Variational Autoencoder

Auto-encoding Variational Bayes by Kingma and Welling [2013]

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Outline

Probabilistic Modeling

- Learn a model that describes the data
- Using Bayes Rule, we can learn and infer about the model and its parameters
- Bayes' Rule : $P(\theta|D) = \frac{P(D|\theta)P(\theta)}{P(D)}$
- Question : How to compute the posterior? (especially when it is not tractable) and how can we compute the predictive distribution based on the updated parameters?
- Answer : Variational Bayes, Markov Chain Mote Carlo (MCMC)..
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What are the problems?

- **Intractability** : We still need the exact solution for simplified cases in Variational Bayes.
- **Inscalability** : MCMC is asymtotically unbiased but it is computationally expensive, so it is not easy to scale up.
- Any ideas?
- Neural Network can be a good candidate.
  - Rather than programming in explicit detail, just write a program how to learn, and show computers many examples. Then, the computer learns it by itself.
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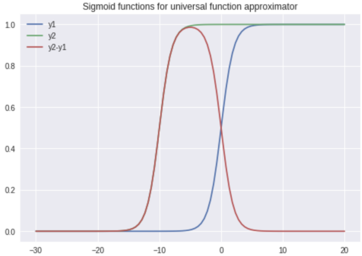
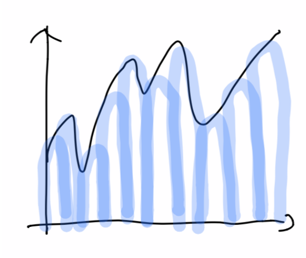
Why Neural Networks?

- Neural Networks with one hidden layer are universal function approximators.





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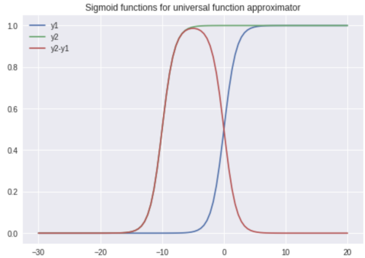

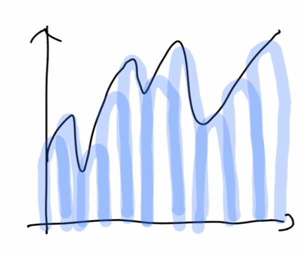

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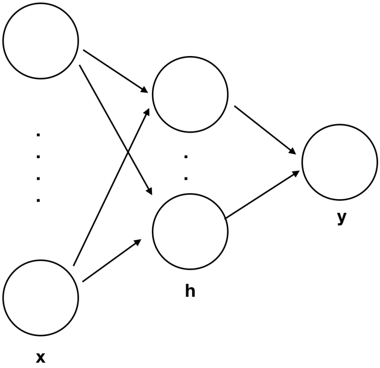
Neural Network - example



- $h_{ik} = a(b^h_k + \sum_j W^h_{jk} x_{ij})$ where $a(x) = \max(x, 0)$, $a(x)$ here is Rectified Linear Unit but it can be other functions.
- $\hat{y} = \sigma(b^o + \sum_k W^o_k h_{ik})$ where $\sigma(x)$ is usually a sigmoid function for binary classification.
- The parameters$(b^h_k, b^o, W^h_{jk}, W^o_k)$ are optimized by Gradient Descent.

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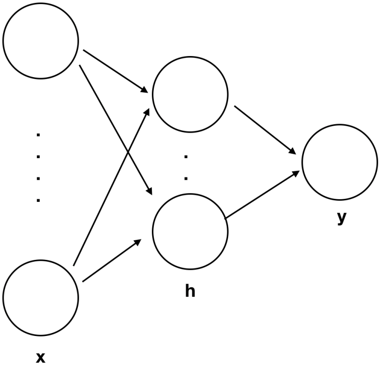

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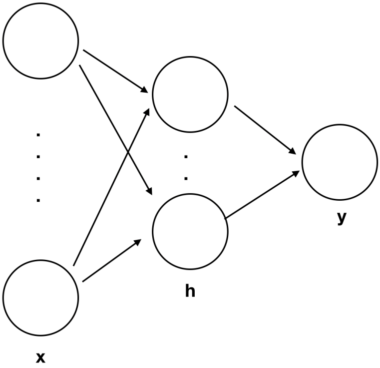

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What is Neural Network?

- **Backpropagation** is used to optimize the parameters. Neural network computes the loss and the gradients, then back-propagate error signals to get derivatives for learning
  - If small changes in parameters increase the probability of the outcome, then keep the change, otherwise drop them.
  - It enables parallel computing, so it is much more efficient. (But, different results for every iterations)
  - After defining the loss function and setting the hyper-parameter for updating the parameter, then the neural network optimizes its parameters automatically.
    $W^h_{jk} = W^h_{jk} - \alpha \frac{\partial J}{\partial W^h_{jk}}, \ \frac{\partial J}{\partial W^h_{jk}} = \frac{\partial J}{\partial \hat{h}} \frac{\partial \hat{h}}{\partial W^h_{jk}}$
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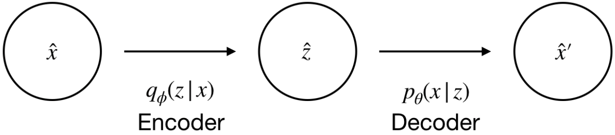
From a Recognition model

- Use the idea from the recognition model : Approximate the posterior as $q_\phi(z|x)$ rather than $p_\theta(z|x)$ directly. Then, use the neural network to approximate it.



- Objective: 1) Maximize the log $p_\theta(\hat{x}')$ and 2) minimize the KL divergence between $q_\phi(z|x)$ and $p_\theta(z|x)$
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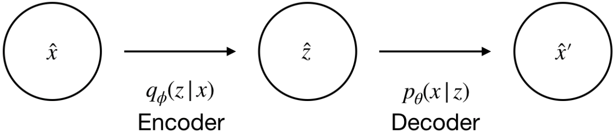

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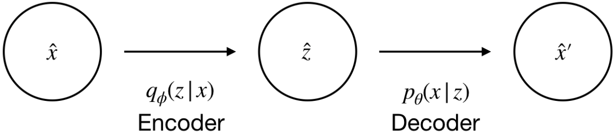

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- Start from $\log p_\theta(x)$

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- Now, go back to Variance Lower Bound again.

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Optimizing the Variance Lower Bound

- By KL-Divergence's non-negativity, $L(\theta, \phi) \leq \log p_\theta(x)$
- Therefore, by optimizing the parameters θ and ϕ, we can increase the evidence lower bound every iteration, similar to Expectation Maximization algorithm.
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Reparameterization Trick

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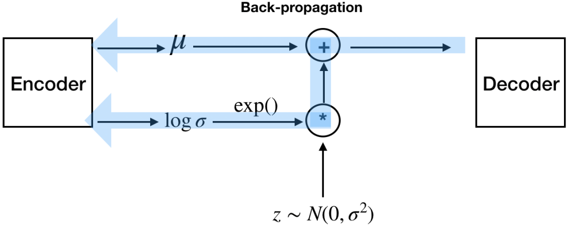

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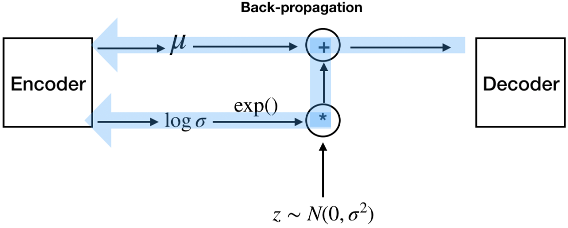

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VAE with MNIST dataset

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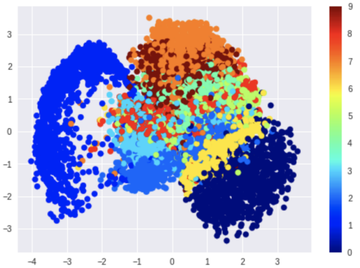

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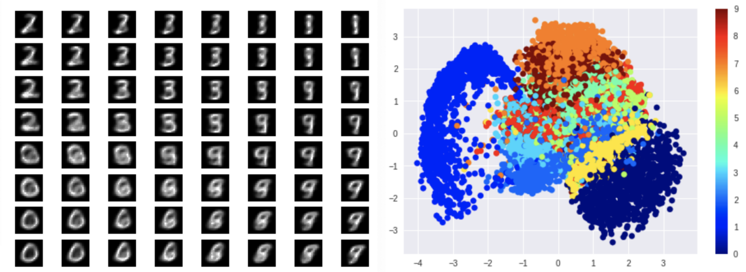

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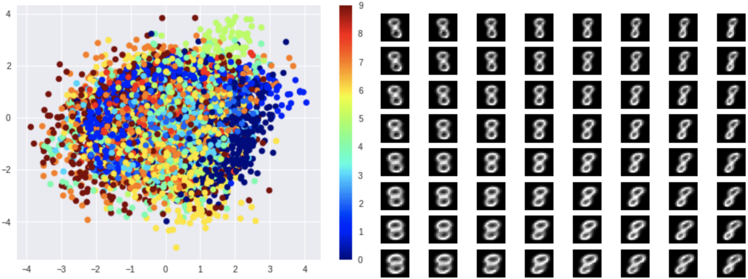

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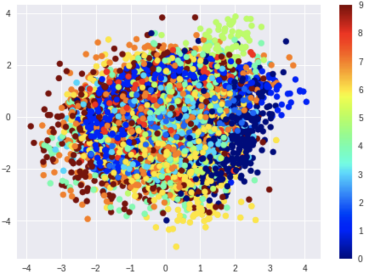

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    - The output on high-frequency parts(e.g. edges) tends to be blurrier than other generative models such as GAN

Disentanglement

- Neural Network suffers from a lack of interpretability. Disentanglement can be a way to interpret the results. Higgins et al. [2016] proposed β-VAE

  $$\max_{\theta,\phi} \mathop{\mathbb{E}}_{x\sim p_D} \mathop{\mathbb{E}}_{z\sim q_\phi(z|x)} \log p_\theta(x|z) \ s.t \ D_{KL}(q_\phi(z|x)||p(z)) \leq \beta$$

  $$E_{x\sim p(x)}[D_{KL}(q(z|x)||p(z))] = I_q(x;z) + D_{KL}(q(z)||p(z))$$

- β can be viewed as how much we penalize the $q_\phi(z|x)$, as we increase β, it is more likely to be disentangled but the quality of the output is also likely to suffer too because $I_q(x;z)$ is also effected.
- Kim and Mnih [2018] proposed factor-VAE which uses additional classifier to check whether the latent space is factorized.

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Flow models

- Use normalizing flow to approximate the posterior distribution. By change of variables, we can derive it as below.

$$\log q(z_T|x) = \log q(z_0|x) - \sum_{t=1}^{T} \log \det \left|\frac{dz_t}{dz_{t-1}}\right|$$

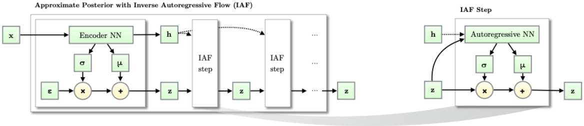

Image from Kingma et al. [2016]

- Using this model, we can approximate the posterior distribution with non-diagonal convariance matrix terms.
- See Germain et al. [2015] Kingma et al. [2016], and Papamakarios et al. [2017] for more developments.

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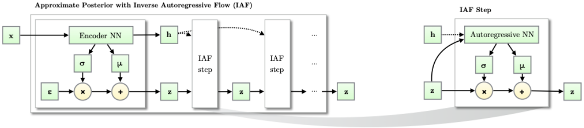

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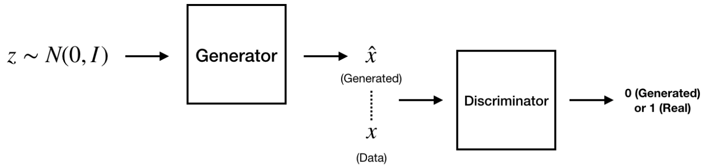
Generative Adversarial Network - GAN

- Now compare with another popular generative model - GAN by Goodfellow et al. [2014]



$$\min_G \max_D L(D, G) = \mathbb{E}_{x \sim p_r(x)} \log D(x) + \mathbb{E}_{z \sim p_z(z)} \log(1 - D(G(z)))$$

- GAN tries to find the Nash Equilibrium between two networks. At the equilibrium, $D(x) = \frac{1}{2}$
- If it is properly trained, the loss function is Jensen-Shannon divergence between two distributions

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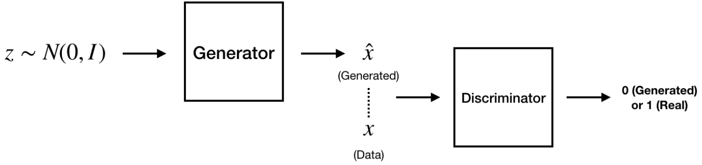

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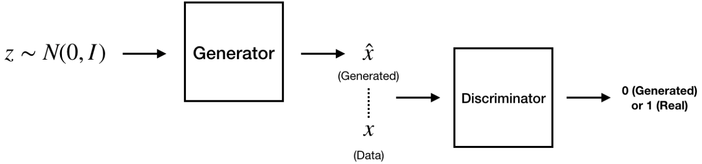

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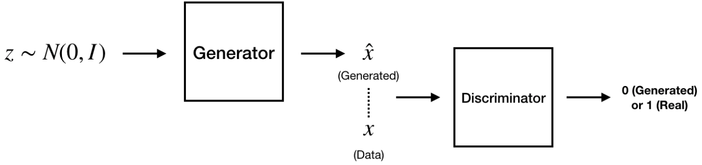

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VAE and GAN

	VAE	GAN
Principles	Optimize Lower Bound	Find the Nash Equilibrium between two Networks (WGAN: find the optimal transport between two distributions)
Strength	See the latent encodings Based on theoretic foundations Training is stable	Generates high-quality & more diverse outputs
Improvements	Output tends to be blurrier on high-freq parts	Training is not stable More like a black-box approach

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