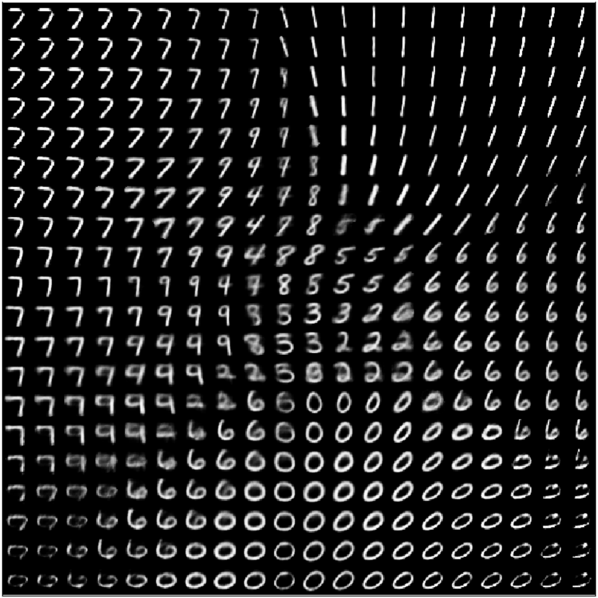
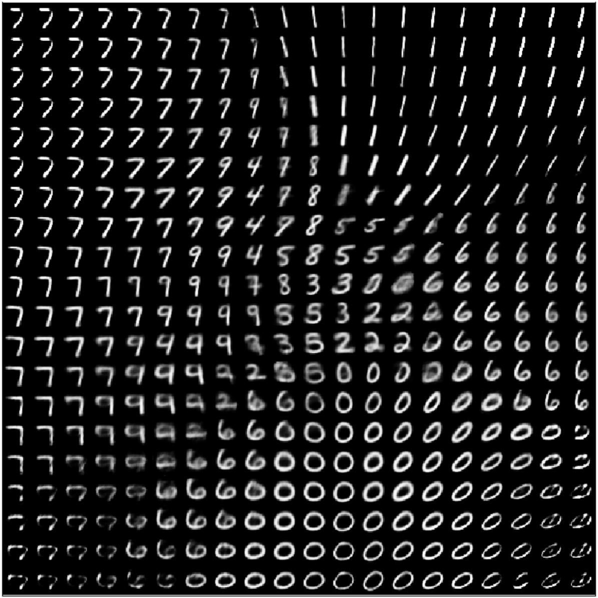


Manifold after 250 epochs

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



Manifold after 500 epochs

Wrapping things up

VAE.ipnyb

Pyro specification of an encoder

```
class Decoder(nn.Module):
    def __init__(self, z_dim, hidden_dim):
        super(Decoder, self).__init__()
        # Setup the two linear transformations used
        self.fc1 = nn.Linear(z_dim, hidden_dim)
        self.fc21 = nn.Linear(hidden_dim, 784)
        # Setup the non-linearities
        self.softplus = nn.Softplus()
        self.sigmoid = nn.Sigmoid()

    def forward(self, z):
        # Define the forward computation on the latent z
        # First compute the hidden units
        hidden = self.softplus(self.fc1(z))
        # Return the parameter for the output Bernoulli
        # Each is of size batch_size x 784
        loc_img = self.sigmoid(self.fc21(hidden))
        return loc_img

# define the model p(x|z)p(z)
def model(self, x):
    # register PyTorch module 'decoder' with Pyro
    pyro.module("decoder", self.decoder)
    with pyro.plate("data", x.shape[0]):
        # setup hyperparameters for prior p(z)
        z_loc = x.new_zeros(torch.Size((x.shape[0], self.z_dim)))
        z_scale = x.new_ones(torch.Size((x.shape[0], self.z_dim)))
        z = pyro.sample("latent", dist.Normal(z_loc, z_scale).to_event(1))
        # decode the latent code z
        loc_img = self.decoder.forward(z)
        # score against actual images
        pyro.sample("obs", dist.Bernoulli(loc_img).to_event(1),
                    obs=x.reshape(-1, 784))
```

Notes

- The PYRO.MODULE call

Pyro specification of a decoder

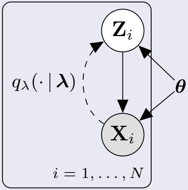
```
class Encoder(nn.Module):
    def __init__(self, z_dim, hidden_dim):
        super(Encoder, self).__init__()
        # Setup the three linear transformations used
        self.fc1 = nn.Linear(784, hidden_dim)
        self.fc21 = nn.Linear(hidden_dim, z_dim)
        self.fc22 = nn.Linear(hidden_dim, z_dim)
        # Setup the non-linearities
        self.softplus = nn.Softplus()

    def forward(self, x):
        # Define the forward computation on the image x
        # First shape the mini-batch to have pixels in
        # the rightmost dimension
        x = x.reshape(-1, 784)
        # then compute the hidden units
        hidden = self.softplus(self.fc1(x))
        # Return a mean vector and a (positive) square
        # root covariance each of size batch_size x z_dim
        z_loc = self.fc21(hidden)
        z_scale = torch.exp(self.fc22(hidden))
        return z_loc, z_scale

# define the guide (i.e. variational distribution) q(z|x)
def guide(self, x):
    # register PyTorch module 'encoder' with Pyro
    pyro.module("encoder", self.encoder)
    with pyro.plate("data", x.shape[0]):
        # use the encoder to get the parameters used to define q(z|x)
        z_loc, z_scale = self.encoder.forward(x)
        # sample the latent code z
        pyro.sample("latent", dist.Normal(z_loc, z_scale).to_event(1))
```

Notes

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



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  - Enormous expressibility.
  - Powerful inference engines (BlackBox Variational Inference)

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  - Requires manual derivation of updating equations.
  - There are tools (variational message passing) that avoid that (Infer.net, Amidst Toolbox, etc).

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  - Requires manual derivation of updating equations.
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- **Beyond Conjugate Exponential Models.**
  - Combine deep learning and probabilistic modeling.
  - Black-Box VI is not so efficient and stable.
  - But it works well in many cases.