Variational Auto-Encoders

October 28, 2022

1 Variational inference

• Representation of the data though a latent variable z:

$$p(\mathbf{x}) = \int_{\mathbf{z}} p(\mathbf{x}|\mathbf{z}) p(\mathbf{z}) d\mathbf{z}.$$

- Neural network to approximate $p(\mathbf{x}|\mathbf{z};\theta)$.
- When evaluating the likelihood on our data, we need samples from \mathbf{z} that will give high values of $p(\mathbf{x}|\mathbf{z})$.
- Instead of computing the distribution, or approximating the real posterior $p(\mathbf{z}|\mathbf{x})$ by sampling from it, we choose an **approximated posterior distribution on z** and try to make it resemble the real posterior as close as possible.

We use a **family** of distributions, parameterized by some parameters ϕ (e.g. they can be, again, the **parameters of a neural network**)

$$q(\mathbf{z}; \phi)$$
.

Variational inference consists in optimizing ϕ simultaneously with θ so that $q(\mathbf{z}; \phi)$ is as close as possible to $p(\mathbf{z}|\mathbf{x}; \theta)$ and maximizing a lower bound on the log-likelihood.

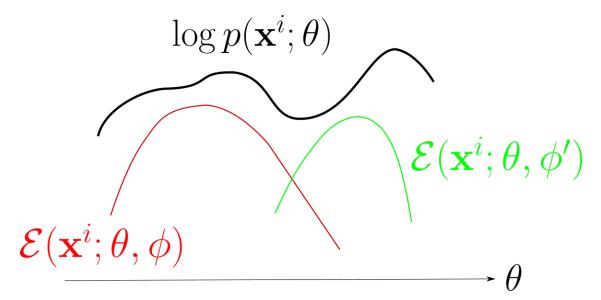
For one training data \mathbf{x}^i

$$\mathcal{L}(\mathbf{x}^i; \theta) \triangleq \log p(\mathbf{x}^i; \theta) \geq \int_{\mathbf{z}} q(\mathbf{z}; \phi) \log p(\mathbf{x}^i, \mathbf{z}; \theta) d\mathbf{z} + H(q(\mathbf{z}; \phi)) \triangleq \mathcal{E}(\mathbf{x}^i; \theta, \phi) \text{ (ELBO)}$$

and

$$\mathcal{L}(\mathbf{x}^i; \theta) = \mathcal{E}(\mathbf{x}^i; \theta, \phi) + D_{KL}(q(\mathbf{z}; \phi) || p(\mathbf{z} | \mathbf{x}^i; \theta))$$

As $q(\mathbf{z}; \phi)$ approximate well the posterior $p(\mathbf{z}|\mathbf{x}^i; \theta)$, the lower bound $\mathcal{E}(\mathbf{x}^i; \theta, \phi)$ will be close to $\log p(\mathbf{x}^i; \theta)$, which means that maximizing the ELBO will be very similar to maximizing the marginal likelihood. This process is called variational inference.



Training a model implies maximizing its log-likelihood over a dataset \mathcal{D}_{train}

$$\mathcal{L}(\mathcal{D}; \theta) = \sum_{\mathbf{x}_i \in \mathcal{D}} \log p(\mathbf{x}_i; \theta).$$

Evidence lower bound (ELBO) holds for any $q(\mathbf{z}; \phi)$

$$\log p(\mathbf{x}; \theta) \ge \sum_{\mathbf{z} \sim q(\mathbf{z}; \phi)} \log p(\mathbf{z}, \mathbf{x}; \theta) + H(q(\mathbf{z}; \phi)) = \mathcal{E}(\mathbf{x}; \theta, \phi).$$

To train the model, we maximize the total likelihood over \mathcal{D}_{train} :

$$\mathcal{L}(\mathcal{D}_{train}; \theta) = \sum_{\mathbf{x}^i \in \mathcal{D}_{train}} \log p(\mathbf{x}^i; \theta) \ge \sum_{\mathbf{x}^i \in \mathcal{D}_{train}} \mathcal{E}(\mathbf{x}^i; \theta, \phi^i)$$

Hence,

$$\max_{\theta} \mathcal{L}(\mathcal{D}_{train}; \theta) \ge \max_{\theta, \phi^1, \dots, \phi^n} \sum_{\mathbf{x}^i \in \mathcal{D}_{train}} \mathcal{E}(\mathbf{x}^i; \theta, \phi^i).$$

Note that we use different variational parameters ϕ^i for every data point \mathbf{x}^i , because the true posterior $p(\mathbf{z}|\mathbf{x}^i;\theta)$ should be different from one data \mathbf{x}^i to another.

To evaluate the bound $\mathcal{E}(\mathbf{x}^i; \theta, \phi^i)$, sample $\mathbf{z}^{(1)}, ..., \mathbf{z}^{(S)}$ from $q(\mathbf{z}; \phi^i)$ and estimate

$$\mathcal{E}(\mathbf{x}^i; \theta, \phi^i) = E_{q(\mathbf{z}; \phi^i)}[\log p(\mathbf{z}, \mathbf{x}^i; \theta) - \log q(\mathbf{z}; \phi^i)] \approx \frac{1}{S} \sum_{s=1}^{S} \log p(\mathbf{z}^{(s)}, \mathbf{x}^i; \theta) - \log q(\mathbf{z}^{(s)}; \phi))$$

Note that for this evaluation to be implemented, we need p and q to be **evaluated and sampled**: simple distributions (**Gaussians**, for example).

To maximize this bound, a general strategy is to follow the stochastic gradient algorithm and, for each data \mathbf{x}^i , alternate the optimization of ϕ^i and the one of θ .

Stochastic variational inference

- 1. Initialize $\theta, \phi^1, ..., \phi^n$.
- 2. Sample a data point \mathbf{x}^i from \mathcal{D}_{train} .
- 3. Optimize $\mathcal{E}(\mathbf{x}^i; \theta, \phi^i)$ with respect to ϕ^i : determine $\phi^{i*} \approx \arg \max_{\phi^i} \mathcal{E}(\mathbf{x}^i; \theta, \phi^i)$ by **gradient** ascent steps:

$$\phi^i = \phi^i + \alpha \nabla_{\phi^i} \mathcal{E}(\mathbf{x}^i; \theta; \phi^i).$$

- 4. Compute $\nabla_{\theta} \mathcal{E}(\mathbf{x}^i; \theta, \phi^{i*})$.
- 5. Update θ in the gradient direction:

$$\theta = \theta + \beta \nabla_{\theta} \mathcal{E}(\mathbf{x}^i; \theta; \phi^i).$$

6. Follow on step 2.

The gradient with respect to θ is simple because **only the first term in the ELBO depends on** θ :

$$\nabla_{\theta} E_{q(\mathbf{z};\phi)}[\log p(\mathbf{z}, \mathbf{x}; \theta) - \log q(\mathbf{z}; \phi)] = E_{q(\mathbf{z};\phi)}[\nabla_{\theta} \log p(\mathbf{z}, \mathbf{x}; \theta)], \tag{1}$$

$$\approx \frac{1}{S} \sum_{s=1}^{S} \nabla_{\theta} \log p(\mathbf{z}^{(s)}, \mathbf{x}; \theta). \tag{2}$$

Now, computing

$$\nabla_{\phi} E_{q(\mathbf{z};\phi)}[\log p(\mathbf{z},\mathbf{x};\theta) - \log q(\mathbf{z};\phi)]$$

is a prori way more complicated because what we have is an expectation over a distribution parameterized through ϕ . How to take the derivative of this kind of expression on ϕ ?

1.1 The reparameterization trick

Consider, more generally, the expectation of a scalar function f:

$$E_{q(\mathbf{z};\phi)}[f(\mathbf{z};\phi)] = \int f(\mathbf{z};\phi)q(\mathbf{z};\phi)d\mathbf{z}$$

and suppose that q is simply a Gaussian with diagonal covariance:

$$q(\mathbf{z}; \phi) \triangleq \mathcal{N}(\mu, \sigma^2 \mathbf{I}).$$

Sampling **z** from q can be written as:

$$\epsilon \sim \mathcal{N}(0, \mathbf{I}) \text{ and } \mathbf{z} = \mu(\phi) + \sigma(\phi)\epsilon.$$

Then

$$E_{q(\mathbf{z};\phi)}[f(\mathbf{z};\phi)] = \int_{\mathbf{z} \sim q(\mathbf{z};\phi)} f(\mathbf{z};\phi) q(\mathbf{z};\phi) d\mathbf{z} = \int_{\epsilon} f(\mu(\phi) + \sigma(\phi)\epsilon;\phi) p(\epsilon) d\epsilon.$$

This way, we **remove the** ϕ **from the integral**! This works more generally whenever you can express

$$\mathbf{z} \sim q(\mathbf{z}; \phi) \text{ as } \mathbf{z} = q(\epsilon; \phi).$$

Then:

$$\nabla_{\phi} E_{q(\mathbf{z};\phi)}[f(\mathbf{z};\phi)] = \qquad \qquad \nabla_{\phi} \int_{\epsilon} f(\mu(\phi) + \sigma(\phi)\epsilon;\phi) p(\epsilon) d\epsilon \qquad (3)$$

$$= \qquad \qquad \int_{\epsilon} \nabla_{\phi} f(\mu(\phi) + \sigma(\phi)\epsilon;\phi) d\epsilon. \qquad (4)$$

From this we can use **Monte-Carlo again**:

$$\nabla_{\phi} E_{q(\mathbf{z};\phi)}[f(\mathbf{z};\phi)] \approx \frac{1}{S} \sum_{s=1}^{S} \nabla_{\phi} f(\mu(\phi) + \sigma(\phi)\epsilon^{(s)};\phi),$$

where $\epsilon^{(1)}, \epsilon^{(2)}, ..., \epsilon^{(S)}$ are sampled from $\mathcal{N}(0, \mathbf{I})$. The last expression should be differentiable if f, μ , σ are differentiable.

Translated in our problem, for a given data point \mathbf{x}^i :

$$\nabla_{\phi^i} E_{q(\mathbf{z};\phi^i)}[\log p(\mathbf{z},\mathbf{x}^i;\theta) - \log q(\mathbf{z};\phi^i)] \approx \frac{1}{S} \sum_{s=1}^{S} \left[\nabla_{\phi^i} \log p(\mu(\phi^i) + \sigma(\phi^i)\epsilon^{(s)},\mathbf{x}^i;\theta) - \log q(\mu(\phi^i) + \sigma(\phi^i)\epsilon^{(s)}) \right].$$

However, this plan of estimating one ϕ^i per data is hardly scalable!

1.2 Amortized inference

Instead of learning one function per data point, what about learning only one function that would depend on the data point \mathbf{x}^i and would change the characteristics of the p.d.f. in function of the data point:

$$\mathbf{x}^i \to q(\mathbf{z}|\mathbf{x}^i;\phi) \approx \phi^{i*}.$$

That would replace the step of optimizing ϕ^i for each data, by learning a function that estimates this optimal value.

- 1. Initialize θ, ϕ .
- 2. Sample a data point \mathbf{x}^i from \mathcal{D}_{train} .
- 3. Optimize $\mathcal{E}(\mathbf{x}^i; \theta, \phi)$ with respect to ϕ : update ϕ by **gradient ascent steps** (with the **reparameterization trick!**):

$$\phi = \phi + \alpha \nabla_{\phi} \mathcal{E}(\mathbf{x}^i; \theta; \phi).$$

- 4. Compute $\nabla_{\theta} \mathcal{E}(\mathbf{x}^i; \theta, \phi)$.
- 5. Update θ in the gradient direction:

$$\theta = \theta + \beta \nabla_{\theta} \mathcal{E}(\mathbf{x}^i; \theta; \phi).$$

6. Follow on step 2.

1.3 The variational auto-encoder

If we rewrite the ELBO:

$$\mathcal{E}(\mathbf{x}^i; \theta, \phi^i) = E_{q(\mathbf{z}; \phi)}[\log p(\mathbf{z}, \mathbf{x}^i; \theta) - \log q(\mathbf{z}|\mathbf{x}; \phi)]$$
 (5)

$$= E_{q(\mathbf{z};\phi)}[\log p(\mathbf{x}^{i}|\mathbf{z};\theta) + \log p(\mathbf{z}) - \log q(\mathbf{z}|\mathbf{x};\phi)]$$
 (6)

$$E_{q(\mathbf{z};\phi)}[\log p(\mathbf{x}^i|\mathbf{z};\theta)] + E_{q(\mathbf{z};\phi)}[\log p(\mathbf{z}) - \log q(\mathbf{z}|\mathbf{x};\phi)]$$
 (7)

$$= E_{q(\mathbf{z};\phi)}[\log p(\mathbf{x}^{i}|\mathbf{z};\theta)] + D_{KL}(q(\mathbf{z}|\mathbf{x};\phi), p(\mathbf{z})), \tag{8}$$

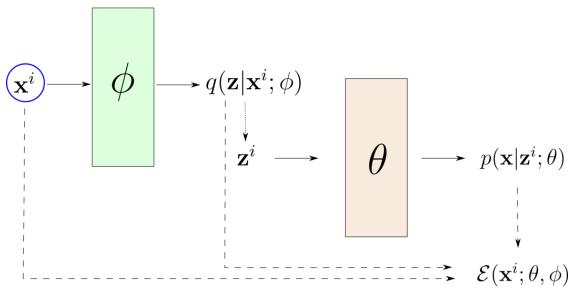
we can re-interpret the objective as:

- a reconstruction term $\log p(\mathbf{x}^i|\mathbf{z};\theta)$ that will favor using sampled \mathbf{z} that produce an \mathbf{x} similar to \mathbf{x}^i ;
- a second term that favors sampled **z** that are likely according to the **prior** $p(\mathbf{z})$.

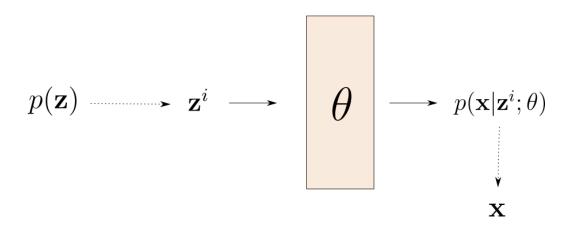
Encoder-decoder structure: during training, for a new data \mathbf{x}^i

- compute the **posterior** on **z** from $q(\mathbf{z}|\mathbf{x}^i;\phi)$ (**encoder**);
- sample a latent variable value z^i from this posterior;
- deduce $p(\mathbf{x}|\mathbf{z}^i;\theta)$ (decoder).

Variational Auto-encoder (training mode)



Variational Auto-encoder (testing mode)



1.4 A useful particular case: Gaussian distributions

Suppose that we limit ourselves to: $z \in \mathbb{R}^d$

$$p(\mathbf{z}) = \qquad \qquad \mathcal{N}(\mathbf{0}, \mathbf{I}) \qquad (9)$$

$$q(\mathbf{z}|\mathbf{x}; \phi) = \qquad \mathcal{N}(\mu_q(\mathbf{x}; \phi), diag(\sigma_q(\mathbf{x}; \phi))) \qquad (10)$$

(11)

In that case,

$$\mathcal{E}(\mathbf{x}^i; \theta, \phi^i) = E_{q(\mathbf{z}; \phi)}[\log p(\mathbf{x}^i | \mathbf{z}; \theta)] + D_{KL}(q(\mathbf{z} | \mathbf{x}; \phi), p(\mathbf{z})),$$

and the D_{KL} has a simple analytic form.

$$D_{KL}(q, p) = -\int q(\mathbf{x}) \log p(\mathbf{x}) d\mathbf{x} + \int q(\mathbf{x}) \log q(\mathbf{x}) d\mathbf{x}$$

First note that in 1D

$$\int q(\mathbf{x}) \log q(\mathbf{x}) d\mathbf{x} = \frac{1}{\sqrt{2\pi\sigma_q^2}} \int \left[-\frac{1}{2\sigma_q^2} (\mathbf{x} - \mu_q)^2 - \frac{1}{2} \log(2\pi\sigma_q^2) \right] \exp(-\frac{1}{2\sigma_q^2} (\mathbf{x} - \mu_q)^2) d\mathbf{x} - \frac{1}{2\sigma_q^2} \int (\mathbf{x} - \mu_q)^2 \frac{1}{\sqrt{2\pi\sigma_q^2}} \exp(-\frac{1}{2\sigma_q^2} (\mathbf{x} - \mu_q)^2) d\mathbf{x} - \frac{1}{2\sigma_q^2} \int (\mathbf{x} - \mu_q)^2 \frac{1}{\sqrt{2\pi\sigma_q^2}} \exp(-\frac{1}{2\sigma_q^2} (\mathbf{x} - \mu_q)^2) d\mathbf{x} - \frac{1}{2\sigma_q^2} \int (\mathbf{x} - \mu_q)^2 \frac{1}{\sqrt{2\pi\sigma_q^2}} \exp(-\frac{1}{2\sigma_q^2} (\mathbf{x} - \mu_q)^2) d\mathbf{x} - \frac{1}{2\sigma_q^2} \int (\mathbf{x} - \mu_q)^2 \frac{1}{\sqrt{2\pi\sigma_q^2}} \exp(-\frac{1}{2\sigma_q^2} (\mathbf{x} - \mu_q)^2) d\mathbf{x} - \frac{1}{2\sigma_q^2} \int (\mathbf{x} - \mu_q)^2 \frac{1}{\sqrt{2\pi\sigma_q^2}} \exp(-\frac{1}{2\sigma_q^2} (\mathbf{x} - \mu_q)^2) d\mathbf{x} - \frac{1}{2\sigma_q^2} \int (\mathbf{x} - \mu_q)^2 \frac{1}{\sqrt{2\pi\sigma_q^2}} \exp(-\frac{1}{2\sigma_q^2} (\mathbf{x} - \mu_q)^2) d\mathbf{x} - \frac{1}{2\sigma_q^2} \int (\mathbf{x} - \mu_q)^2 \frac{1}{\sqrt{2\pi\sigma_q^2}} \exp(-\frac{1}{2\sigma_q^2} (\mathbf{x} - \mu_q)^2) d\mathbf{x} - \frac{1}{2\sigma_q^2} \int (\mathbf{x} - \mu_q)^2 \frac{1}{\sqrt{2\pi\sigma_q^2}} \exp(-\frac{1}{2\sigma_q^2} (\mathbf{x} - \mu_q)^2) d\mathbf{x} - \frac{1}{2\sigma_q^2} \int (\mathbf{x} - \mu_q)^2 \frac{1}{\sqrt{2\pi\sigma_q^2}} \exp(-\frac{1}{2\sigma_q^2} (\mathbf{x} - \mu_q)^2) d\mathbf{x} - \frac{1}{2\sigma_q^2} \int (\mathbf{x} - \mu_q)^2 \frac{1}{\sqrt{2\pi\sigma_q^2}} \exp(-\frac{1}{2\sigma_q^2} (\mathbf{x} - \mu_q)^2) d\mathbf{x} - \frac{1}{2\sigma_q^2} \int (\mathbf{x} - \mu_q)^2 \frac{1}{\sqrt{2\pi\sigma_q^2}} \exp(-\frac{1}{2\sigma_q^2} (\mathbf{x} - \mu_q)^2) d\mathbf{x} - \frac{1}{2\sigma_q^2} \int (\mathbf{x} - \mu_q)^2 \frac{1}{\sqrt{2\pi\sigma_q^2}} \exp(-\frac{1}{2\sigma_q^2} (\mathbf{x} - \mu_q)^2) d\mathbf{x} - \frac{1}{2\sigma_q^2} \int (\mathbf{x} - \mu_q)^2 \frac{1}{\sqrt{2\pi\sigma_q^2}} \exp(-\frac{1}{2\sigma_q^2} (\mathbf{x} - \mu_q)^2) d\mathbf{x} - \frac{1}{2\sigma_q^2} \int (\mathbf{x} - \mu_q)^2 \frac{1}{\sqrt{2\pi\sigma_q^2}} \exp(-\frac{1}{2\sigma_q^2} (\mathbf{x} - \mu_q)^2) d\mathbf{x} - \frac{1}{2\sigma_q^2} \int (\mathbf{x} - \mu_q)^2 \frac{1}{\sqrt{2\pi\sigma_q^2}} \exp(-\frac{1}{2\sigma_q^2} (\mathbf{x} - \mu_q)^2) d\mathbf{x} - \frac{1}{2\sigma_q^2} \int (\mathbf{x} - \mu_q)^2 \frac{1}{\sqrt{2\pi\sigma_q^2}} \exp(-\frac{1}{2\sigma_q^2} (\mathbf{x} - \mu_q)^2) d\mathbf{x} - \frac{1}{2\sigma_q^2} \int (\mathbf{x} - \mu_q)^2 \frac{1}{\sqrt{2\pi\sigma_q^2}} \exp(-\frac{1}{2\sigma_q^2} (\mathbf{x} - \mu_q)^2) d\mathbf{x} - \frac{1}{2\sigma_q^2} \int (\mathbf{x} - \mu_q)^2 \frac{1}{\sqrt{2\pi\sigma_q^2}} \exp(-\frac{1}{2\sigma_q^2} (\mathbf{x} - \mu_q)^2) d\mathbf{x} - \frac{1}{2\sigma_q^2} \int (\mathbf{x} - \mu_q)^2 \frac{1}{\sqrt{2\pi\sigma_q^2}} \exp(-\frac{1}{2\sigma_q^2} (\mathbf{x} - \mu_q)^2) d\mathbf{x} - \frac{1}{2\sigma_q^2} \int (\mathbf{x} - \mu_q)^2 \frac{1}{\sqrt{2\sigma_q^2}} \exp(-\frac{1}{2\sigma_q^2} (\mathbf{x} - \mu_q)^2) d\mathbf{x} - \frac{1}{2\sigma_q^2} \int (\mathbf{x} - \mu_q)^2 \frac{1}{2\sigma_q^2} (\mathbf{x} - \mu_q)^2 d\mathbf{x} + \frac{1}{2\sigma_q^2} \int (\mathbf{x} - \mu_q)^2 d\mathbf{x} + \frac{1}{2\sigma_q^2} (\mathbf{x} - \mu_q)^2 d\mathbf{x} + \frac{1}{2\sigma_q^2} (\mathbf{x} -$$

And

$$\int q(\mathbf{x}) \log p(\mathbf{x}) d\mathbf{x} = \int \left[-\frac{1}{2\sigma_p^2} (\mathbf{x} - \mu_p)^2 - \frac{1}{2} \log(2\pi\sigma_p^2) \right] q(\mathbf{x}) d\mathbf{x} \right]$$
(16)
$$= \frac{1}{2} \log(2\pi\sigma_p^2) - \frac{1}{2\sigma_p^2} \int (\mathbf{x}^2 - 2\mu_p \mathbf{x} + \mu_p^2) q(\mathbf{x}) d\mathbf{x} \right]$$
(17)
$$= -\frac{1}{2} \log(2\pi\sigma_p^2) - \frac{1}{2\sigma_p^2} \int \mathbf{x}^2 q(\mathbf{x}) d\mathbf{x} + 2\frac{1}{2\sigma_p^2} \int \mu_p \mathbf{x} q(\mathbf{x}) d\mathbf{x} - \frac{1}{2\sigma_p^2} \int \mu_p^2 q(\mathbf{x}) d\mathbf{x}$$
(18)
$$= \frac{1}{2} \log(2\pi\sigma_p^2) - \frac{1}{2\sigma_p^2} (\sigma_q^2 + \mu_q^2) + \frac{1}{\sigma_p^2} \mu_q \mu_p - \frac{1}{2\sigma_p^2} \mu_p^2$$
(19)
$$= \frac{1}{2} \log(2\pi\sigma_p^2) - \frac{1}{2\sigma_p^2} (\sigma_q^2 + (\mu_q - \mu_p)^2)$$
(20)

Then:

$$D_{KL}(q, p) = -\int q(\mathbf{x}) \log p(\mathbf{x}) d\mathbf{x} + \int q(\mathbf{x}) \log q(\mathbf{x}) d\mathbf{x}$$
 (21)

$$= \frac{1}{2}\log(2\pi\sigma_p^2) + \frac{1}{2\sigma_p^2}(\sigma_q^2 + (\mu_q - \mu_p)^2) - \frac{1}{2}(1 + \log(2\pi\sigma_q^2))$$
 (22)

$$\log(\frac{\sigma_p}{\sigma_q}) + \frac{1}{2} \frac{\sigma_q^2}{\sigma_p^2} + \frac{1}{2\sigma_p^2} (\mu_q - \mu_p)^2 - \frac{1}{2}.$$
 (23)

When $\mu_p = 0$ and $\sigma_p = 1$, we get

$$D_{KL}(q, p) = -\log(\sigma_q) + \frac{1}{2}\sigma_q^2 + \frac{1}{2}(\mu_q)^2 - \frac{1}{2},$$

hence, in our problem (where we can decouple each dimension j)

$$D_{KL}(q(\mathbf{z}|\mathbf{x};\phi),p(\mathbf{z})) = -\frac{1}{2}\sum_{j=1}^{d}\log(\sigma_{q,j}^{2}(\mathbf{x};\phi)) + \frac{1}{2}\sum_{j=1}^{d}\sigma_{q,j}^{2}(\mathbf{x};\phi) + \frac{1}{2}\sum_{j=1}^{d}\mu_{q,j}^{2}(\mathbf{x};\phi) - \frac{d}{2}.$$

This expression can be differentiated easily.

For ensuring that $\sigma_{q,j} > 0$ during the optimization process, the network outputs instead:

$$logvar_i(\mathbf{x}; \phi) \triangleq \log(\sigma_{q,i}^2(\mathbf{x}; \phi))$$

and the KL becomes:

$$D_{KL}(q(\mathbf{z}|\mathbf{x};\phi),p(\mathbf{z})) = -\frac{1}{2}\sum_{j=1}^{d}logvar_{j}(\mathbf{x};\phi) + \frac{1}{2}\sum_{j=1}^{d}exp(logvar_{j}(\mathbf{x};\phi)) + \frac{1}{2}\sum_{j=1}^{d}\mu_{q,j}^{2}(\mathbf{x};\phi) - \frac{d}{2}.$$

1.5 Example

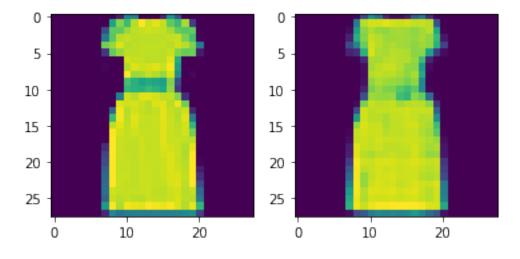
```
[1]: import matplotlib.pyplot as plt
  import numpy as np
  import pandas as pd
  import torch
  import torch.nn as nn
  import torch.nn.functional as F
  import torchvision
  from torchvision import datasets, transforms
  from torchvision.utils import save_image
  import numpy as np
  import random
  import tqdm
```

```
[2]: device = torch.device('cuda' if torch.cuda.is_available() else 'cpu')
     device
[2]: device(type='cuda')
[3]: # Load the csv files
     test_data = pd.read_csv('data/fashion-mnist_test.csv').values
     train_data = pd.read_csv('data/fashion-mnist_train.csv').values
[4]: # Get the normalized images (as vectors) and the labels
     x_train = train_data[:,1:]/255
     y_train = train_data[:,0]
     x_test = test_data[:,1:]/255
     y_test = test_data[:,0]
[5]: # Sanity check: random samples from the training data
     indices = np.random.randint(len(y_train), size=16)
     plt.figure(figsize=(15, 10))
     for i in range(16):
         plt.subplot(4, 4, i + 1)
         plt.xticks([])
         plt.yticks([])
         plt.imshow(x_train[indices[i]].reshape((28,28)),cmap='gray')
         plt.title(y_train[indices[i]])
```

```
[12]: # Our VAE class
      class VAE(nn.Module):
          nFeatures = 64
          imgWidth = 28
          imgHeight = 28
          dimLatent = 64
          # Constructor
          def __init__(self, dimChannels=1,__
       →dimFeatures=nFeatures*(imgWidth-6)*(imgHeight-6), dimLatent=dimLatent):
              super(VAE, self).__init__()
              self.dimFeatures = dimFeatures
              self.dimLatent = dimLatent
              self.dimChannels = dimChannels
              # 16 filters, 5x5
              self.enConv1 = nn.Conv2d(self.dimChannels, 16, 5)
              # 32 filters, 3x3
              self.enConv2 = nn.Conv2d(16, self.nFeatures, 3)
              # Fully connected layers to produce the posterior parameters
              self.enFC1 = nn.Linear(self.dimFeatures, dimLatent)
              self.enFC2 = nn.Linear(self.dimFeatures, dimLatent)
              # Decoder
              self.deFC1 = nn.Linear(dimLatent, dimFeatures)
              self.deConv1 = nn.ConvTranspose2d(self.nFeatures, 16, 3)
              self.deConv2 = nn.ConvTranspose2d(16, dimChannels, 5)
          # Encoding: produce q(z|x;phi)
          def encode(self, x):
              x = F.relu(self.enConv1(x))
              x = F.relu(self.enConv2(x))
              x = x.view(-1,self.dimFeatures)
              # Produce q(z|x;phi)
                       = self.enFC1(x)
              logsigma = self.enFC2(x)
              return mu, logsigma
          # Sampling through the reparameterization trick
          def sample(self, mu, logsigma):
              std = torch.exp(logsigma /2)
              eps = torch.rand_like(std)
              return mu + eps* std
          # Decoding: produce image
          def decode(self, z):
              x = F.relu(self.deFC1(z))
              x = x.view(-1, self.nFeatures,(self.imgWidth-6),(self.imgHeight-6))
```

```
x = F.relu(self.deConv1(x))
              x = torch.sigmoid(self.deConv2(x))
              return x
          # Forward
          def forward(self,x_in):
              mu, logsigma= self.encode(x_in)
                        = self.sample(mu, logsigma)
                        = self.decode(z)
              x_{out}
              return x_out, mu, logsigma
[14]: batch_size
                  = 1024
      learning_rate = 1e-3
      num_epochs
                   = 200
[15]: train_loader = torch.utils.data.DataLoader(torch.utils.data.TensorDataset(torch.
      →Tensor(x_train),torch.Tensor(y_train)),batch_size=batch_size)
      test_loader = torch.utils.data.TensorDataset(torch.Tensor(x_test),torch.
       →Tensor(y_test))
[16]: net = VAE().to(device)
[17]: optimizer = torch.optim.Adam(net.parameters(), lr=learning_rate)
 []: for epoch in range(num_epochs):
          for idx, data in enumerate(tqdm.tqdm(train_loader)):
              imgs, _ = data
                     = imgs.view(-1, 1, 28, 28)
              imgs
                   = imgs.float()
              imgs
                   = imgs.to(device)
              imgs
              out, mu, logVar = net(imgs)
              # loss function
              kl_divergence = 0.5 * torch.sum(-1 - logVar + mu.pow(2) + logVar.exp())
              loss = F.binary_cross_entropy(out, imgs, size_average=False) +__
       →kl_divergence
              optimizer.zero_grad()
              loss.backward()
              optimizer.step()
          print('Epoch {}: Loss {}'.format(epoch, loss))
[19]: net.eval()
      with torch.no_grad():
          for data in random.sample(list(test_loader), 1):
              imgs, _ = data
```

```
imgs = imgs.view(-1, 1, 28, 28)
imgs = imgs.float()
imgs = imgs.to(device)
out, mu, logVAR = net(imgs)
plt.subplot(121)
plt.imshow(imgs[0, 0].cpu().numpy())
plt.subplot(122)
plt.imshow(out[0, 0].cpu().numpy())
break
```



```
[21]: net.eval()
plt.figure(figsize=(15, 10))

with torch.no_grad():
    for i in range(16):
        mu, sigma = 0.0,1.0
        z = torch.Tensor(np.random.normal(mu, sigma, 64))
        z = z.to(device)
        img = net.decode(z).cpu().numpy()
        plt.subplot(4, 4, i + 1)
        plt.xticks([])
        plt.yticks([])
        plt.imshow(img[0,0],cmap='gray')
```



```
[72]: net.eval()
      dim = 2
      with torch.no_grad():
          for data in random.sample(list(test_loader), 1):
              img_in, _ = data
              img_in = img_in.view(-1, 1, 28, 28)
              plt.figure(figsize=(10, 8))
              plt.subplot(1, 2, 1)
              plt.imshow(img_in[0,0].cpu().numpy(),cmap='gray')
              plt.subplot(1, 2, 2)
              img_in = img_in.float()
              img_in = img_in.to(device)
              mu, logsigma= net.encode(img_in)
              img_out = net.decode(mu)
              plt.imshow(img_out.view(-1, 1, 28, 28)[0,0].cpu().numpy(),cmap='gray')
              plt.show()
              plt.figure(figsize=(15, 10))
              for i,var in enumerate(np.linspace(-1.0,1.0, num=9)):
                  plt.subplot(3, 3, i +1 )
                          = mu
```

```
z[0,dim]+= var
img_out = net.decode(z)
plt.imshow(img_out[0,0].cpu().numpy(),cmap='gray')
break
```

