CS7015 (Deep Learning) : Lecture 21

Variational Autoencoders

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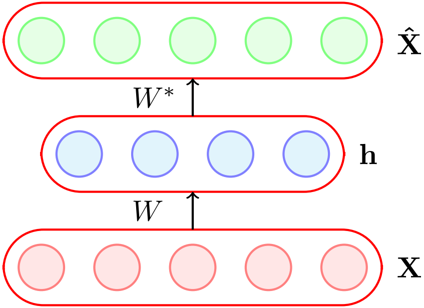
Acknowledgments

- Tutorial on Variational Autoencoders by Carl Doersch[1]
- Blog on Variational Autoencoders by Jaan Altosaar[2]

[1] Tutorial
[2] Blog

Module 21.1: Revisiting Autoencoders



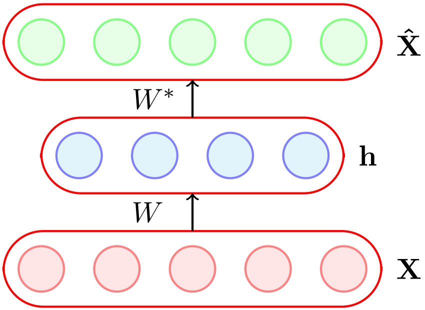
$$\mathbf{h} = g(W\mathbf{X} + \mathbf{b})$$

$$\hat{\mathbf{X}} = f(W^*\mathbf{h} + \mathbf{c})$$

- Before we start talking about VAEs, let us quickly revisit autoencoders
- An autoencoder contains an encoder which takes the input X and maps it to a hidden representation
- The decoder then takes this hidden representation and tries to reconstruct the input from it as $\hat{X}$
- The training happens using the following objective function

$$\min_{W,W^*,\mathbf{c},\mathbf{b}} \frac{1}{m} \sum_{i=1}^{m} \sum_{j=1}^{n} (\hat{x}_{ij} - x_{ij})^2$$

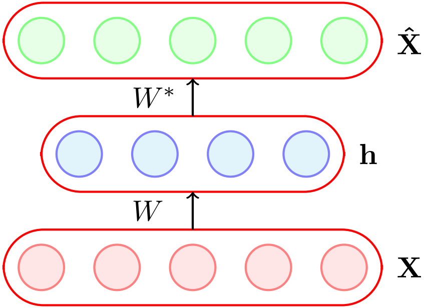
- where m is the number of training instances, $\{x_i\}_{i=1}^{m}$ and each $x_i \in R^n$ (x_{ij} is thus the j-th dimension of the i-th training instance)



$$\mathbf{h} = g(W\mathbf{X} + \mathbf{b})$$

$$\hat{\mathbf{X}} = f(W^*\mathbf{h} + \mathbf{c})$$

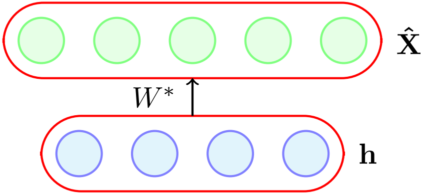
- But where's the fun in this ?
- We are taking an input and simply reconstructing it
- Of course, the fun lies in the fact that we are getting a good *abstraction* of the input
- But RBMs were able to do something more besides abstraction (they were able to do *generation*)
- Let us revisit *generation* in the context of autoencoders



$$\mathbf{h} = g(W\mathbf{X} + \mathbf{b})$$

$$\hat{\mathbf{X}} = f(W^*\mathbf{h} + \mathbf{c})$$

- Can we do generation with autoencoders ?
- In other words, once the autoencoder is trained can I remove the encoder, feed a hidden representation h to the decoder and decode a $\hat{X}$ from it ?
- In principle, yes! But in practice there is a problem with this approach
- h is a very high dimensional vector and only a few vectors in this space would actually correspond to meaningful latent representations of our input
- So of all the possible value of h which values should I feed to the decoder (we had asked a similar question before: slide 67, bullet 5 of lecture 19)



$$\hat{\mathbf{X}} = f(W^*\mathbf{h} + \mathbf{c})$$

- Ideally, we should only feed those values of h which are highly *likely*
- In other words, we are interested in sampling from $P(h|X)$ so that we pick only those h's which have a high probability
- But unlike RBMs, autoencoders do not have such a probabilistic interpretation
- They learn a hidden representation h but not a distribution $P(h|X)$
- Similarly the decoder is also deterministic and does not learn a distribution over X (given a h we can get a X but not $P(X|h)$)

We will now look at variational autoencoders which have the same structure as autoencoders but they learn a distribution over the hidden variables

Module 21.2: Variational Autoencoders: The Neural Network Perspective

Figure: Abstraction

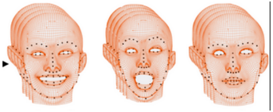
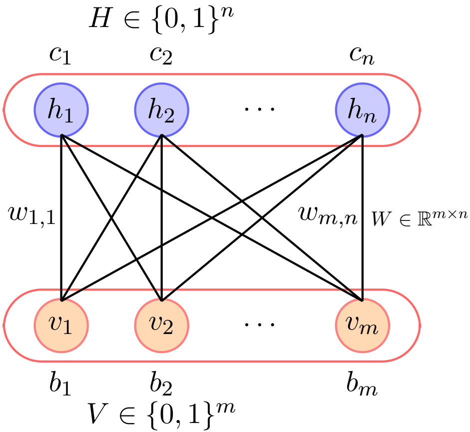
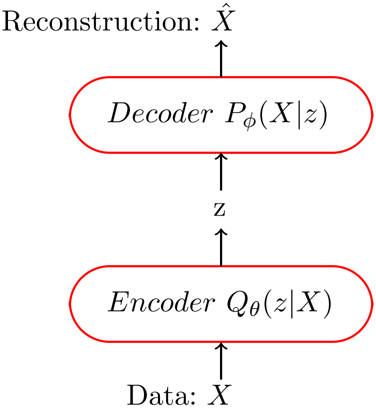


Figure: Generation

- Let $\{X = x_i\}_{i=1}^N$ be the training data
- We can think of X as a random variable in R^n
- For example, X could be an image and the dimensions of X correspond to pixels of the image
- We are interested in learning an abstraction (i.e., given an X find the hidden representation z)
- We are also interested in generation (*i.e.*, given a hidden representation generate an X)
- In probabilistic terms we are interested in $P(z|X)$ and $P(X|z)$ (to be consistent with the literation on VAEs we will use z instead of H and X instead of V)

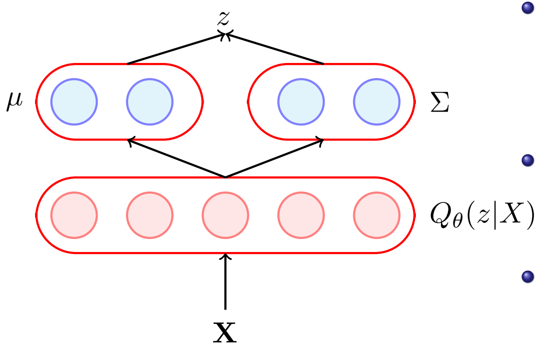


- Earlier we saw RBMs where we learnt $P(z|X)$ and $P(X|z)$
- Below we list certain characteristics of RBMs
- **Structural assumptions:** We assume certain independencies in the Markov Network
- **Computational:** When training with Gibbs Sampling we have to run the Markov Chain for many time steps which is expensive
- **Approximation:** When using Contrastive Divergence, we approximate the expectation by a point estimate
- (Nothing wrong with the above but we just mention them to make the reader aware of these characteristics)



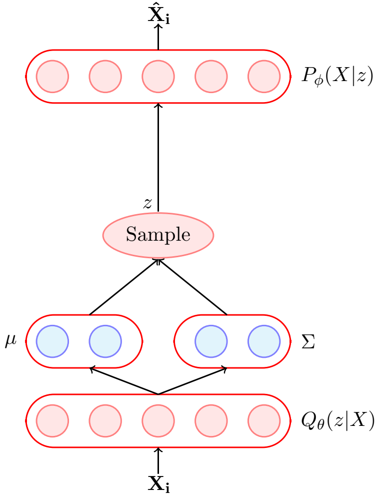
θ: the parameters of the encoder neural network
ϕ: the parameters of the decoder neural network

- We now return to our goals
- **Goal 1:** Learn a distribution over the latent variables ($Q(z|X)$)
- **Goal 2:** Learn a distribution over the visible variables ($P(X|z)$)
- VAEs use a neural network based encoder for Goal 1
- and a neural network based decoder for Goal 2
- We will look at the encoder first

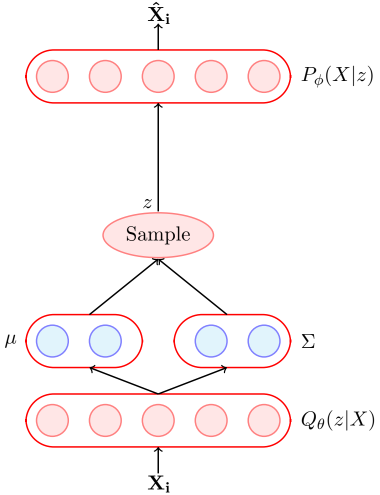


$X \in \mathbb{R}^n$, $\mu \in \mathbb{R}^m$ and $\Sigma \in \mathbb{R}^{m \times m}$

- **Encoder:** What do we mean when we say we want to learn a distribution? We mean that we want to learn the parameters of the distribution
- But what are the parameters of $Q(z|X)$? Well it depends on our modeling assumption!
- In VAEs we assume that the latent variables come from a standard normal distribution $\mathcal{N}(0, I)$ and the job of the encoder is to then predict the parameters of this distribution



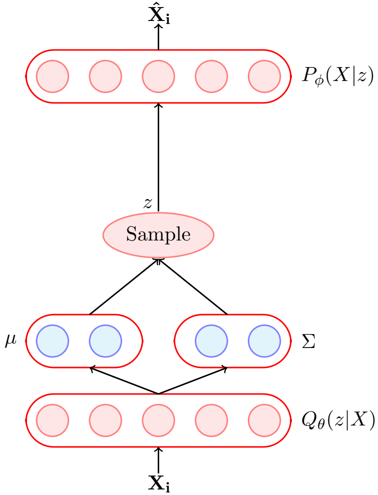
- Now what about the decoder?
- The job of the decoder is to predict a probability distribution over $X : P(X|z)$
- Once again we will assume a certain form for this distribution
- For example, if we want to predict 28 x 28 pixels and each pixel belongs to $\mathbb{R}$ (*i.e.*, $X \in \mathbb{R}^{784}$) then what would be a suitable family for $P(X|z)$?
- We could assume that $P(X|z)$ is a Gaussian distribution with unit variance
- The job of the decoder f would then be to predict the mean of this distribution as $f_\phi(z)$



- What would be the objective function of the decoder ?
- For any given training sample x_i it should maximize $P(x_i)$ given by

$$P(x_i) = \int P(z)P(x_i|z)dz$$
$$= -\mathbb{E}_{z\sim Q_\theta(z|x_i)}[\log P_\phi(x_i|z)]$$

- (As usual we take log for numerical stability)



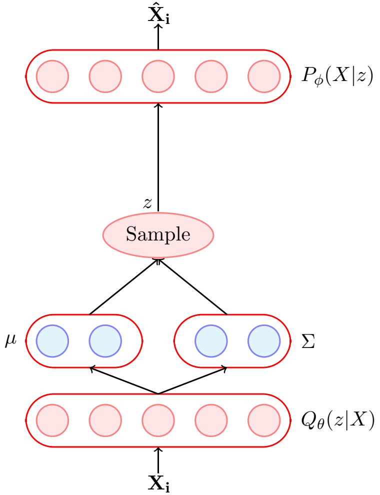
- KL divergence captures the difference (or distance) between 2 distributions

- This is the loss function for one data point ($l_i(\theta)$) and we will just sum over all the data points to get the total loss $\mathscr{L}(\theta)$

$$\mathscr{L}(\theta) = \sum_{i=1}^{m} l_i(\theta)$$

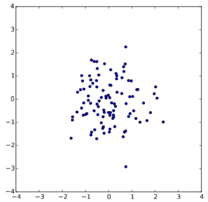
- In addition, we also want a constraint on the distribution over the latent variables
- Specifically, we had assumed $P(z)$ to be $\mathcal{N}(0, I)$ and we want $Q(z|X)$ to be as close to $P(z)$ as possible
- Thus, we will modify the loss function such that

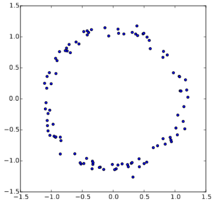
$$l_i(\theta, \phi) = -\mathbb{E}_{z \sim Q_\theta(z|x_i)}[\log P_\phi(x_i|z)] \\ + KL(Q_\theta(z|x_i)||P(z))$$



$$l_i(\theta, \phi) = -\mathbb{E}_{z \sim Q_\theta(z|x_i)}[\log P_\phi(x_i|z)] + KL(Q_\theta(z|x_i)||P(z))$$

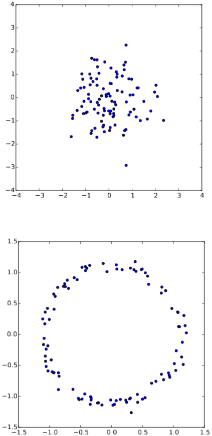
- The second term in the loss function can actually be thought of as a regularizer
- It ensures that the encoder does not cheat by mapping each x_i to a different point (a normal distribution with very low variance) in the Euclidean space
- In other words, in the absence of the regularizer the encoder can learn a unique mapping for each x_i and the decoder can then decode from this unique mapping
- Even with high variance in samples from the distribution, we want the decoder to be able to reconstruct the original data very well (motivation similar to the adding noise)
- To summarize, for each data point we predict a distribution such that, with high probability a sample from this distribution should be able to reconstruct the original data point
- But why do we choose a normal distribution? Isn't it too simplistic to assume that z follows a normal distribution





$$l_i(\theta, \phi) = -\mathbb{E}_{z \sim Q_\theta(z|x_i)}[\log P_\phi(x_i|z)] + KL(Q_\theta(z|x_i)||P(z))$$

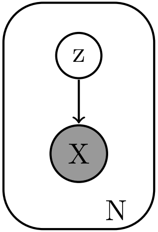
- Isn't it a very strong assumption that $P(z) \sim \mathcal{N}(0, I)$?
- For example, in the 2-dimensional case how can we be sure that $P(z)$ is a normal distribution and not any other distribution
- The key insight here is that any distribution in d dimensions can be generated by the following steps
- Step 1: Start with a set of d variables that are normally distributed (that's exactly what we are assuming for $P(z)$)
- Step 2: Mapping these variables through a sufficiently complex function (that's exactly what the first few layers of the decoder can do)



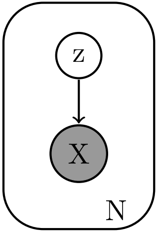
$$l_i(\theta,\phi) = -\mathbb{E}_{z\sim Q_\theta(z|x_i)}[\log P_\phi(x_i|z)] \\ +KL(Q_\theta(z|x_i)||P(z))$$

- In particular, note that in the adjoining example if z is 2-D and normally distributed then $f(z)$ is roughly ring shaped (giving us the distribution in the bottom figure)
$$f(z) = \frac{z}{10} + \frac{z}{||z||}$$
- A non-linear neural network, such as the one we use for the decoder, could learn a complex mapping from z to $f_\phi(z)$ using its parameters ϕ
- The initial layers of a non linear decoder could learn their weights such that the output is $f_\phi(z)$
- The above argument suggests that even if we start with normally distributed variables the initial layers of the decoder could learn a complex transformation of these variables say $f_\phi(z)$ if required
- The objective function of the decoder will ensure that an appropriate transformation of z is learnt to reconstruct X

Module 21.3: Variational autoencoders: (The graphical model perspective)



- Here we can think of z and X as random variables
- We are then interested in the joint probability distribution $P(X, z)$ which factorizes as $P(X, z) = P(z)P(X|z)$
- This factorization is natural because we can imagine that the latent variables are fixed first and then the visible variables are drawn based on the latent variables
- For example, if we want to draw a digit we could first fix the latent variables: *the digit, size, angle, thickness, position and so on* and then draw a digit which corresponds to these latent variables
- And of course, unlike RBMs, this is a directed graphical model



- Now at inference time, we are given an X (observed variable) and we are interested in finding the most likely assignments of latent variables z which would have resulted in this observation
- Mathematically, we want to find

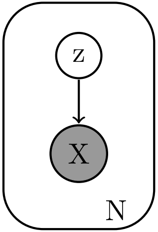
$$P(z|X) = \frac{P(X|z)P(z)}{P(X)}$$

- This is hard to compute because the LHS contains $P(X)$ which is intractable

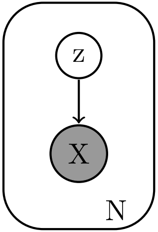
$$P(X) = \int P(X|z)P(z)dz$$

$$= \int\int ... \int P(X|z_1, z_2, ..., z_n)P(z_1, z_2, ..., z_n)dz_1, ...dz_n$$

- In RBMs, we had a similar integral which we approximated using Gibbs Sampling
- VAEs, on the other hand, cast this into an optimization problem and learn the parameters of the optimization problem



- Specifically, in VAEs, we assume that instead of $P(z|X)$ which is intractable, the posterior distribution is given by $Q_\theta(z|X)$
- Further, we assume that $Q_\theta(z|X)$ is a Gaussian whose parameters are determined by a neural network $\mu, \Sigma = g_\theta(X)$
- The parameters of the distribution are thus determined by the parameters θ of a neural network
- Our job then is to learn the parameters of this neural network



- But what is the objective function for this neural network
- Well we want the proposed distribution $Q_\theta(z|X)$ to be as close to the true distribution
- We can capture this using the following objective function

$$minimize \ \ KL(Q_\theta(z|X)||P(z|X))$$

- What are the parameters of the objective function ? (they are the parameters of the neural network - we will return back to this again)

- Let us expand the KL divergence term

$$\begin{aligned} D[Q_\theta(z|X)||P(z|X)] &= \int Q_\theta(z|X)\log Q_\theta(z|X)dz - \int Q_\theta(z|X)\log P(z|X)dz \\ &= \mathbb{E}_{z\sim Q_\theta(z|X)}[\log Q_\theta(z|X) - \log P(z|X)] \end{aligned}$$

- For shorthand we will use $\mathbb{E}_Q = \mathbb{E}_{z\sim Q_\theta(z|X)}$
- Substituting $P(z|X) = \frac{P(X|z)P(z)}{P(X)}$, we get

$$\begin{aligned} D[Q_\theta(z|X)||P(z|X)] &= \mathbb{E}_Q[\log Q_\theta(z|X) - \log P(X|z) - \log P(z) + \log P(X)] \\ &= \mathbb{E}_Q[\log Q_\theta(z|X) - \log P(z)] - \mathbb{E}_Q[\log P(X|z)] + \log P(X) \\ &= D[Q_\theta(z|X)||p(z)] - \mathbb{E}_Q[\log P(X|z)] + \log P(X) \end{aligned}$$

$$\therefore \log p(X) = \mathbb{E}_Q[\log P(X|z)] - D[Q_\theta(z|X)||P(z)] + D[Q_\theta(z|X)||P(z|X)]$$

- So, we have

$$\log P(X) = \mathbb{E}_Q[\log P(X|z)] - D[Q_\theta(z|X)||P(z)] + D[Q_\theta(z|X)||P(z|X)]$$

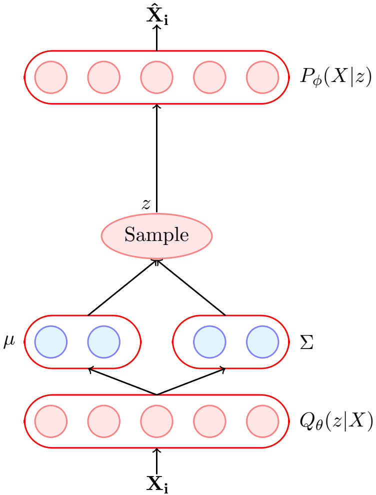
- Recall that we are interested in maximizing the log likelihood of the data *i.e.* $P(X)$
- Since KL divergence (the red term) is always >= 0 we can say that

$$\mathbb{E}_Q[\log P(X|z)] - D[Q_\theta(z|X)||P(z)] <= \log P(X)$$

- The quantity on the LHS is thus a lower bound for the quantity that we want to maximize and is knows as the Evidence lower bound (ELBO)
- Maximizing this lower bound is the same as maximizing $\log P(X)$ and hence our equivalent objective now becomes

$$maximize \;\; \mathbb{E}_Q[\log P(X|z)] - D[Q_\theta(z|X)||P(z)]$$

- And, this method of learning parameters of probability distributions associated with graphical models using optimization (by maximizing ELBO) is called variational inference
- Why is this any easier? It is easy because of certain assumptions that we make as discussed on the next slide



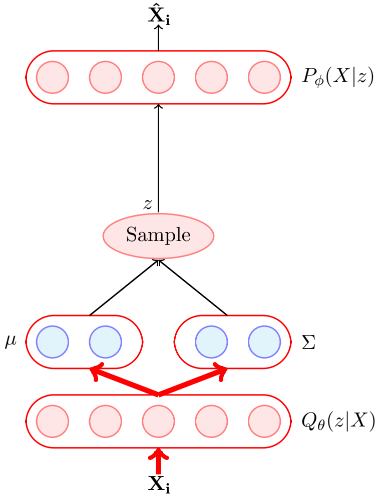
- First we will just reintroduce the parameters in the equation to make things explicit

$$maximize \;\; \mathbb{E}_Q[\log P_\phi(X|z)] - D[Q_\theta(z|X)||P(z)]$$

- At training time, we are interested in learning the parameters θ which maximize the above for every training example ($x_i \in \{x_i\}_{i=1}^N$)
- So our total objective function is

$$\underset{\theta}{maximize} \sum_{i=1}^{N} \mathbb{E}_Q[\log P_\phi(X = x_i|z)] - D[Q_\theta(z|X = x_i)||P(z)]$$

- We will shorthand $P(X = x_i)$ as $P(x_i)$
- However, we will assume that we are using stochastic gradient descent so we need to deal with only one of the terms in the summation corresponding to the current training example



- So our objective function w.r.t. one example is

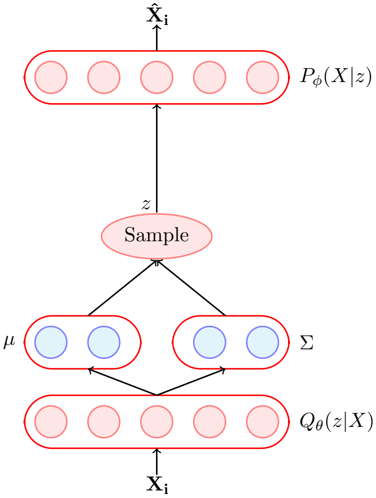
$$\underset{\theta}{maximize} \ \mathbb{E}_Q[\log P_\phi(x_i|z)] - D[Q_\theta(z|x_i)||P(z)]$$

- Now, first we will do a forward prop through the encoder using X_i and compute $\mu(X)$ and $\Sigma(X)$
- The second term in the above objective function is the difference between two normal distribution $\mathcal{N}(\mu(X), \Sigma(X))$ and $\mathcal{N}(0, I)$
- With some simple trickery you can show that this term reduces to the following expression (Seep proof here)

$$D[\mathcal{N}(\mu(X), \Sigma(X))||\mathcal{N}(0, I)]$$
$$= \frac{1}{2}(tr(\Sigma(X)) + (\mu(X))^T[\mu(X)) - k - \log det(\Sigma(X))]$$

where k is the dimensionality of the latent variables

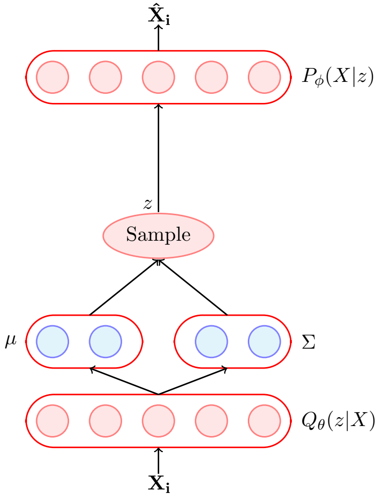
- This term can be computed easily because we have already computed $\mu(X)$ and $\Sigma(X)$ in the forward pass



- Now let us look at the other term in the objective function

$$\sum_{i=1}^{n} \mathbb{E}_Q[\log P_\phi(X|z)]$$

- This is again an expectation and hence intractable (integral over z)
- In VAEs, we approximate this with a single z sampled from $\mathcal{N}(\mu(X), \Sigma(X))$
- Hence this term is also easy to compute (of course it is a nasty approximation but we will live with it!)



- Further, as usual, we need to assume some parametric form for $P(X|z)$
- For example, if we assume that $P(X|z)$ is a Gaussian with mean $\mu(z)$ and variance I then

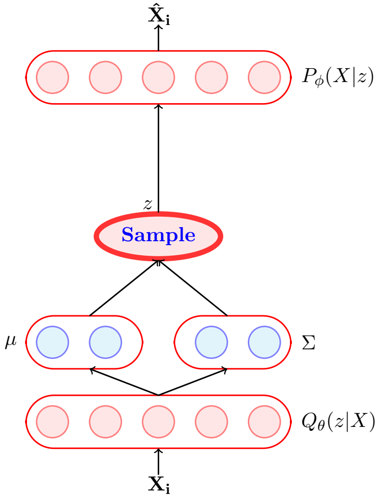
$$\log P(X = X_i|z) = C - \frac{1}{2}||X_i - \mu(z)||^2$$

- $\mu(z)$ in turn is a function of the parameters of the decoder and can be written as $f_\phi(z)$

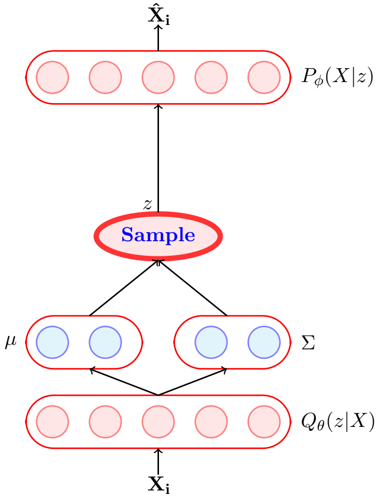
$$\log P(X = X_i|z) = C - \frac{1}{2}||X_i - f_\phi(z)||^2$$

- Our effective objective function thus becomes

$$\underset{\theta,\phi}{minimize} \quad \sum_{n=1}^{N} \Big[\frac{1}{2}(tr(\Sigma(X_i)) + (\mu(X_i))^T[\mu(X_i)) - k$$
$$- \log det(\Sigma(X_i))] + ||X_i - f_\phi(z)||^2\Big]$$



- The above loss can be easily computed and we can update the parameters θ of the encoder and ϕ of decoder using backpropagation
- However, there is a catch !
- The network is not end to end differentiable because the output $f_\phi(z)$ is not an end to end differentiable function of the input X
- Why? because after passing X through the network we simply compute $\mu(X)$ and $\Sigma(X)$ and then sample a z to be fed to the decoder
- This makes the entire process non-deterministic and hence $f_\phi(z)$ is not a continuous function of the input X



- VAEs use a neat trick to get around this problem
- This is known as the reparameterization trick wherein we move the process of sampling to an input layer
- For 1 dimensional case, given μ and σ we can sample from $\mathcal{N}(\mu, \sigma)$ by first sampling $\epsilon \sim \mathcal{N}(0, 1)$, and then computing

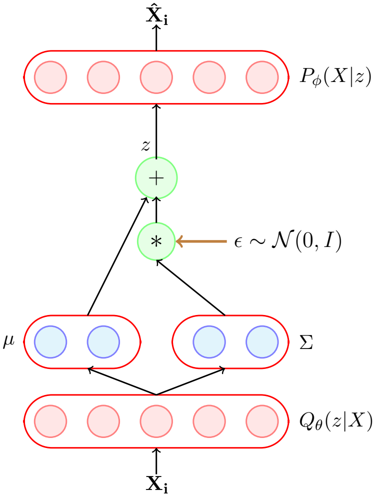
$$z = \mu + \sigma * \epsilon$$

- The adjacent figure shows the difference between the original network and the reparamterized network
- The randomness in $f_\phi(z)$ is now associated with ϵ and not X or the parameters of the model

- **Data:** $\{X_i\}_{i=1}^N$
- **Model:** $\hat{X} = f_\phi(\mu(X) + \Sigma(X) * \epsilon)$
- **Parameters:** θ, ϕ
- **Algorithm:** Gradient descent
- **Objective:**

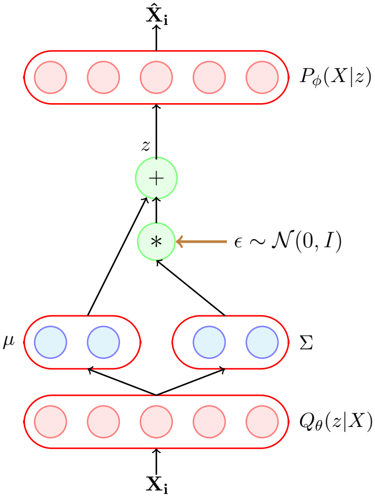
$$\sum_{n=1}^{N} \left[\frac{1}{2}(tr(\Sigma(X_i)) + (\mu(X_i))^T [\mu(X_i)) - k - \log det(\Sigma(X_i))] + ||X_i - f_\phi(z)||^2 \right]$$

- With that we are done with the process of training VAEs
- Specifically, we have described the data, model, parameters, objective function and learning algorithm
- Now what happens at test time? We need to consider both *abstraction* and *generation*
- In other words we are interested in computing a z given a X as well as in generating a X given a z
- Let us look at each of these goals



- After the model parameters are learned we feed a X to the encoder
- By doing a forward pass using the learned parameters of the model we compute $\mu(X)$ and $\Sigma(X)$
- We then sample a z from the distribution $\mu(X)$ and $\Sigma(X)$ or using the same reparameterization trick
- In other words, once we have obtained $\mu(X)$ and $\Sigma(X)$, we first sample $\epsilon \sim \mathcal{N}(\mu(X), \Sigma(X))$ and then compute z

$$z = \mu + \sigma * \epsilon$$



Generation

- After the model parameters are learned we remove the encoder and feed a $z \sim \mathcal{N}(0, I)$ to the decoder
- The decoder will then predict $f_\phi(z)$ and we can draw an $X \sim \mathcal{N}(f_\phi(z), I)$
- Why would this work ?
- Well, we had trained the model to minimize $D(Q_\theta(z|X)||p(z))$ where $p(z)$ was $\mathcal{N}(0, I)$
- If the model is trained well then $Q_\theta(z|X)$ should also become $\mathcal{N}(0, I)$
- Hence, if we feed $z \sim \mathcal{N}(0, I)$, it is almost as if we are feeding a $z \sim Q_\theta(z|X)$ and the decoder was indeed trained to produce a good $f_\phi(z)$ from such a z
- Hence this will work !