Machine Learning Workshop 2

Variational Autoencoder

Jonathan Guymont

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Outline

- Autoencoders
 - An example to keep in mind
 - Autoencoders
- Variational autoencoder
 - Generative Model
 - Latent variable models
 - Variational Lower Bound
- Experiment
 - Unsupervised Spam Detection
 - Preprocessing
 - Binary Cross Entropy
 - Bernoulli MLP as Decoder
 - Spam Detector



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3/57

An example to keep in mind



Figure: Conversion of a greyscale image to an matrix

Note: In the workshop, we will mostly work with linear layer, so we also need to flatten the image.

```
from PIL import Image
def image_to_array(image_path):
    with Image.open(image_path) as img:
        image = img.convert()
        array_image = np.asarray(image, np.float)
    return array_image
```

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Autoencoers are neural network that are trained to learn how to map their input to their input. Internally, it has an hidden layer h that contains a lossy summary of the relevant feature for the task.

An autoencoder can be seen has a two parts network

ullet Encoder function: $oldsymbol{z} = f_\phi(oldsymbol{x})$

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The simplest autoencoder is a one layer MLP:

$$\mathbf{z} = \text{relu} (\mathbf{W}_{xz} \mathbf{x} + \mathbf{b}_{xz}) \quad [\text{encoder}]$$

$$\tilde{\mathbf{x}} = \text{sigmoid} (\mathbf{W}_{zx} \mathbf{z} + \mathbf{b}_{zx}) \quad [\text{decoder}]$$
(1)

Pytorch simple autoencoder

```
class Autoencoder:
        def __init__(self, **kargs):
            """constructor"""
            pass
        def encoder(self, x):
            pass
        def decoder(self, z)
            pass
        def forward(self, x):
            pass
```

Parameter initialization

$$\mathbf{z} = \text{relu} (\mathbf{W}_{xz} \mathbf{x} + \mathbf{b}_{xz})$$

$$\tilde{\mathbf{x}} = \text{sigmoid} (\mathbf{W}_{zx} \mathbf{z} + \mathbf{b}_{zx})$$
(2)

```
class Autoencoder:
    def __init__(self, x_dim, z_dim):
        # encoder parameters \phi
        self.Wxz = xavier_init(size=[x_dim, z_dim])
        self.bxz = Variable(torch.zeros(z_dim), requires_grad=True)
        # decoder parameters \theta
        self.Wzx = xavier_init(size=[z_dim, x_dim])
        self.bzx = Variable(torch.zeros(x_dim), requires_grad=True)
```

Encoder $f_{\phi}(x)$

$$\mathbf{z} = \text{relu} \left(\mathbf{W}_{xz} \mathbf{x} + \mathbf{b}_{xz} \right) \tag{3}$$

$$\phi = \{\mathbf{W}_{xz}, \mathbf{b}_{xz}\} \tag{4}$$

```
class Autoencoder:
    def encoder(self, x):
        z = F.relu(self.Wxz @ z + self.bxz.repeat(x.size(0), 1))
        return z
```

Decoder $g_{\theta}(x)$

$$\mathbf{z} = \sigma \left(\mathbf{W}_{zx} \mathbf{z} + \mathbf{b}_{zx} \right) \tag{5}$$

$$\boldsymbol{\theta} = \{ \mathbf{W}_{zx}, \mathbf{b}_{zx} \} \tag{6}$$

```
class Autoencoder:
    def decoder(self, z):
        x_recon = F.sigmoid(z @ self.Wzx + self.bzx.repeat(z.size(0), 1))
        return x_recon
```

Forward propagation

$$\mathbf{z} = \text{relu} (\mathbf{W}_{xz} \mathbf{x} + \mathbf{b}_{xz})$$

$$\tilde{\mathbf{x}} = \text{sigmoid} (\mathbf{W}_{zx} \mathbf{z} + \mathbf{b}_{zx})$$
(7)

```
class Autoencoder:
    ...
    def forward(self, x):
        z = self.encoder(x)
        x_recon = self.decoder(z)
        return x_recon
```

Pytorch simple autoencoder

```
class Autoencoder:
   def __init__(self, x_dim, z_dim):
        # encoder parameters
        Wxz = xavier init(size=[x dim, z dim])
        bxz = Variable(torch.zeros(z_dim), requires_grad=True)
        # decoder parameters
        Wzx = xavier init(size=[h dim, x dim])
        bzx = Variable(torch.zeros(X_dim), requires_grad=True)
    def encoder(self, x):
        z = F.relu(x @ self.Wxh + self.bxh.repeat(x.size(0), 1))
       return z
   def decoder(self, z):
       x_recon = F.sigmoid(z @ self.Wzx + self.bzx.repeat(z.size(0), 1))
       return x_recon
   def forward(self, x):
       z = self.encoder(x)
       x recon = self.decoder(z)
        return x recon
```

Autoencoder - Loss Function

If you treat the problem like a $regression^1$, use the mean square error between the input and the reconstruction

$$\mathcal{L} = \sum_{i=1}^{d} (x_i - \tilde{x}_i)^2 \tag{8}$$

Training Autoencoders

Algorithm 1 Pseudocode for Stochastic Gradient Training

```
Require: Learning rate \eta
Require: Initial parameter \omega_0
Require: Number of epochs T
   for i = 1 to T do
      X = X^{train}.copy() and Y = Y^{train}.copy()
      while X is not empty do
         Sample \{x^{(1)},...,x^{(m)}\}\ from X and \{y^{(1)},...,y^{(m)}\}\ from Y
         Remove samples from X and Y
         Compute gradient g_t = \frac{1}{m} \nabla_{\omega} \sum_i \mathcal{L}(\tilde{x}^{(i)}, x^{(i)})
         Apply update: \omega_t = \boldsymbol{\omega}_{t-1} - \eta \cdot \boldsymbol{q}_t
      end while
   end for
```

Pytorch Stochastic Gradient

```
def train(self, trainloader, num epochs, learning rate):
    for epoch in range(num_epochs):
        for inputs, targets in trainloader:
            batch_size = inputs.size(0)
            x_tilde = self.forward(x)
            loss = F.mse loss(x, x tilde)
            # Use autograd to compute the derivative of the loss w.r.t
            # all Tensors with requires_grad=True. After calling `loss.backward()`,
            # conv_weight.grad, dense_weight.grad, and dense_bias.grad
            # will be Tensors equal to the gradient of the loss with respect
            # to the filters of the cnn layer, the weight of the fully connected layer, and
            # the bias of the fully connected layer respectively.
            loss.backward()
            # Apply gradient descent to all the leaned parameters
            # The derivative of the loss is giving us the direction
            # where the funtion increase. Thus we go in the
            # opposite direction. Using torch.no_grad() tells pytorch
            # to not include thes operation in the computational graph.
            # Instead, gradient descent is goning to be applied `inplace`.
            with torch.no grad():
                self.W_xz -= learning_rate * self.W_xz.grad
                self.b_xz -= learning_rate * self.b_xz.grad
                self.W zx -= learning rate * self.W zx.grad
                self.b zx -= learning rate * self.b zx.grad
```

To summarize

- ullet A neural network encode x in a hidden state z of smaller dimension
- ullet Another neural network decode z to reconstruct x
- A sound loss function could be the mean square error between the input and its reconstruction.
- Both network can be train at the same time with gradient method.

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Generative Models

Represent the probability distribution of either P(X,Y) or P(X). In the case of *density estimation*, we are looking for a representation of

$$x \sim P_{\theta}(X)$$

For example, $x \sim \mathcal{N}(x; \boldsymbol{\mu}_{\mathsf{mle}}, \boldsymbol{\sigma}_{\mathsf{mle}})$

Problem: Most parametric distribution make strong (and often wrong) assumption about the distribution.

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We can model the distribution of x as a function of a latent variable z

$$p(x) = \int p_{\theta}(x|z)p(z)dz$$

where the distribution of z is chosen. A typical choice for z is

$$z \sim \mathcal{N}(z; \mathbf{0}, \boldsymbol{I})$$

Then we can train a model to learn a good representation of $p_{\theta}(x|z)$ with stochastic gradient.

$$p(x) = \int p_{\theta}(x|z)p(z)dz$$

Once we have a good representation of $p_{\theta}(x|z)$, we can sample from p(x) by first sampling

$$z' \sim p(z)$$

and then sampling

$$x' \sim p(x|z')$$



Problem 1: To learn $p_{\theta}(x|z)$ using stochastic gradient, we need to know a good mapping

$$f: \mathcal{Z} \times \Theta \mapsto \mathcal{X}$$

In other word when we sample $x \sim p(x|z')$ we need to know which x is likely to be generated by this particular z' in order to train the model.

Solution: the prior of the latent space can be written has

$$p(z) = \int p(z|x)p(x)dx$$

During training, We can sample z by sampling

$$x' \sim p(x)$$

and then

$$z \sim p(z|x')$$

The training set comes from p(x) so we can sample from it. This will reduce the space of the latent variable a lot and allow the model to learn efficiently.



Problem 2: p(z|x) is intractable.

Solution: use an approximation $q_{\phi}(z|x)$

To summarize

- Sample $x \sim D_n$
- Sample $z \sim q_{\phi}(z|x)$
- Sample $\tilde{x} \sim p_{\theta}(x|z)$

The parameter to learn are ϕ and θ and they should be learn such that the marginal likelihood p(x) is maximized.

Before looking at how we can train this model efficiently, let's take a closer look at how it works concretely.

Probabilistic Encoder $q_{\phi}(z|x)$

Example: Gaussian MLP as encoder

```
• \mu_z, \log \sigma_z^2 = f(\mathbf{x}; \phi)

• \mathbf{h} = \text{relu}(xW_{xh} + b_{xh})

• \mu = hW_{hz}^{(1)} + b_{hz}^{(1)}

• \log \sigma^2 = hW_{hz}^{(2)} + b_{hz}^{(2)}

• q_{\phi}(z|x) = \mathcal{N}(\mathbf{z}; \mu_z, \sigma_z^2)

• \phi = \{W_{hz}^{(1)}, b_{hz}^{(1)}, W_{hz}^{(2)}, b_{hz}^{(2)}, W_{xh}, b_{xh}\}
```

```
class VAE:
...
def encoder(self, x):
    # Encoder network. Return the parameter of q(z|x)
    h = relu(x @ self.Wxh + self.bxh.repeat(x.size(0), 1))
    mu = h @ self.Whz_mu + self.bhz_mu.repeat(x.size(0), 1)
    log_var = h @ self.Whz_var + self.bhz_var.repeat(x.size(0), 1)
    reture mu, log_var
```

Sampling $z \sim q_{\phi}(z|x)$

Example: Sampling z from $q_{\phi}(z|x)$

- $\mathbf{z} \sim \mathcal{N}(\boldsymbol{\mu}_z, \boldsymbol{\sigma}_z)$
 - μ_z , $\log \sigma_z^2 = f(\mathbf{x}; \boldsymbol{\phi})$
 - $\epsilon \sim \mathcal{N}(\mathbf{0}, \mathbf{I})$
 - $\mathbf{z} = \boldsymbol{\mu}_z + \boldsymbol{\sigma}_z \odot \boldsymbol{\epsilon}$

```
class VAE:
```

```
. . .
```

```
def _sample_z(self, mu, log_var):
    epsilon = Variable(torch.randn(mu.size()).to(self._device)
    sigma = torch.exp(log_var / 2)
   return mu + sigma * epsilon
```

Probabilistic Decoder $p_{\theta}(x|z)$

Example: Gaussian MLP as decoder

 $\bullet \ \mu_{x}, \ \log \sigma_{x}^{2} = g(\mathbf{x}; \boldsymbol{\theta})$ $\bullet \ \mathbf{h} = \text{relu}(\mathbf{W}_{zh}\mathbf{x} + \mathbf{b}_{zh})$ $\bullet \ \mu_{x} = W_{hz}^{(1)}\mathbf{h} + \mathbf{b}_{hz}^{(1)}$ $\bullet \ \log \sigma_{x}^{2} = W_{hz}^{(2)}\mathbf{h} + \mathbf{b}_{hz}^{(2)}$ $\bullet \ p_{\boldsymbol{\theta}}(x|z) = \mathcal{N}(x; \boldsymbol{\mu}_{x}, \log \sigma_{x}^{2})$ $\bullet \ \boldsymbol{\theta} = \{W_{zh}, b_{zh}, W_{zx}, b_{zx}\}$

```
class VAE:
...
def decoder(self, z):
    # Decoder network. Reconstruct the input from
    # the latent variable z
    h = relu(z @ self.Whx + self.bhx.repeat(x.size(0), 1))
    gamma = h @ self.Whx_mu + self.bhx.repeat(x.size(0), 1)
    reture gamma
```

To summarize

- Sample $x \sim D_n$
- Sample $z \sim q_{\phi}(z|x)$
- Sample $\tilde{x} \sim p_{\theta}(x|z)$

The parameter to learn are ϕ and θ and they should be learn such that the marginal likelihood p(x) is maximized.

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Training VAE

We need $p_{\theta}(x|z)$ to be such that the marginal likelihood p(x) is maximized.

In other word the lost function should be

$$\mathcal{L}(x; \phi, \theta) = -\log p(x)$$

Kullback-Leibler divergence

Kullback-Leibler divergence

Let p(x) and q(x) be probability measures over a set X, and q(x) is absolutely continuous with respect to p(x), then the Kullback?Leibler divergence from p to q is defined as

$$\mathcal{D}_{KL}[q(x)||p(x)] = \mathbb{E}_{x \sim q(x)}[\log q(x) - \log p(x)]$$

$$= \int q(x)(\log q(x) - \log p(x))dx$$

$$= \int q(x)\log q(x)dx - \int q(x)\log p(x)dx$$

Gibbs' inequality

$$\mathcal{D}_{KL}[q(x)||p(x)] \ge 0$$



Variational Lower Bound

Corollary

The marginal log-likelihood $\log p(x)$ is lower bounded by the variational lower bound i.e

$$\log p(x) \ge \mathrm{E}_{z \sim q(z|x)} \log p(x|z) - \mathcal{D}_{KL}[q(z|x)||p(z)]$$

Hence, our loss function is

$$\mathcal{L}(x; \phi, \theta) = \mathcal{E}_{z \sim q(z|x)} \log p(x|z) - \mathcal{D}_{KL}[q(z|x)||p(z)]$$

Proof of the Variational Lower Bound

Proof.

First, let's compute de Kullback-Leibler divergence \mathcal{D}_{KL} between p(z|x) and q(z|x)

$$\begin{split} \mathcal{D}_{KL}[q(z|x)||p(z|x)] = & \mathbf{E}_{z \sim q(z|x)}[\log q(z|x) - \log p(z|x)] \\ = & \mathbf{E}_{z \sim q(z|x)}[\log q(z|x) - \log p(x|z) - \log p(z) + \log p(x)] \\ = & \log p(x) + \mathbf{E}_{z \sim q(z|x)}[\log q(z|x) - \log p(z)] - \mathbf{E}_{z \sim q(z|x)}\log p(x|z) \\ = & \log p(x) - \mathcal{D}_{KL}[q(z|x)||p(z|x)] - \mathbf{E}_{z \sim q(z|x)}\log p(x|z) \end{split}$$

Sending all the terms on the right except $\log p(x)$ gives

$$\log p(x) = \mathbf{E}_{z \sim q(z|x)} \log p(x|z) - \mathcal{D}_{KL}[q(z|x)||p(z)] + \mathcal{D}_{KL}[q(z|x)||\log p(z|x)]$$

Finally, because of Gibbs' inequality we have

$$\log p(x) \geq \mathbf{E}_{z \sim q(z|x)} \log p(x|z) - \mathcal{D}_{KL}[q(z|x)||p(z)]$$



Solution of $\mathcal{D}_{KL}[q(z|x)||p(z)]$

Lemma

Let $z \in \mathbb{R}^J$ be a standard multivariate Gaussian distribution and let z|x be a multivariate Gaussian distribution with mean μ_z and standard deviation σ_z . Then the KL-divergence from p(z) to $q_\phi(z|x)$ is

$$\mathcal{D}_{KL}[q(z|x)||p(z)] = \frac{1}{2} \sum_{j=1}^{J} \mu_j^2 + \sigma_j^2 - 1 - \log \sigma_j^2$$

```
def kl_divergence(mu, log_sigma):
    sigma = torch.exp(log_sigma)
    return .5 * torch.sum(mu**2 + sigma**2 - 1 - 2*log_sigma, axis=1)
```

Proof for the Solution of $\mathcal{D}_{KL}[q(z|x)||p(z)]$

Proof.

According to the definition of the KL-divergence we have

$$\mathcal{D}_{KL}[q_{\phi}(z|x)||p(z)] = \int q_{\phi}(z|x) \log q_{\phi}(z|x) dx - \int q_{\phi}(z|x) \log p(z)) dx$$

Solving the first integral gives

$$\int q(z|x) \log q(z|x) dz = \int \mathcal{N}(z;\mu,\sigma) \log \mathcal{N}(z;\mu,\sigma)$$

$$= -\frac{J}{2} \log 2\pi - \frac{1}{2} \sum_{j=1}^{J} (1 + \log \sigma_j^2)$$
(9)

Now solving the second integral

$$\int q(z|x) \log p(z) dz = \int \mathcal{N}(z; \mu, \sigma) \log \mathcal{N}(z; 0, I)$$

$$= -\frac{J}{2} \log 2\pi - \frac{1}{2} \sum_{j=1}^{J} (\mu_j^2 + \sigma_j^2)$$
(10)

where J is the dimension of z. Finally, subtracting (10) from (9) gives

$$\mathcal{D}_{KL}[q(z|x)||p(z)] = \frac{1}{2} \sum_{j=1}^{J} \mu_j^2 + \sigma_j^2 - 1 - \log \sigma_j^2$$

ш

VAE Loss Function

The loss function for a standard Gaussian latent variable and a multivariate Gaussian posterior distribution on \boldsymbol{x} is given by

$$\mathcal{L}(x; \phi, \theta) = -\operatorname{E}_{z \sim q(z|x)} \log p(x|z) + \mathcal{D}_{KL}[q(z|x)||p(z)]$$

$$= -\log \mathcal{N}(x; \boldsymbol{\mu}_x, \boldsymbol{\sigma}_x) + \frac{1}{2} \sum_{i=1}^{J} \mu_j^2 + \sigma_j^2 - 1 - \log \sigma_j^2$$
(11)

In our example, we used $p_{\theta}(x|z) = \mathcal{N}(x; \mu_z, \sigma_z)$. In practice you can use any distribution you want.

Some important aspect to consider

• The image of the distribution must correspond to the input space.

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Some important aspect to consider

- The image of the distribution must correspond to the input space.
- Choose a distribution that make sense base on you knowledge of the problem.

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Some important aspect to consider

- The image of the distribution must correspond to the input space.
- Choose a distribution that make sense base on you knowledge of the problem.
- If the domain is continuous on the real number a normal distribution can make sense

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Some important aspect to consider

- The image of the distribution must correspond to the input space.
- Choose a distribution that make sense base on you knowledge of the problem.
- If the domain is continuous on the real number a normal distribution can make sense
- If the domain is discrete, choose a discrete distribution like a Bernoulli or a Poisson.

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Unsupervised Spam Detection

- SMS Spam Collection Data Set²
 - Number of instances: 5574
 - Number of spams: 747 ($\sim 13\%$)
- Spam detection
 - Estimate the distribution of all the text messages
 - Evaluate the density of each text message
 - Text message with low density are classified as spam

Data

Examples of non spams

- What you doing?how are you?
- Ok lar... Joking wif u oni...
- Cos i was out shopping wif darren jus now n i called him 2 ask wat present he wan lor. Then he started guessing who i was wif n he finally guessed darren lor.

• Examples of **spams**

- FreeMsg: Txt: CALL to No: 86888 & claim your reward of 3 hours talk time to use from your phone now! ubscribe6GBP/ mnth inc 3hrs 16 stop?txtStop
- Sunshine Quiz! Win a super Sony DVD recorder if you canname the capital of Australia? Text MQUIZ to 82277. B
- URGENT! Your Mobile No 07808726822 was awarded a L2,000 Bonus Caller Prize on 02/09/03! This is our 2nd attempt to contact YOU! Call 0871-872-9758 BOX95QUm



Performance Metric

$$F_{1} - Score = \left(\frac{\operatorname{recall}^{-1} + \operatorname{precision}^{-1}}{2}\right)^{-1}$$

$$= 2 \cdot \frac{\operatorname{precision} \cdot \operatorname{recall}}{\operatorname{precision} + \operatorname{recall}}$$
(12)

where

$$precision = \frac{|\{spams \ detected\}|}{|\{spams \ classified\}|} \qquad recall = \frac{|\{spams \ detected\}|}{|\{spams\}|}$$

Motivation: Both precision and recall metric are important. Take the harmonic mean between them.

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Preprocessing

- Some terminology
 - Vocabulary: Set of all the word types in the training set $\{w_1,...,w_{|\mathsf{Vocabulary}|}\}.$
 - Training corpus: Set of all text messages in the training set $\{x^{(1)},...,x^{(n)}\}.$
 - Bag of words: Vector representation of a sentence.

Bag of words

- $x^{(i)} = What you doing?how are you?$ (original sentence)
- $x^{(i)} = what you do how be you (after preprocessing)$
- $x^{(i)} = [0 \cdots 0 \ 1 \ 0 \cdots \ 0 \ 2 \ 0 \cdots 0]$ (vector representation)

```
x = 'What you doing?how are you?'

x = preprocess(x)
print(x)
>>> 'what you do how be you'

x = vectorize(x)
print(x)
>>> [0 0 0 ... 0 0 0]
```

Bag of words

- Bag of words
 - All examples in the corpus have the same length.
 - The value of a position in the vector is equal to the frequency of this word it the example.
 - $x^{(i)} = [0 \cdots 0 \ 1 \ 0 \cdots \ 0 \ 2 \ 0 \cdots 0]$
- Binary bag of words
 - All examples in the corpus have the same length.
 - Each element in the vector is either 0 or 1.
 - $x^{(i)} = [0 \cdots 0 \ 1 \ 0 \cdots \ 0 \ 1 \ 0 \cdots 0]$

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Recall that the density of a Bernoulli distribution is given by

Bernoulli
$$(x; \gamma) = \gamma^x (1 - \gamma)^{1-x}$$
 (13)

where $\gamma \equiv p(x=1)$.

Thus the log-likelihood of a Bernoulli distribution is

$$\log p(x) = x \log \gamma + (1 - x) \log(1 - \gamma) \tag{14}$$

If your have binary features, i.e. $x_i \in \{0,1\}$ for i=1,...,d, then the output of the decoder can be interpreted has the parameter of a Bernoulli. Thus the likelihood of the input x can be compute has

$$p(x|z) = \prod_{i=1}^{d} p(x_i|z) = \prod_{i=1}^{d} \gamma_i^{x_i} (1 - \gamma_i)^{1 - x_i}$$
 (15)

Note that this works only if $\gamma_i \in (0,1)$. To ensure it, apply sigmoid element wise on the output of the decoder.

And the log-likelihood is given by

$$\log p(x|z) = -\sum_{i=1}^{d} x_i \log \gamma_i + (1 - x_i) \log(1 - \gamma_i)$$

in pytorch
functional.binary_cross_entropy(param, x)

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Probabilistic Decoder $p_{\theta}(x|z)$

Bernoulli MLP as decoder

```
• \gamma = g(z; \boldsymbol{\theta})

• h = \text{relu}(W_{zh}x + b_{zh})

• \gamma = \sigma(W_{hx}h + b_{hx})
```

- $p_{\theta}(x|z) = \text{Bernoulli}(x; \gamma)$
- $\theta = \{W_{zh}, b_{zh}, W_{zx}, b_{zx}\}$

Outline

- Autoencoders
 - An example to keep in mind
 - Autoencoders
- Variational autoencoder
 - Generative Model
 - Latent variable models
 - Variational Lower Bound
- Experiment
 - Unsupervised Spam Detection
 - Preprocessing
 - Binary Cross Entropy
 - Bernoulli MLP as Decoder
 - Spam Detector



Anomaly detection

Algorithm 2 Pseudocode for Batch Gradient Descent

```
Require: Learning rate \epsilon_k Require: Initial parameter \boldsymbol{w}_0 Require: Number of epochs T for i=1 to T do Compute gradient \boldsymbol{g}_t = \frac{1}{m} \nabla_w \sum_i L(h_{w_{t-1}}(\boldsymbol{x}^{(i)}), \boldsymbol{y}^{(i)}) Apply update: \boldsymbol{w}_t = \boldsymbol{w}_{t-1} - \epsilon \boldsymbol{g}_t end for
```