# CS109B Advanced Section : A Tour of Variational Inference

Professor : Pavlos Protopapas, TF : Srivatsan Srinivasan

CS109B, IACS

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# Information Theory

# Information Theory

How much information can be communicated between any two components of any system ?

**QUESTION :** Assume you have N forks (left or right) on road. An oracle tells you which paths you take to reach a final destination. How many prompts do you need ?

**SHANNON INFORMATION (SI) :** Consider a coin which lands heads 90% times. What is the surprise when you see its outcome?

SI Quantifies surprise of information - $SI = -\log_2 p(x_h)$

# Entropy

Assume I transmit 1000 bits (0s and 1s) of information from A to B. What is the quantum of information that has been transmitted ?

- When all the bits are known ? (0 shannons)
- When each bit is i.i.d. and equally distributed (P(0) = P(1) =0.5) i.e. all messages are equi-probable? (1000 shannons)
- Entropy defines a general uncertainty measure over this information. When is it maximized ?

$$H(X) = -\mathbb{E}_X \log p(x) = -\sum_x p(x) \log p(x) \quad \text{or} \quad -\int_x p(x) \log p(x) dx \tag{1}$$

**EXERCISE :** Calculate entropy of a dice roll.

**REMEMBER THIS ?** $-p(x) \log p(x) - (1 - p(x)) \log p(x)$

# Joint and Conditional Entropy

- Joint Entropy - Entropy of joint distribution

$$H^{joint}(X,Y) = -\mathbb{E}_{X,Y} \log p(X,Y) = -\sum_{x,y} p(x,y) \log p(x,y) \tag{2}$$

- Conditional Entropy - Conditional Uncertainty of X given Y

$$\begin{aligned} H(X|Y) &= -\mathbb{E}_Y H(X|Y=y) \\ &= -\sum_y p(y) \sum_x p(x|y) \log p(x|y) \\ &= -\sum_{x,y} p(x,y) \log p(x|y) \end{aligned} \tag{3}$$

$$H(X|Y) = H(X,Y) - H(Y)$$

# Mutual Information

Pointwise Mutual Information - Between two events, the discrepancy between joint likelihood and independent joint likelihood

$$pmi(x, y) = \log \frac{p(x, y)}{p(x)p(y)} \tag{4}$$

Mutual Information - Expected amount of information that can be obtained about one random variable by observing another.

$$\begin{aligned} I(X;Y) &= \mathbb{E}_{x,y}\, pmi(x, y) = \mathbb{E}_{x,y} \log \frac{p(x, y)}{p(x)p(y)} \\ I(X;Y) &= I(Y;X) \quad \text{(symmetric)} \\ &= H(X) - H(X|Y) = H(Y) - H(Y|X) \\ &= H(X) + H(Y) - H(X, Y) \end{aligned} \tag{5}$$

# Cross Entropy

Average number of bits needed to identify an event drawn from $p$ when a coding scheme used is for optimizing a different distribution $q$.

$$H(p,q) = \mathbb{E}_p - \log(q) = \sum_x -p(x) \log q(x) \tag{6}$$

Example : Take any code over which you communicate a equiprobable number between 1 and 8 (true). But your receiver uses a different code scheme and hence needs a longer message length to get the message.

**REMEMBER ?** $y \log \hat{y} + (1-y) \log(1-\hat{y})$

# Understanding cross entropy

- Game 1 : 4 coins of different color each(blue, yellow, red, green) - probability each 0.25. Ask me yes/no questions to figure out the answer.
  - Q1 : Is it green or blue ?
  - Q2 : Yes : Is it green? No : Is it red ?
  - Expected number of questions 2 H(P)
- Game 2 : 4 coins of different color each - probability each [0.5 -blue, 0.125-red, 0.125-green, 0.25-yellow]. Ask me yes/no questions to figure out the answer.
  - Q1 : Is it blue ?
  - Q2 : Yes : over, No : Is it red ?
  - Q3 : Yes : over, No : Is it yellow ?
  - Expected number of questions 1.75. H(Q)
- Game 3 : Use strategy used in game 1 on game 2 and the expected number of questions is $2 > 1.75$. H(Q,P)

# KL Divergence

Measure of Discrepancy between two probability distributions.

$$\begin{aligned} D_{KL}(p(X)||q(X)) &= -\mathbb{E}_P \log \frac{q(X)}{p(X)} \\ &= -\sum_x p(x) \log \frac{q(x)}{p(x)} \quad \text{or} \quad -\int_x p(x) \log \frac{q(x)}{p(x)} dx \end{aligned} \tag{7}$$

$$D_{KL}(P||Q) = H(P,Q) - H(P) \geq 0 \tag{8}$$

Remember entropy of P quantifies the least possible message length for encoding information from P.

KL - Extra message-length per datum that must be communicated if a code that is optimal for a given (wrong) distribution Q is used, compared to using a code based on the true distribution P.

# Variational Inference

# Latent Variable Inference

- Latent Variables - Random variables which are not observed.
- Example - Data of Children's score on an exam - Latent Variable : Intelligence of a child
- Example

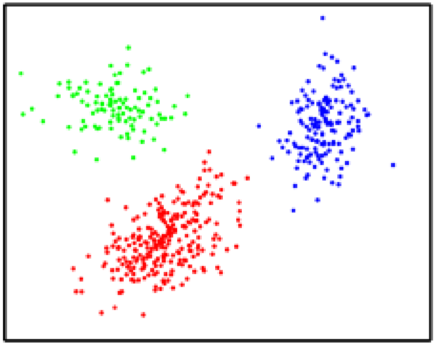


Figure 1: Mixture of cluster centers

- Break down :

$$p(x,z) = \underbrace{p(z)}_{\text{latent}}\,p(x|z) = p(z|x)p(x); \quad p(x) = \int_z p(x,z)dz$$

# Latent Variable Inference

- Assuming a prior on z since it is under our control.
- **INFERENCE :** Learn posterior of the latent distribution - $p(z|x)$. How does our belief about the latent variable change after observing data ?

$$p(z|x) = \frac{p(x|z)p(z)}{p(x)} = \underbrace{\frac{p(x|z)p(z)}{\sum_z p(x|z)p(z)}}_{\text{Could be intractable}} \tag{9}$$

# Variational Inference - Central Idea

Minimize $KL(q(z)||p(z|x))$

$$q^*(\mathbf{z}) = \arg\min_{q\sim\mathcal{Q}} \mathrm{KL}(q(\mathbf{z})||p(\mathbf{z}|\mathbf{x})) \tag{10}$$

$$\begin{aligned}
\mathrm{KL}(q(\mathbf{z})||p(\mathbf{z}|\mathbf{x})) &= \mathbb{E}_{\mathbf{z}\sim q}\log q(\mathbf{z}) - \mathbb{E}_{\mathbf{z}\sim q}\log p(\mathbf{z}|\mathbf{x}) \\
&= \underbrace{\mathbb{E}_{\mathbf{z}\sim q}\log q(\mathbf{z}) - \mathbb{E}_{\mathbf{z}\sim q}\log p(\mathbf{z},\mathbf{x})}_{\text{(a) --- -1*ELBO}} + \underbrace{\log p(\mathbf{x})}_{\text{(b)}} \\
&= -\mathrm{ELBO}(q) + \underbrace{\log p(\mathbf{x})}_{\text{Does not depend on z}}
\end{aligned} \tag{11}$$

**Idea**

*Minimizing* $KL(q(z)||p(z|x))$ = *Maximizing ELBO !*

# ELBO

$$\begin{aligned}\mathrm{ELBO}(p,q) &= \mathbb{E}_q \log p(\mathbf{z},\mathbf{x}) - \mathbb{E}_q \log q(\mathbf{z}) \\ &= \mathbb{E}_q \log p(\mathbf{z}) + \mathbb{E}_q \log p(\mathbf{x}|\mathbf{z}) - \mathbb{E}_q \log q(\mathbf{z}) \\ &= \mathbb{E}_q \log p(\mathbf{x}|\mathbf{z}) - \mathrm{KL}(q(\mathbf{z})||p(\mathbf{z}))\end{aligned} \tag{12}$$

## Idea

$\mathbb{E}_q \log p(\boldsymbol{z},\boldsymbol{x}) - \mathbb{E}_q \log q(\boldsymbol{z})$- *Energy encourages q to focus probability mass where the joint mass is, $p(\mathbf{x},\mathbf{z})$. The entropy encourages q to spread probability mass and avoid concentration to one location.*

## Idea

*ELBO Term* $\mathbb{E}_q \log p(\boldsymbol{x}|\boldsymbol{z}) - KL(q(\boldsymbol{z})||p(\boldsymbol{z})$- *Conditional Likelihood Term and KL Term. Trade-off between maximizing the conditional likelihood and not deviating from the true latent distribution (prior).*

# Variational Parameters

- Parametrize q(z) using variational parameters $\lambda$ - $q(z;\lambda)$
- Learn variational parameters during training (using some gradient based optimization for example)
- Example - $q(z;\lambda=[\mu,\sigma]) \sim \mathcal{N}(\mu,\sigma)$. Here $\mu,\sigma$ are variational parameters $\lambda=[\mu,\sigma]$.
- $ELBO(\lambda) = \mathbb{E}_{q(z;\lambda)} \log p(\mathbf{x}|\mathbf{z}) - \mathrm{KL}(q(\mathbf{z};\lambda)||p(\mathbf{z}))$
- Gradients :
  $\nabla_\lambda ELBO(\lambda) = \nabla_\lambda\big[\mathbb{E}_{q(z;\lambda)} \log p(\mathbf{x}|\mathbf{z}) - \mathrm{KL}(q(\mathbf{z};\lambda)||p(\mathbf{z}))\big]$
- Not directly differentiable via backpropagation : WHY ?

# VI Gradients and Reparametrization

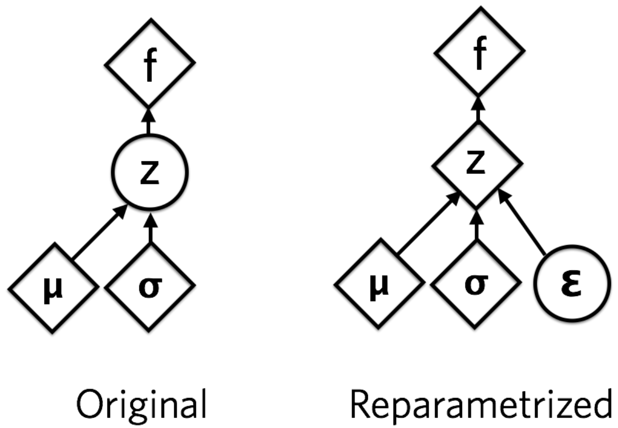



Figure 2: Reparametrization Trick : $z = \mu + \sigma * \epsilon; \quad \epsilon \sim \mathcal{N}(0, 1)$

- Gradients : $\nabla_\lambda ELBO(\lambda) = \mathbb{E}_\epsilon \Big[ \nabla_\lambda \big[ \log p(\mathbf{x}|\mathbf{z}) - \mathrm{KL}(q(\mathbf{z};\lambda)||p(\mathbf{z})) \big] \Big]$
- Disadvantage : Not flexible for any black box distribution.

# VI Gradients and Score Function a.k.a REINFORCE

$$
\begin{aligned}
\nabla_\lambda ELBO(\lambda) &= \nabla_\lambda \mathbb{E}_{q(z;\lambda)}\left[-\log q_\lambda(z) + \log p(z) + \log p(x|z)\right] \\
&= \int_z \nabla_\lambda q_\lambda(z)\left[-\log q_\lambda(z) + \log p(z) + \log p(x|z)\right] dz \\
&\text{Use} \nabla_\lambda(q_\lambda(z)) = q_\lambda(z) \log q_\lambda(z) \\
&= \mathbb{E}_{q(z;\lambda)}\left[\left(\nabla_\lambda q_\lambda(z)\right) \cdot \left(-\log q_\lambda(z) + \log p(z) + \log p(x|z)\right)\right]
\end{aligned} \tag{13}
$$

- Only need ability to take derivative of q with respect to $\lambda$.
- Works for any black box variational family.
- Use MC sampling to update parameters in each step and take empirical mean.

# Mean Field Variational Inference

- Mean Field Approximation - A simplifying approximation for the variational distribution.
- Assumes all the variational components are independent of each other.
- Then, mean field assumption assumes

$$p(z|X) \approx q(z) = \prod_{i=1}^{N} q_i(z_i) \tag{14}$$

# Mean Field VI - GMM

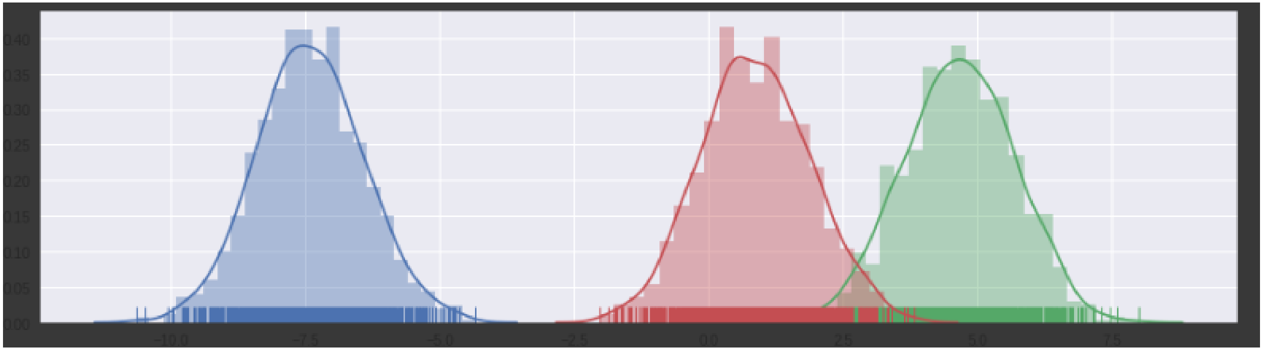



Figure 3: 1-D GMM with three cluster centers

Generative Model : For each datapoint $x^{(i)}$ where i = 1,2......N

- Sample a cluster assignment i.e. the membership of a given point to a mixture component $c^{(i)}$ uniformly. $c^{(i)} \sim Uniform(K)$
- Sample its value from the correpsonding component: $x^{(i)} \sim \mathcal{N}(\mu_{c^{(i)}}, 1)$

# Mean Field VI - GMM

To reiterate, the full parametrization of the model could be written as

- $\mu_j \sim \mathcal{N}(0, \sigma^2)\ \forall j = 1, 2....K$ - totally K (3) cluster centers. Known variance $\sigma$ - Not learning them.
- $c_i \sim \mathcal{U}(K)\ \forall i = 1, 2....N$ - one cluster assignment for each point.
- $x_i \sim \mathcal{N}(c_i^T \mu, 1) \forall i = 1, 2....N$ - each datapoint comes from a Gaussian whose mean is a mixture of the cluster centers with a known variance.
- **PROBLEM :** You are provided X($x_1, ...x_n$). You need to eventually learn P(X) using latent variables $\mu, \mathbf{c}$ which you don't observe. You don't know any of the information that you see above in real life.

# Mean Field Approximations

- Mean Field Definition : $q(z) = \prod_j q_j(z_j)$ .
- Latent variables in this case :
  $q(\mu, c) = q(\mu; m, s^2) = \prod_j q(\mu_j; m_j, s_j^2) \times \prod_i q(c_i, \phi_i)$
- $\mu_j; m_j, s_j^2 \sim \mathcal{N}(m_j, s_j^2)$
- $c_i; \phi_i \sim MultiNomial(\phi_i)$
- Thus, $\phi_i$ is a vector of probabilities such that $p(c_i = j) = \phi_{ij}$ such that $\sum_j \phi_{ij} = 1$. Learns the likelihood of each point belonging to one cluster center.

# Mean Field VI for GMM - A sketch

- Use $ELBO(\lambda) = \mathbb{E}_{q(z;\lambda)} \log p(x,z) + H(q;\lambda)$
- Calculate $\log p(x,c,\mu) = \log p(\mu) \log p(c) \log p(x|c,\mu)$ based on our mean field approximations.
- Calculate the entropy term.

$$\log q(c,\mu) = \log q(c) + \log q(\mu) = \sum_{i=1}^{N} \log q(c_i;\phi_i) + \sum_{j=1}^{K} \log q(\mu_j; m_j, s_j^2)$$

.

- Final ELBO is an expectation over sum of both these terms i.e.

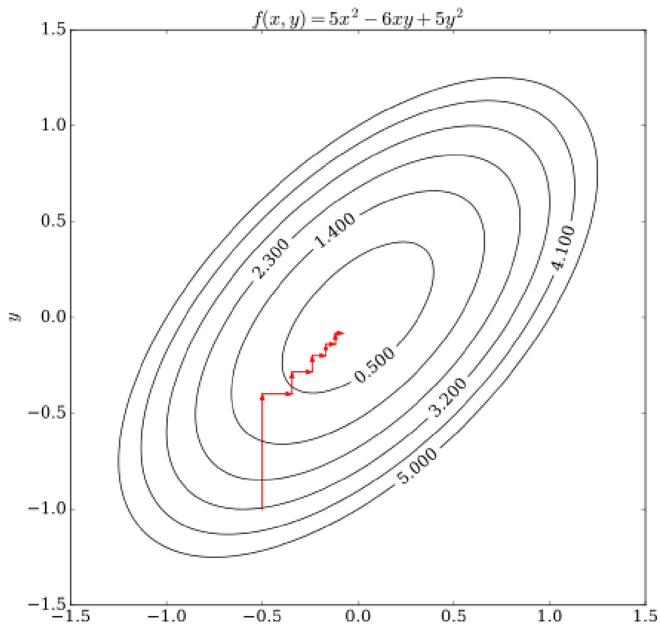
$$\begin{aligned} ELBO \propto \sum_j -\mathbb{E}_q \frac{\mu_j}{2\sigma^2} + \sum_i \sum_j \mathbb{E}_q[C_{ij}] \mathbb{E}_q\left[\frac{(x_i-\mu_j)^2}{2}\right] - \\ \sum_i \sum_j \mathbb{E}_q[\log \phi_{ij}] + \sum_j \frac{1}{2} \log(s_j^2) \end{aligned} \tag{15}$$

# Parameter Updates and CAVI

- Gradient Update $\phi_{ij}$ using $\frac{\partial ELBO}{\partial \phi_{ij}}$
- Gradient update $m_j$ using $\frac{\partial ELBO}{\partial m_j}$
- Gradient Update $s_j^2$ using $\frac{\partial ELBO}{\partial s_j^2}$
- Remember we are doing Coordinate Ascent here (Maximization Problem).

# Coordinate Ascent

1. Choose initial parameter vector x. Repeat steps 2 to 4.
2. Choose an index i from 1 to n.
3. Choose a step size $\alpha$.
4. Update $x_i$ to $x_i + \alpha \frac{\partial F(\mathbf{x})}{\partial x_i}$



# Variational Autoencoders

# Generative Models

- Learns the generative form of the data distribution - P(X)
- Remember AutoEncoders learned in class.
- Why latent variable models are needed ?
- What are the latent variables expected to learn ? Eg: MNIST
- Remember $p(x) = \int_z p(x, z; \theta) p(z; \theta) dz$. $\theta$ can be any parametric form - could be a neural network.

# VAEs

- Define $p(z) = \mathcal{N}(0, I)$
- Transform a simple $p(z)$ into a complicated $p(x)$

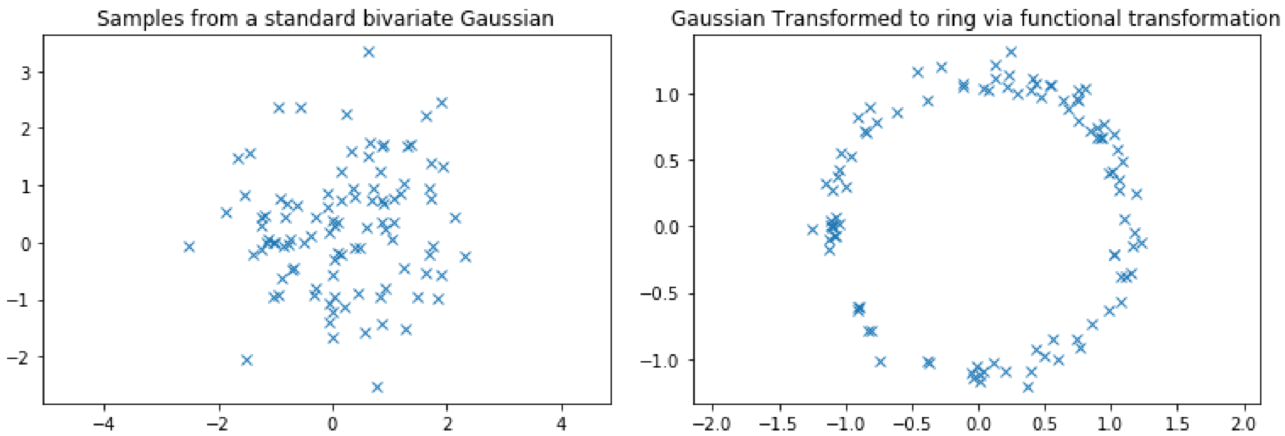



Figure 5: Given a random variable Z with one distribution (on the left - standard bivariate Gaussian), we can always create another random variable X = g(Z) with an entirely different distribution through appropriate functional transformation(on the right. $g(z) \rightarrow z/10 + z/||z||$.

**Where is the Autoencoder?**

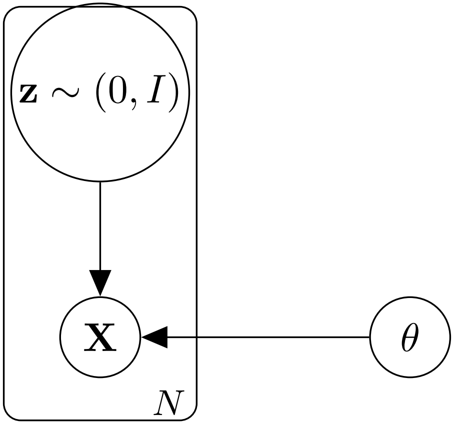



Figure 6: Graphical Model of VAE

Need to infer the posterior after observing data.

$$p(z|x) = \frac{p(x|z)p(z)}{\underbrace{\int_z p(x|z;\theta)p(z)dz}_{\text{Intractable}}} \tag{16}$$

# VAEs

Assume variational approximation for p(z—x). We have got our encoder decoder setup back. q is the encoder and p is the decoder.

$$\mathcal{L}(\mathbf{x};\theta,\lambda) = D_{KL}\big(\underbrace{q(\mathbf{z}|\mathbf{x};\lambda)}_{\text{decoder}}\,||p(\mathbf{z})\big) - \mathbb{E}_{\mathbf{z}\sim q}\log \underbrace{p(\mathbf{x}|\mathbf{z};\theta)}_{\text{encoder}} \tag{17}$$

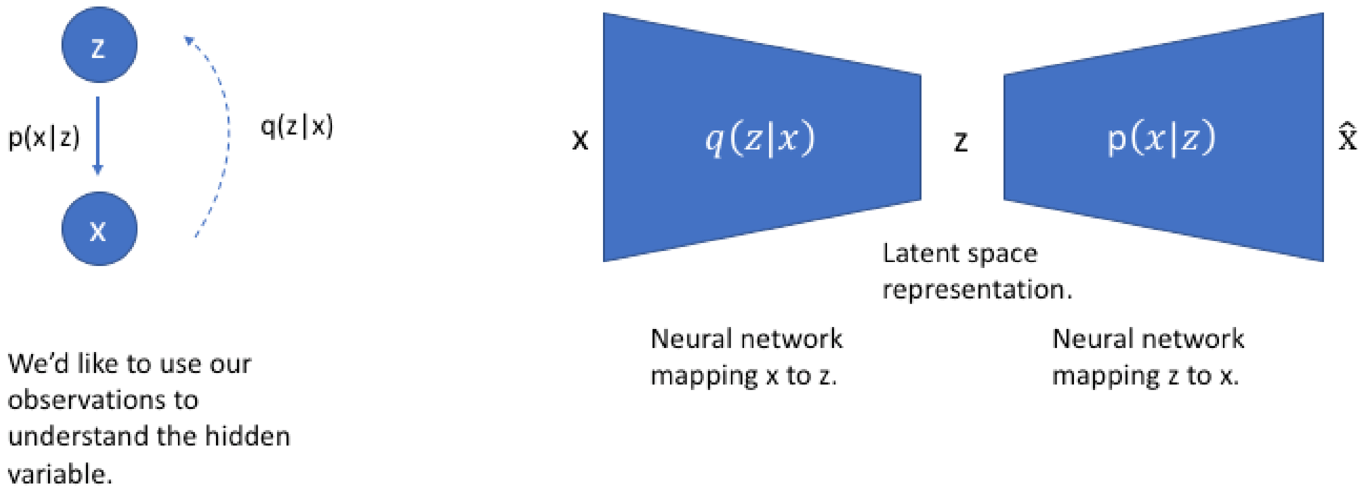



Figure 7: VAE in a nutshell

# VAEs

$$\mathcal{L}(\mathbf{x};\theta,\lambda) = D_{KL}\Big(\underbrace{q(\mathbf{z}|\mathbf{x};\lambda)}_{\text{decoder}}||p(\mathbf{z})\Big) - \mathbb{E}_{\mathbf{z}\sim q}\log \underbrace{p(\mathbf{x}|\mathbf{z};\theta)}_{\text{encoder}}$$

$$D_{KL}((\mathcal{N}(\mu(X),\Sigma(X))||\mathcal{N}(0,I)) = \frac{1}{2}\Big(\mathrm{Tr}(\Sigma(X)) + (\mu(X))^T(\mu(X)) - k - \log\det(\Sigma(X))\Big) \tag{18}$$

What about the reconstruction term ?

# VAE Reconstruction - Training

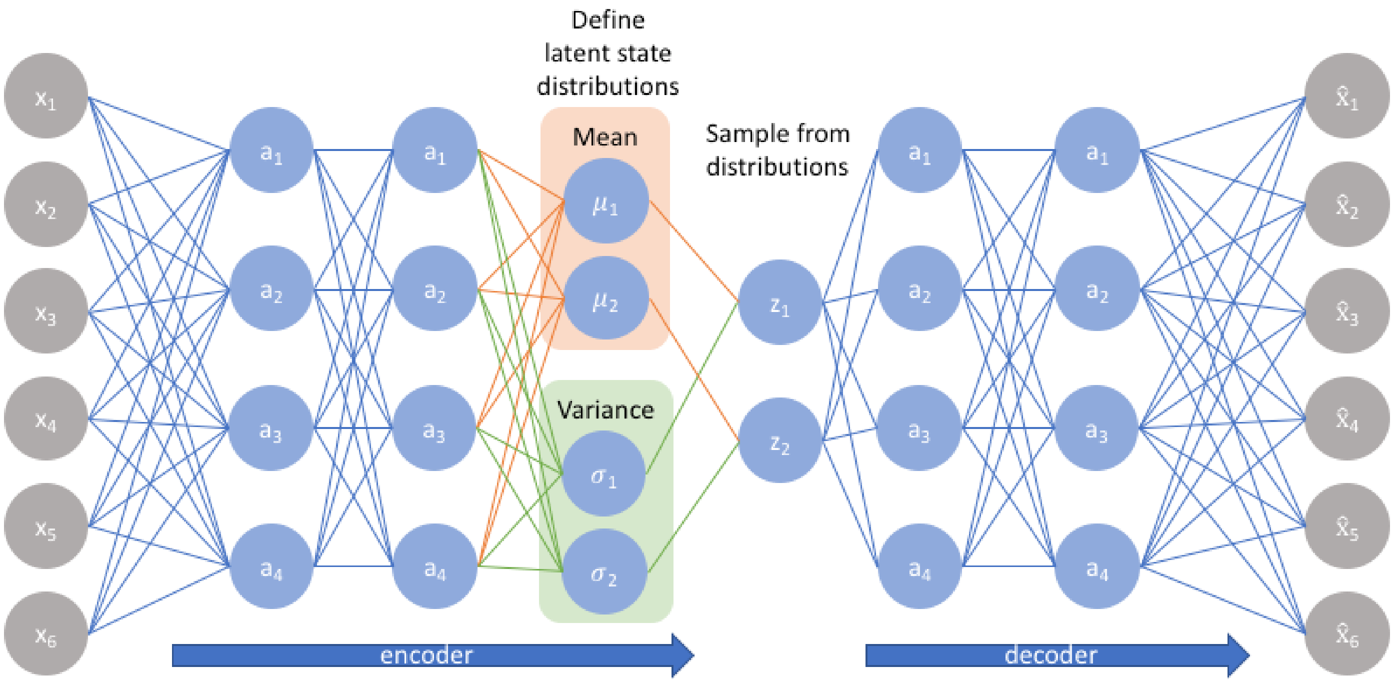



Figure 8: Training of VAE with Gaussian Variational Family

# Reparametrization

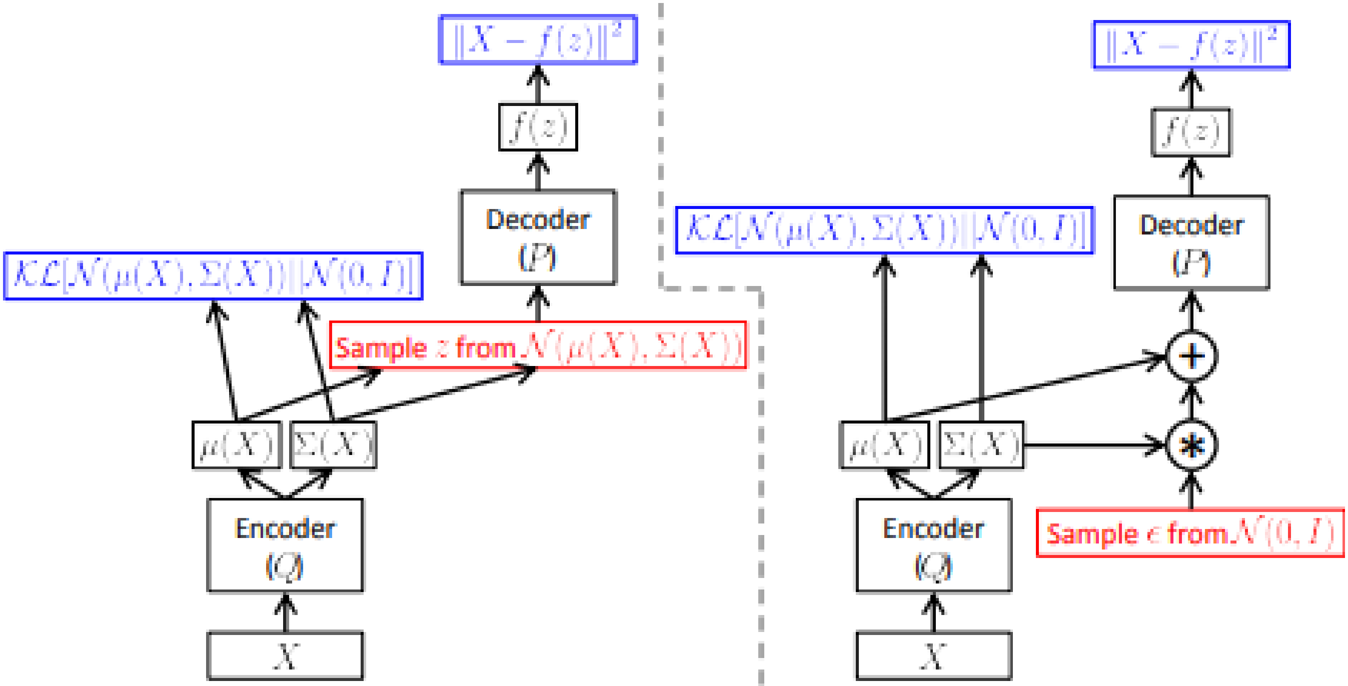



Figure 9: Reparametrization(Right)

# VAE - Visualization

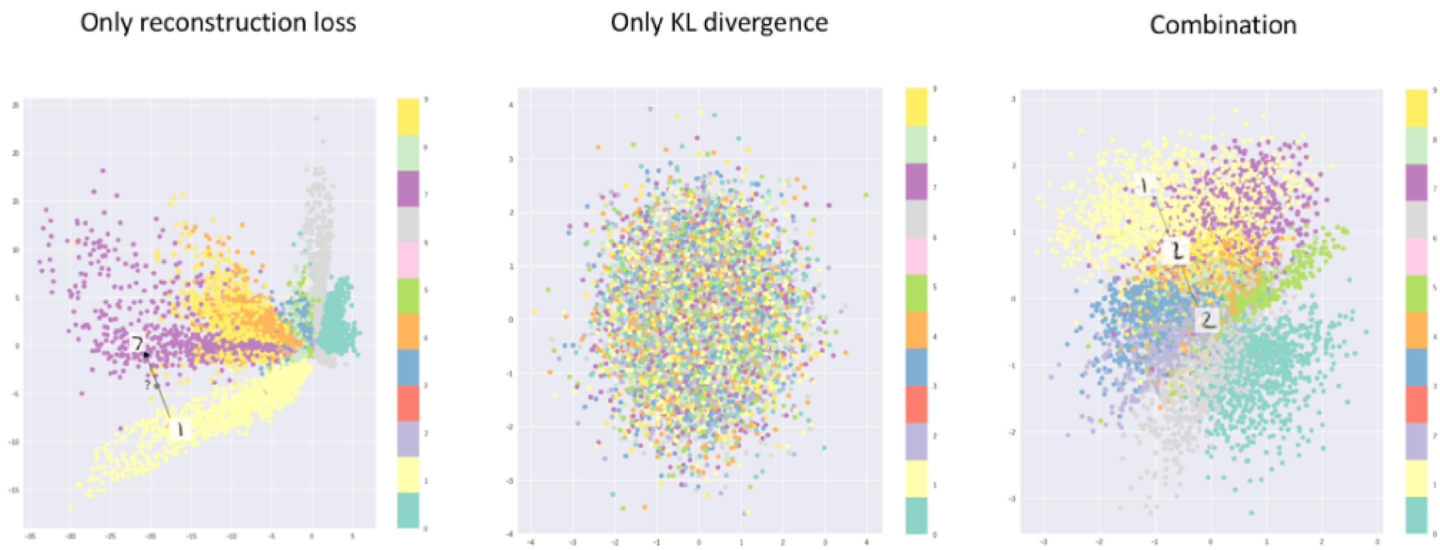



Figure 10: Contributions of reconstruction and KL

# VAE - Visualization

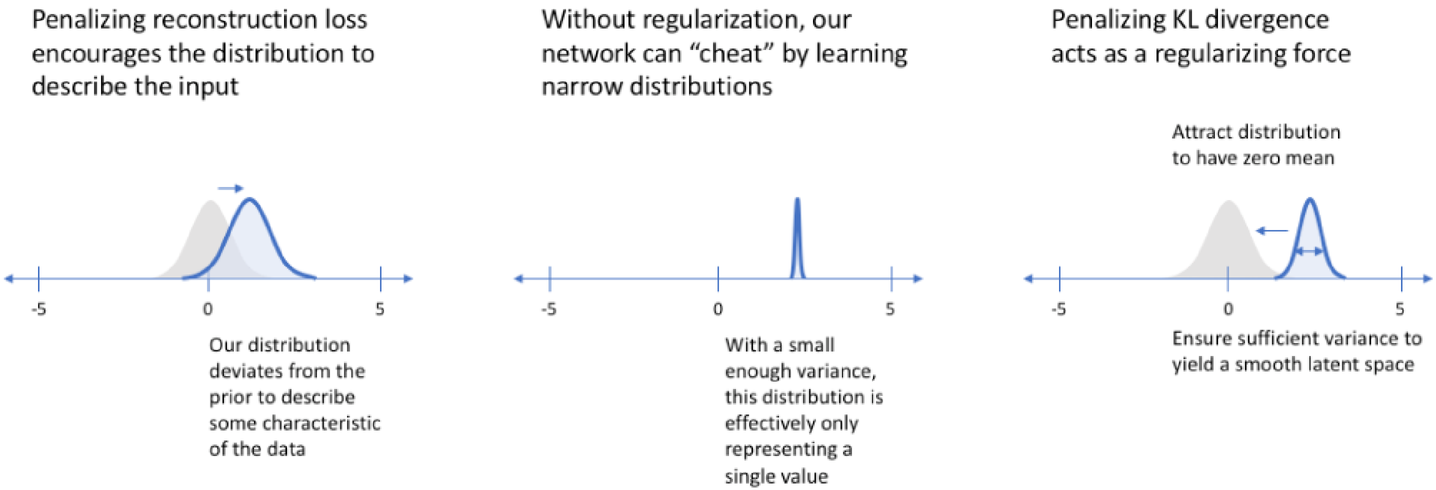



Figure 11: Contributions of reconstruction and KL

# VAE-Results

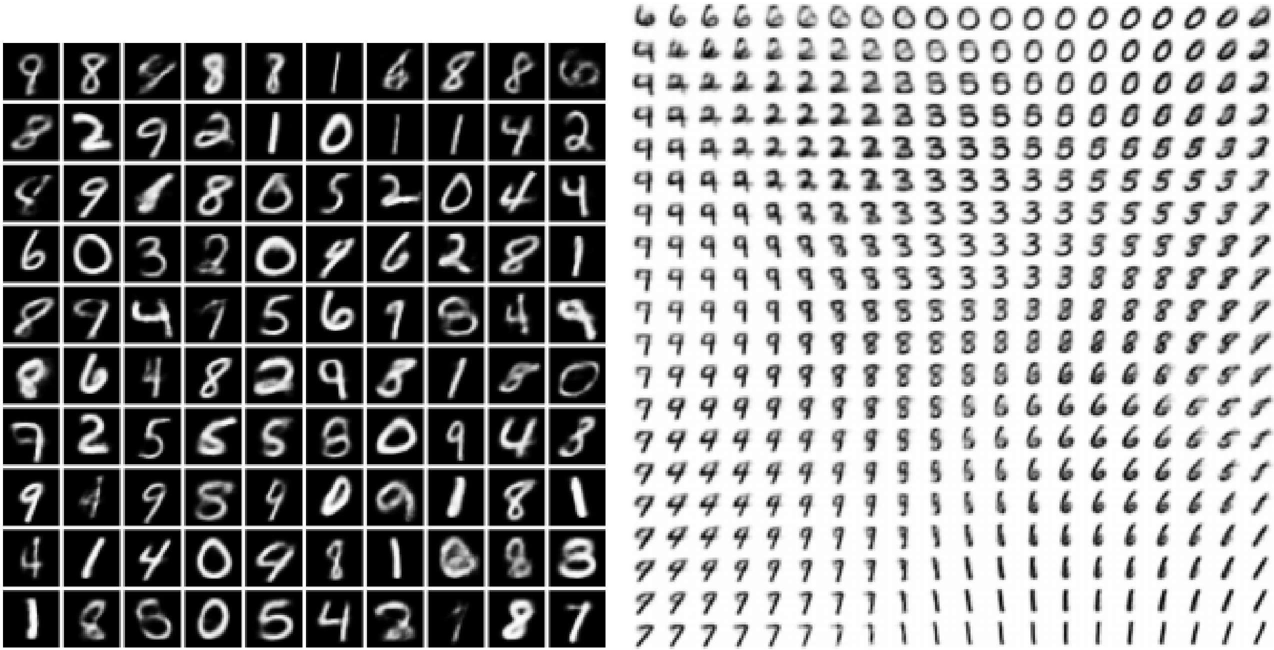
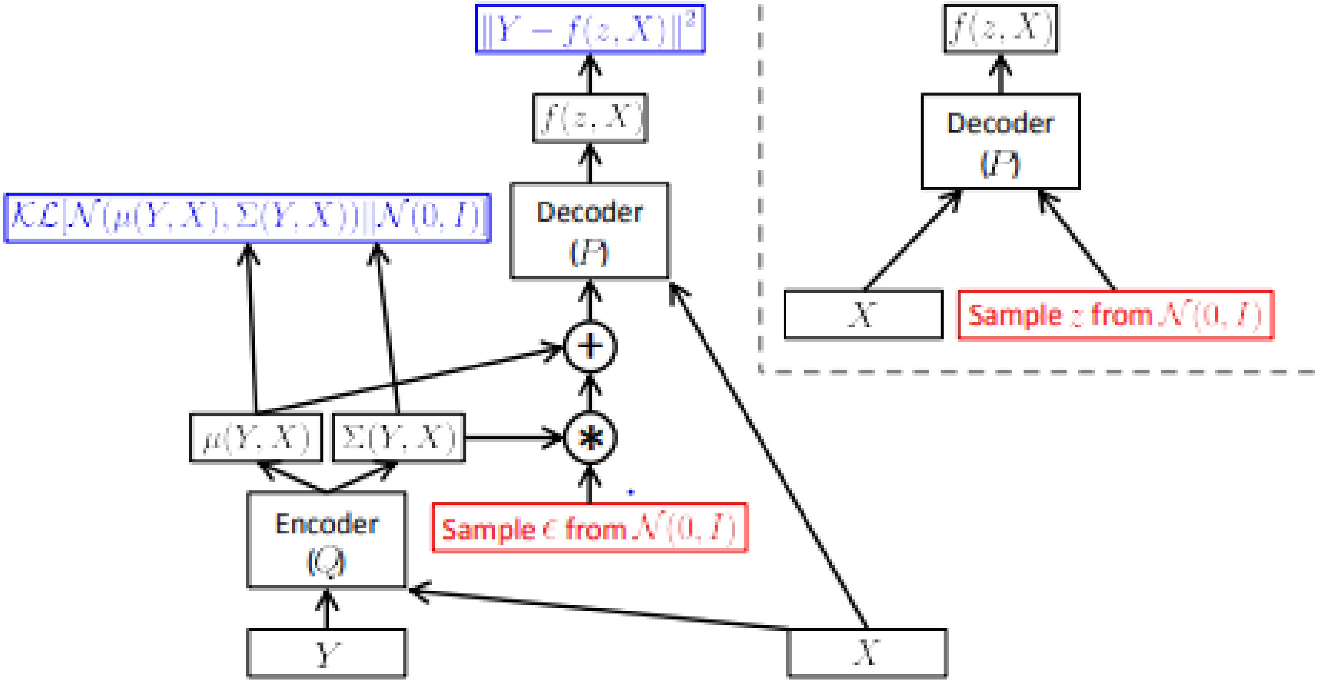


Figure 12: Left: MNIST generative results from VAE. Right : Latent code interpolation - Results generated from sampling latent codes and interpolating between those two codes.

# Music-VAE (Google, 2018)

https://youtu.be/G5JT16flZwM

# Conditional VAE



# Conditional VAE

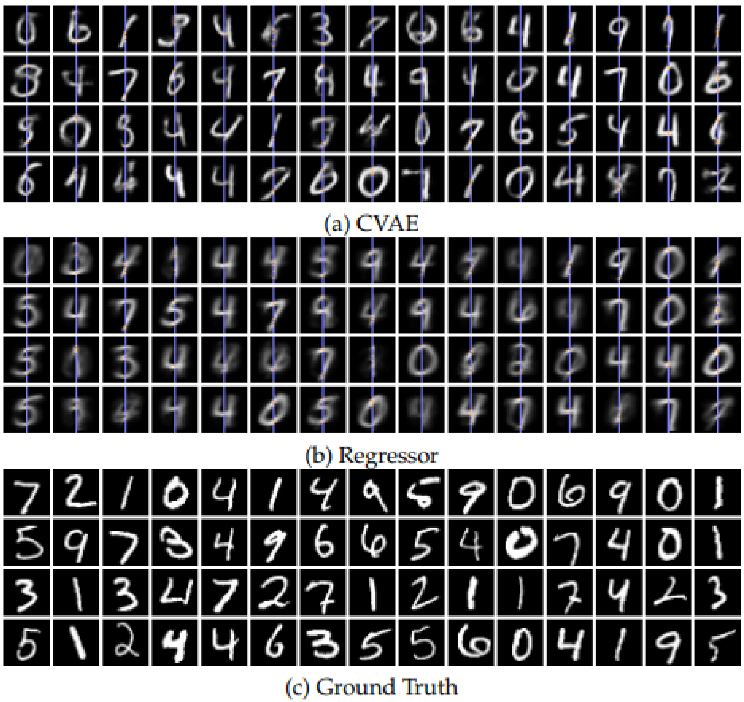



Figure 14: A Conditional VAE. Image Completion - The inputs(incomplete image) to CVAE are the pixels in the middle column shown in the images in blue.

# Bayesian Neural Networks

**QUESTION :** How do you learn uncertainty of what your deep network learns ?

**IDEA :** Have a prior over weights and do MAP inference.

- Confidence of your predictions.
- Richer and regularized representation of weights since you control the prior
- Model Averaging (since the lilely prediction of y is the expected value of distribution over functions)

# How does it look like ?

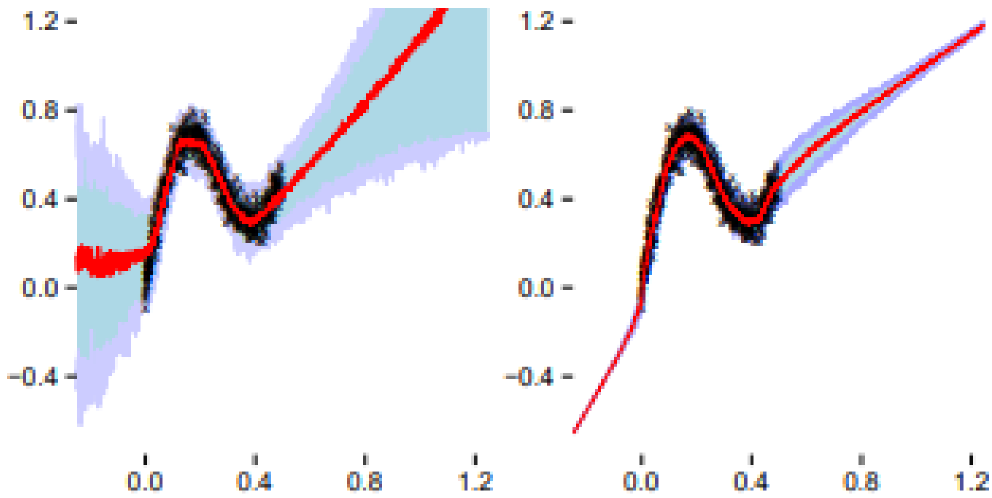



Figure 15: Left : Fit via BBB. Right:Fit via Neural Nets. Red indicates the median prediction. Blue boundaries indicate quartile ranges. Look how BBB is less confident in out of distribution regions and more confident around evidence.Credits

# How do you do it ?

$$p(\mathbf{w}|\mathbf{x},\mathbf{y}) \propto \mathbb{P}\Big(\mathbf{y}_{1:n}|\mathbf{x}_{1:n},;\mathbf{w}\Big) * p(\mathbf{w})$$
$$\mathbf{w}^* = \arg\max_{\mathbf{w}} \quad \underbrace{P(\mathbf{w}|\mathbf{x},\mathbf{y})}_{\text{As usual, intractable}} \tag{19}$$

$$\theta^* = \arg\min_{\theta} D_{KL}\big(q(\mathbf{w};\theta)||p(\mathbf{w}|\mathcal{D})\big)$$
$$= \arg\min_{\theta} \underbrace{D_{KL}\big[q(\mathbf{w};\theta)||p(\mathbf{w})\big] - \mathbb{E}_{q(\mathbf{w};\theta)} \log p(\mathcal{D}|\mathbf{w})}_{\mathcal{L}(\mathcal{D},\theta)} \tag{20}$$

(derived similar to VI)

Perform SGD via re-parametrization to train the network. Bayes by backpropagation - $https://arxiv.org/pdf/1505.05424.pdf$.(pseudo-code)

# Credits

1. https://www.jeremyjordan.me/variational-autoencoders/ (Images and Text)
2. https://arxiv.org/abs/1606.05908 (Images and Text)
3. Other references in the notes (Largely text)