

CS 3750 Advanced Machine Learning

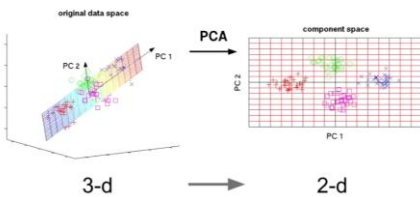
Deep Generative Models

Hung Chau
hkc6@pitt.edu

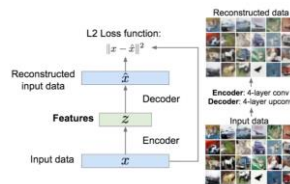
Unsupervised Learning

Data: x
Just data, no labels

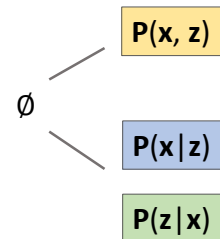
Goal: Learn some underlying hidden structure of the data



Principle Component Analysis
(Dimensionality reduction)



Autoencoders
(Feature learning)



Generative Models

Generative Models

Given training data, generate new samples from same distribution

CIFAR-10 dataset (*Krizhevsky and Hinton, 2009*)



Training data $\sim p_{\text{data}}(\mathbf{x})$

Generated sampled $\sim p_{\text{model}}(\mathbf{x})$

Want to learn $p_{\text{model}}(\mathbf{x})$ similar to $p_{\text{data}}(\mathbf{x})$

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Deep Generative Models

Why Generative Models?

- Realistic samples for artwork, super-resolution, colorization, etc.

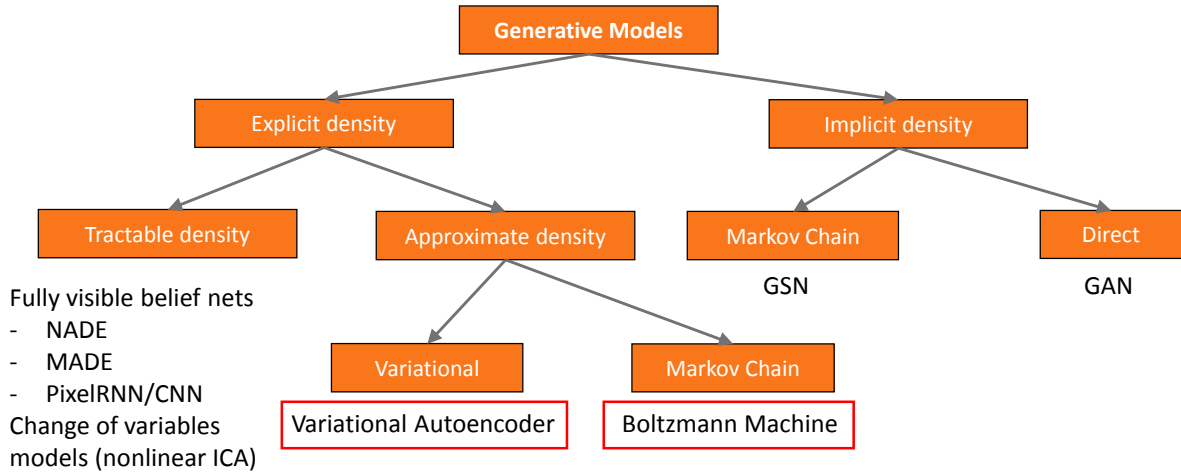


- Generative models of time-series data can be used for simulation and planning (reinforcement learning applications!)
- Training generative models can also enable inference of latent representation that can be useful as general features

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Deep Generative Models

Taxonomy of Generative Models



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Deep Generative Models

Restricted Boltzmann Machines (RBM)

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Restricted Boltzmann Machines

Many interesting theoretical results about undirected models depends on the assumption that $\forall x, \tilde{p}(x) > 0$. A convenient way to enforce this condition is to use an *energy-based model* where

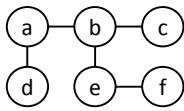
$$\tilde{p}(x) = \exp(-E(x))$$

Remember: normalized probability distribution

$$p(x) = \frac{1}{Z} \tilde{p}(x)$$

- $E(x)$ is known as the *energy function*

Any distribution of this form is an example of a *Boltzmann distribution*. For this reason, many energy-based models are called *Boltzmann machines*.



$E(a, b, c, d, e, f)$ can be written as

$$E_{a,b}(a,b) + E_{b,c}(b,c) + E_{a,d}(a,d) + E_{b,e}(b,e) + E_{e,f}(e,f)$$

$$\phi_{a,b}(a, b) = \exp(-E(a, b))$$

Restricted Boltzmann Machines

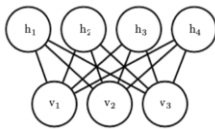
- *Boltzmann machines* were originally introduced as a general “connectionist” approach to learning arbitrary probability distributions over binary vectors
- While Boltzmann machines were defined to encompass both models with and without latent variables, the term Boltzmann machine is today most often used to designate models with latent variables

Joint probability distribution: $p(\mathbf{x}, \mathbf{h}) = \frac{1}{Z} \exp(-E(\mathbf{x}, \mathbf{h}))$

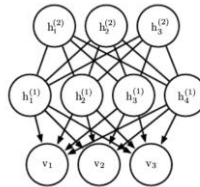
Energy function: $E(\mathbf{x}, \mathbf{h}) = -\mathbf{x}^T \mathbf{R} \mathbf{x} - \mathbf{x}^T \mathbf{W} \mathbf{h} - \mathbf{h}^T \mathbf{S} \mathbf{h} - \mathbf{c}^T \mathbf{x} - \mathbf{b}^T \mathbf{h}$

Restricted Boltzmann Machines

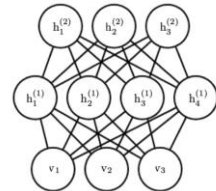
- *Restricted Boltzmann machines (RBMs)* are undirected probabilistic graphical models containing a layer of observable variables and a single layer of latent variables
- RBM is a bipartite graph, with no connections permitted between any variables in the observed layer or between any units in the latent layer



Restricted Boltzmann machine



Deep belief network

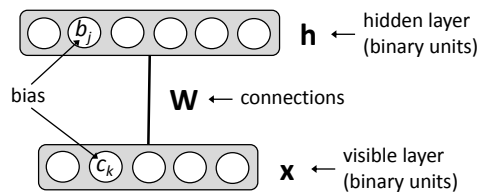


Deep Boltzmann machine

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Deep Generative Models

Restricted Boltzmann Machines



$$\begin{aligned}
 p(\mathbf{x}, \mathbf{h}) &= \exp(-E(\mathbf{x}, \mathbf{h})) / Z \\
 &= \exp(\mathbf{h}^T \mathbf{W} \mathbf{x} + \mathbf{c}^T \mathbf{x} + \mathbf{b}^T \mathbf{h}) / Z \\
 &= \underbrace{\exp(\mathbf{h}^T \mathbf{W} \mathbf{x}) \exp(\mathbf{c}^T \mathbf{x}) \exp(\mathbf{b}^T \mathbf{h})}_{\text{Factors}} / Z
 \end{aligned}$$

$$Z = \sum_{\mathbf{x}, \mathbf{h}} \exp(-E(\mathbf{x}, \mathbf{h}))$$

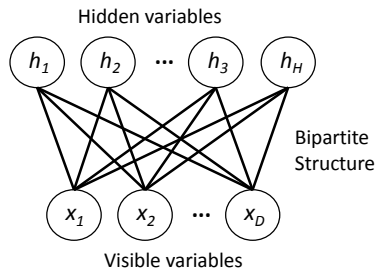
partition function (intractable)

The notation based on an **energy function** is simply an alternative to the representation as the product of factors

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Restricted Boltzmann Machines



$$p(\mathbf{x}, \mathbf{h}) = \frac{1}{Z} \prod_j \prod_k \exp(W_{j,k} h_j x_k)$$

Pair-wise Factors

$$\prod_k \exp(c_k x_k)$$

$$\prod_j \exp(b_j h_j)$$

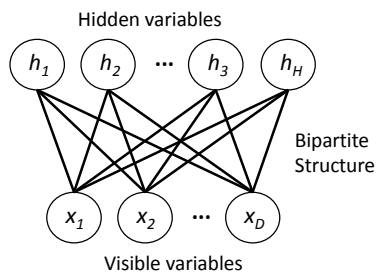
Unary Factors

The scalar visualization is more informative of the structure within the vectors

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Deep Generative Models

RBM: Inference



Restricted: No interaction between hidden variables

Inferring the distribution over the hidden variables is easy

$$p(\mathbf{h}|\mathbf{x}) = \prod_j p(h_j|\mathbf{x})$$

Factorizes: easy to compute

Similarly:

$$p(\mathbf{x}|\mathbf{h}) = \prod_k p(x_k|\mathbf{h})$$

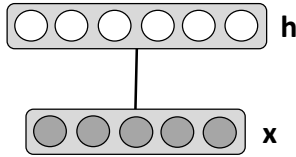
Markov random fields, Boltzmann machines, log-linear models

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Deep Generative Models

RBM: Inference

Conditional Distributions

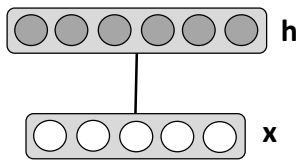


$$p(\mathbf{h}|\mathbf{x}) = \prod_j p(h_j|\mathbf{x})$$

$$p(h_j = 1|\mathbf{x}) = \frac{1}{1 + \exp(-(b_j + \mathbf{W}_j \cdot \mathbf{x}))}$$

$$= \text{sigm}(b_j + \mathbf{W}_j \cdot \mathbf{x})$$

jth row if W



$$p(\mathbf{x}|\mathbf{h}) = \prod_k p(x_k|\mathbf{h})$$

$$p(x_k = 1|\mathbf{h}) = \frac{1}{1 + \exp(-(c_k + \mathbf{h}^T \mathbf{W}_{\cdot k}))}$$

$$= \text{sigm}(c_k + \mathbf{h}^T \mathbf{W}_{\cdot k})$$

kth column if W

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Deep Generative Models

RBM: Free Energy

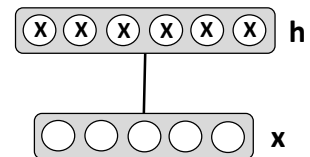
What about computing **marginal** $p(\mathbf{x})$?

$$p(\mathbf{x}) = \sum_{\mathbf{h} \in \{0,1\}^H} p(\mathbf{x}, \mathbf{h}) = \sum_{\mathbf{h} \in \{0,1\}^H} \exp(-E(\mathbf{x}, \mathbf{h}))/Z$$

$$= \exp\left(\mathbf{c}^T \mathbf{x} + \sum_{j=1}^H \log(1 + \exp(b_j + \mathbf{W}_j \cdot \mathbf{x}))\right) / Z$$

$$= \exp(-F(\mathbf{x})) / Z$$

Free energy



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Deep Generative Models

RBM: Free Energy

What about computing **marginal** $p(\mathbf{x})$?

$$\begin{aligned}
 p(\mathbf{x}) &= \sum_{\mathbf{h} \in \{0,1\}^H} \exp(\mathbf{h}^T \mathbf{W} \mathbf{x} + \mathbf{c}^T \mathbf{x} + \mathbf{b}^T \mathbf{h}) / Z \\
 &= \exp(\mathbf{c}^T \mathbf{x}) \sum_{h_1 \in \{0,1\}} \dots \sum_{h_H \in \{0,1\}} \exp\left(\sum_j h_j \mathbf{W}_j \cdot \mathbf{x} + b_j h_j\right) / Z \\
 &= \exp(\mathbf{c}^T \mathbf{x}) \left(\sum_{h_1 \in \{0,1\}} \exp(h_1 \mathbf{W}_1 \cdot \mathbf{x} + b_1 h_1) \right) \dots \left(\sum_{h_H \in \{0,1\}} \exp(h_H \mathbf{W}_H \cdot \mathbf{x} + b_H h_H) \right) / Z \\
 &= \exp(\mathbf{c}^T \mathbf{x}) (1 + \exp(b_1 + \mathbf{W}_1 \cdot \mathbf{x})) \dots (1 + \exp(b_H + \mathbf{W}_H \cdot \mathbf{x})) / Z \\
 &= \exp(\mathbf{c}^T \mathbf{x}) \exp(\log(1 + \exp(b_1 + \mathbf{W}_1 \cdot \mathbf{x}))) \dots \exp(\log(1 + \exp(b_H + \mathbf{W}_H \cdot \mathbf{x}))) / Z \\
 &= \exp\left(\mathbf{c}^T \mathbf{x} + \sum_{j=1}^H \log(1 + \exp(b_j + \mathbf{W}_j \cdot \mathbf{x}))\right) / Z
 \end{aligned}$$

Also known as **Product of Experts** model

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Deep Generative Models

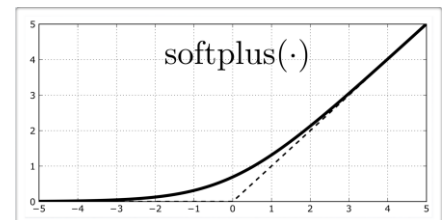
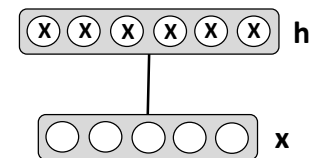
RBM: Free Energy

$$\begin{aligned}
 p(\mathbf{x}) &= \exp\left(\mathbf{c}^T \mathbf{x} + \sum_{j=1}^H \log(1 + \exp(b_j + \mathbf{W}_j \cdot \mathbf{x}))\right) / Z \\
 &= \exp\left(\mathbf{c}^T \mathbf{x} + \sum_{j=1}^H \text{softplus}(b_j + \mathbf{W}_j \cdot \mathbf{x})\right) / Z
 \end{aligned}$$

bias of the probability of each x_i

bias of each feature

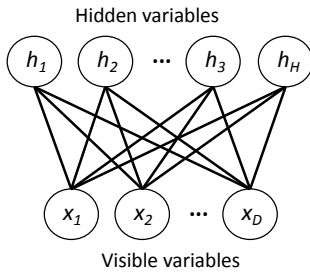
feature expected in \mathbf{x}



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Deep Generative Models

RBM: Model Learning



Given a set of *i.i.d.* training examples we want to minimize the average negative log-likelihood:

$$\frac{1}{T} \sum_t l(f(x^{(t)})) = \frac{1}{T} \sum_t -\log p(x^{(t)})$$

Remember:

$$\begin{aligned} \log p(x^{(t)}) &= \log \left(\sum_h p(x^{(t)}, h) \right) \\ &= \log \left(\sum_h \frac{\exp(-E(x^{(t)}, h))}{Z} \right) \\ &= \log \left(\sum_h \exp(-E(x^{(t)}, h)) \right) - \log Z \end{aligned}$$

Derivative of the negative log-likelihood objective (stochastic gradient descent):

$$\frac{\partial -\log p(x^{(t)})}{\partial \theta} = E_h \left[\frac{\partial E(x^{(t)}, \mathbf{h})}{\partial \theta} | x^{(t)} \right] - E_{x, h} \left[\frac{\partial E(x, \mathbf{h})}{\partial \theta} \right]$$

Positive phase
Negative phase

Hard to compute

Restricted Boltzmann machines Tutorial - Chris Maddison

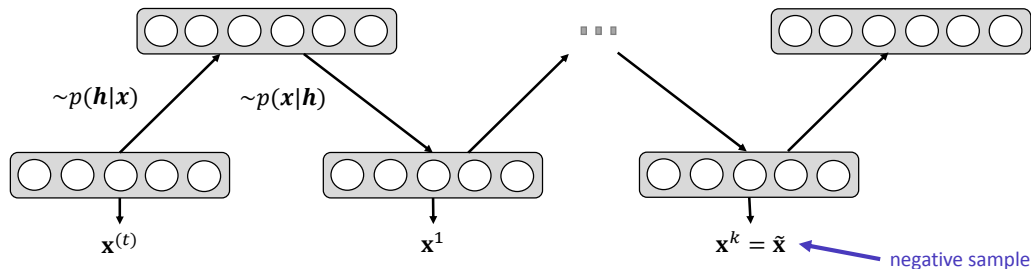
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Deep Generative Models

RBM: Contrastive Divergence

Key idea behind Contrastive Divergence:

- Replace the expectation by a **point estimate** at $\tilde{\mathbf{x}}$
- Obtain the point $\tilde{\mathbf{x}}$ by Gibbs sampling
- Start sampling chain at $\mathbf{x}^{(t)}$



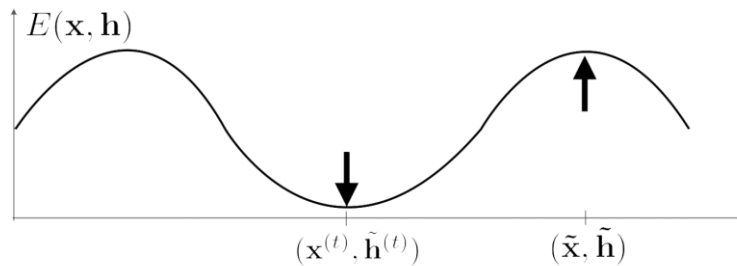
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RBM: Contrastive Divergence

$$\text{Intuition: } \frac{\partial -\log p(\mathbf{x}^{(t)})}{\partial \theta} = E_{\mathbf{h}} \left[\frac{\partial E(\mathbf{x}^{(t)}, \mathbf{h})}{\partial \theta} \mid \mathbf{x}^{(t)} \right] - E_{\mathbf{x}, \mathbf{h}} \left[\frac{\partial E(\mathbf{x}, \mathbf{h})}{\partial \theta} \right]$$

$$E_{\mathbf{h}} \left[\frac{\partial E(\mathbf{x}^{(t)}, \mathbf{h})}{\partial \theta} \mid \mathbf{x}^{(t)} \right] \approx \frac{\partial E(\mathbf{x}^{(t)}, \tilde{\mathbf{h}}^{(t)})}{\partial \theta} \quad E_{\mathbf{x}, \mathbf{h}} \left[\frac{\partial E(\mathbf{x}, \mathbf{h})}{\partial \theta} \right] \approx \frac{\partial E(\tilde{\mathbf{x}}, \tilde{\mathbf{h}})}{\partial \theta}$$



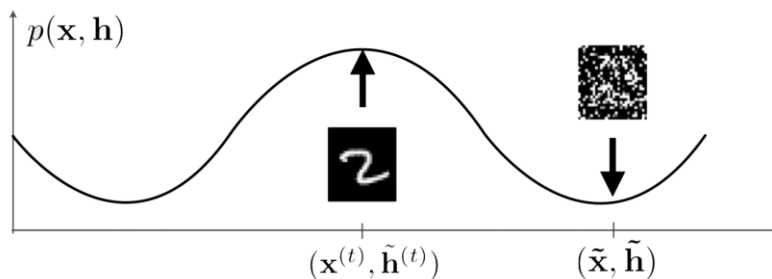
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RBM: Contrastive Divergence

$$\text{Intuition: } \frac{\partial -\log p(\mathbf{x}^{(t)})}{\partial \theta} = E_{\mathbf{h}} \left[\frac{\partial E(\mathbf{x}^{(t)}, \mathbf{h})}{\partial \theta} \mid \mathbf{x}^{(t)} \right] - E_{\mathbf{x}, \mathbf{h}} \left[\frac{\partial E(\mathbf{x}, \mathbf{h})}{\partial \theta} \right]$$

$$E_{\mathbf{h}} \left[\frac{\partial E(\mathbf{x}^{(t)}, \mathbf{h})}{\partial \theta} \mid \mathbf{x}^{(t)} \right] \approx \frac{\partial E(\mathbf{x}^{(t)}, \tilde{\mathbf{h}}^{(t)})}{\partial \theta} \quad E_{\mathbf{x}, \mathbf{h}} \left[\frac{\partial E(\mathbf{x}, \mathbf{h})}{\partial \theta} \right] \approx \frac{\partial E(\tilde{\mathbf{x}}, \tilde{\mathbf{h}})}{\partial \theta}$$



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Deep Generative Models

RBM: Deriving Learning Rule

Let us look at derivative of $\frac{\partial E(\mathbf{x}, \mathbf{h})}{\partial \theta}$ for $\theta = W_{jk}$

$$\begin{aligned}\frac{\partial E(\mathbf{x}, \mathbf{h})}{\partial \theta} &= \frac{\partial}{\partial W_{jk}} \left(- \sum_{jk} W_{j,k} h_j x_k - \sum_k c_k x_k - \sum_j b_j h_j \right) \\ &= - \frac{\partial}{\partial W_{jk}} \sum_{jk} W_{j,k} h_j x_k \\ &= -h_j x_k\end{aligned}$$

Remember:

$$E(\mathbf{x}, \mathbf{h}) = -\mathbf{h}^T \mathbf{W} \mathbf{x} - \mathbf{c}^T \mathbf{x} - \mathbf{b}^T \mathbf{h}$$

Hence:

$$\nabla_{\mathbf{W}} E(\mathbf{x}, \mathbf{h}) = -\mathbf{h} \mathbf{x}^T$$

RBM: Deriving Learning Rule

Let us now derive $\mathbb{E}_{\mathbf{h}} \left[\frac{\partial E(\mathbf{x}, \mathbf{h})}{\partial \theta} \mid \mathbf{x} \right]$

$$\begin{aligned}\mathbb{E}_{\mathbf{h}} \left[\frac{\partial E(\mathbf{x}, \mathbf{h})}{\partial W_{j,k}} \mid \mathbf{x} \right] &= \mathbb{E}_{\mathbf{h}} [-h_j x_k \mid \mathbf{x}] = \sum_{h_j \in \{0,1\}} -h_j x_k p(h_j \mid \mathbf{x}) \\ &= -x_k p(h_j = 1 \mid \mathbf{x})\end{aligned}$$

Hence:

$$E_{\mathbf{h}} [\nabla_{\mathbf{W}} E(\mathbf{x}, \mathbf{h}) \mid \mathbf{x}] = -\mathbf{h}(\mathbf{x}) \mathbf{x}^T$$

$$\begin{aligned}h(\mathbf{x}) &= \begin{pmatrix} p(h_1 = 1 \mid \mathbf{x}) \\ \vdots \\ p(h_H = 1 \mid \mathbf{x}) \end{pmatrix} \\ &= \text{sigm}(\mathbf{b} + \mathbf{W} \mathbf{x})\end{aligned}$$

RBM: Deriving Learning Rule

$$x^{(t)} \quad \tilde{x} \quad \theta = W$$

$$\begin{aligned} W &\Leftarrow W - \alpha(\nabla_W \log p(x^{(t)})) \\ &\Leftarrow W - \alpha(E_h[\nabla_W E(x^{(t)}, h)|x^{(t)}] - E_{x,h}[\nabla_W E(x, h)]) \\ &\Leftarrow W - \alpha(E_h[\nabla_W E(x^{(t)}, h)|x^{(t)}] - E_h[\nabla_W E(\tilde{x}, h)|\tilde{x}]) \\ &\Leftarrow W + \alpha \left(h(x^{(t)})x^{(t)T} - h(\tilde{x})\tilde{x}^T \right) \end{aligned}$$

Learning rate

RBM: CD-k Algorithm

For each training example $x^{(t)}$

- Generate a negative sample \tilde{x} using k steps of Gibbs sampling, starting at the data point $x^{(t)}$
- Update model parameters:

$$W \Leftarrow W + \alpha \left(h(x^{(t)})x^{(t)T} - h(\tilde{x})\tilde{x}^T \right)$$

$$b \Leftarrow b + \alpha \left(h(x^{(t)}) - h(\tilde{x}) \right)$$

$$c \Leftarrow c + \alpha \left(x^{(t)} - \tilde{x} \right)$$

- Go back to the first step until **stopping criteria**

RBM: CD-k Algorithm

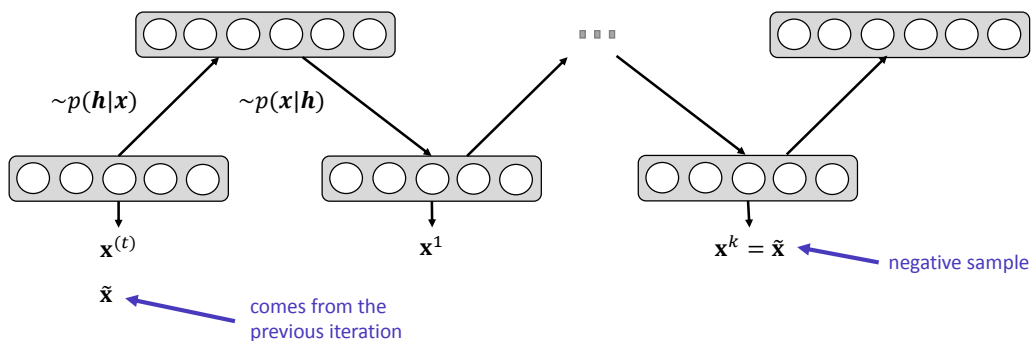
- CD-k: contrastive divergence with k iterations of Gibbs sampling
- In general, the bigger k is, the less biased the estimate of the gradient will be
- In practice, k = 1 works pretty well for learning good features and for pre-training

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RBM: Persistent CD: Stochastic ML Estimator

- Idea: instead of initializing the chain of $x^{(t)}$, initialize the chain to the negative sample of the last iteration



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Deep Generative Models

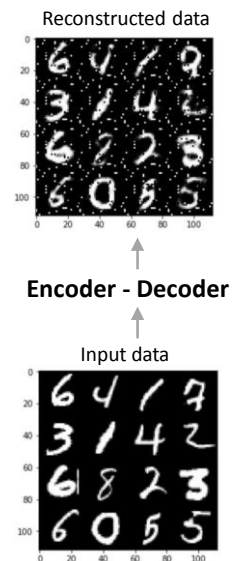
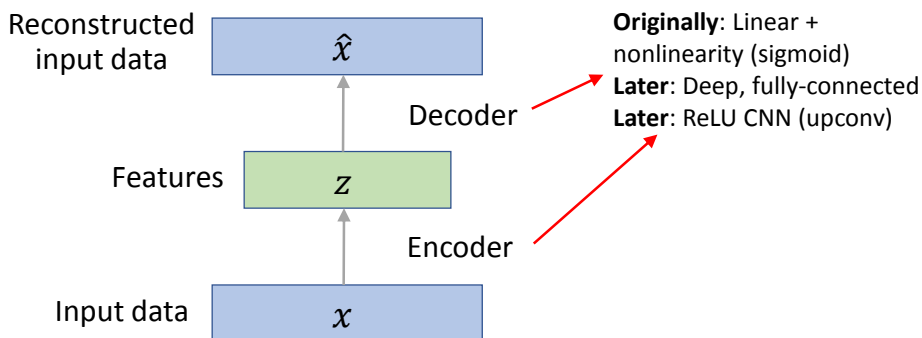
Variational Autoencoders (VAE)

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Deep Generative Models

Autoencoders (Recap)

Unsupervised approach for learning a lower-dimensional feature representation from unlabeled training data

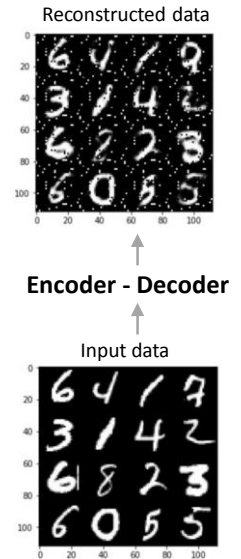
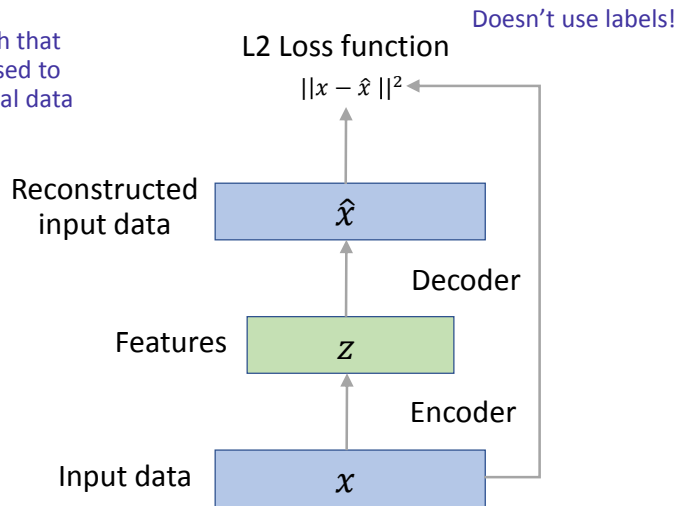


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Autoencoders (Recap)

Train a model such that features can be used to reconstruct original data

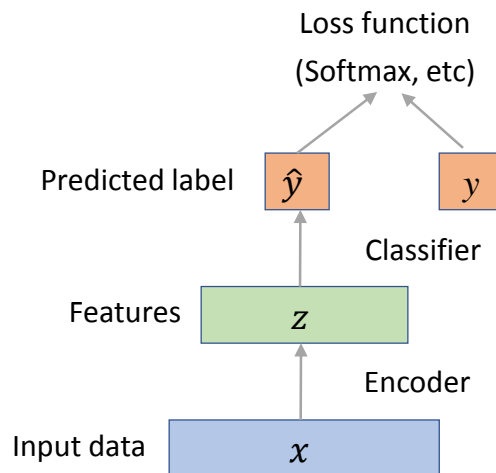


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Autoencoders (Recap)

Encoder can be used to initialize a **supervised** model



bird plane
panther truck dog



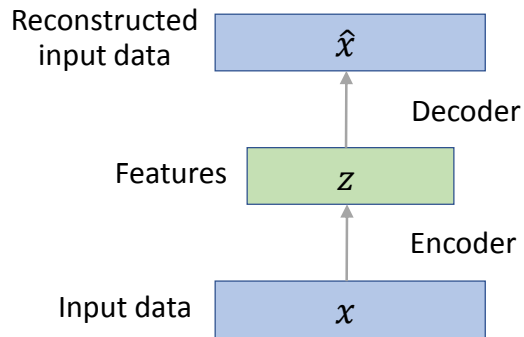
Fine-tune encoder jointly with classifier

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Autoencoders (Recap)

Autoencoders can reconstruct data, and can learn features to initialize a supervised model



Features capture factors of variation in training data. Can we generate new data from an autoencoder?

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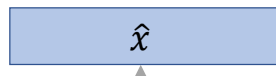
Deep Generative Models

Variational Autoencoders

Probabilistic spin on autoencoders - will let us sample from the model to generate data!

Assume training data $\{x^{(i)}\}_{i=1}^N$ is generated from underlying unobserved (latent) representation \mathbf{Z}

Sample from true conditional
 $p_{\theta^*}(x|z^{(i)})$



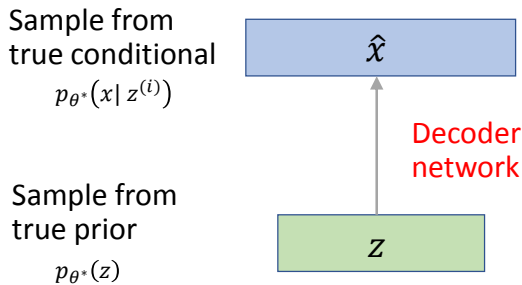
Intuition: x is an image, z is latent factors used to generate x : attributes, orientation, etc.

Sample from true prior
 $p_{\theta^*}(z)$

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Deep Generative Models

Variational Autoencoders



We want to estimate the true parameters θ^* of this generative model

How should we represent this model?

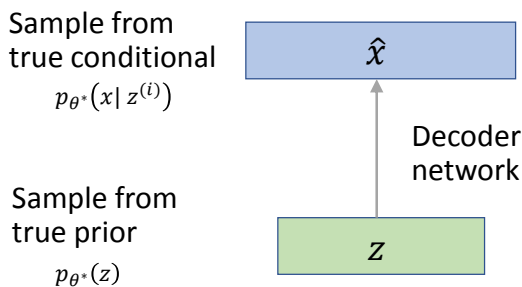
Choose prior $p(z)$ to be simple, e.g. Gaussian

Conditional $p(x|z)$ is complex (generates image) => represent with neural network

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Deep Generative Models

Variational Autoencoders



We want to estimate the true parameters θ^* of this generative model

How train this model?

Learn model parameters to maximize likelihood of training data

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

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Deep Generative Models

Variational Autoencoders

Data likelihood: $p_{\theta}(x) = \int p_{\theta}(z)p_{\theta}(x|z)dz$

Intractable to compute $p(x|z)$ for every z !

Posterior density also intractable: $p_{\theta}(z|x) = \frac{p_{\theta}(x|z)p_{\theta}(z)}{p_{\theta}(x)}$

Solution: in addition to decoder network modeling $p_{\theta}(x|z)$, define additional encoder network $q_{\phi}(z|x)$ that approximates $p_{\theta}(z|x)$

Will see that this allows us to derive a lower bound on the data likelihood that is tractable, which we can optimize

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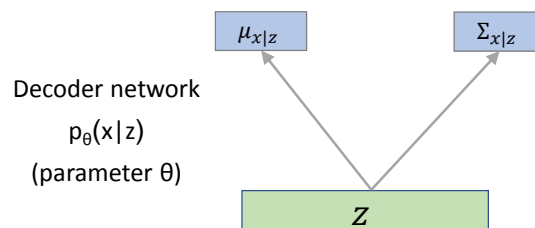
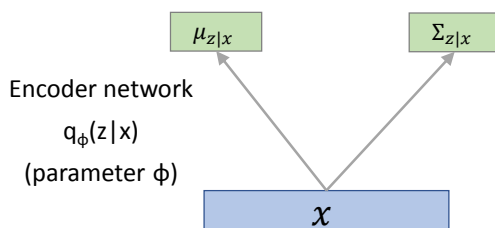
Deep Generative Models

Variational Autoencoders

Since we're modeling probabilistic generation of data, encoder and decoder networks are probabilistic

Mean and (diagonal) covariance of $z|x$

Mean and (diagonal) covariance of $x|z$

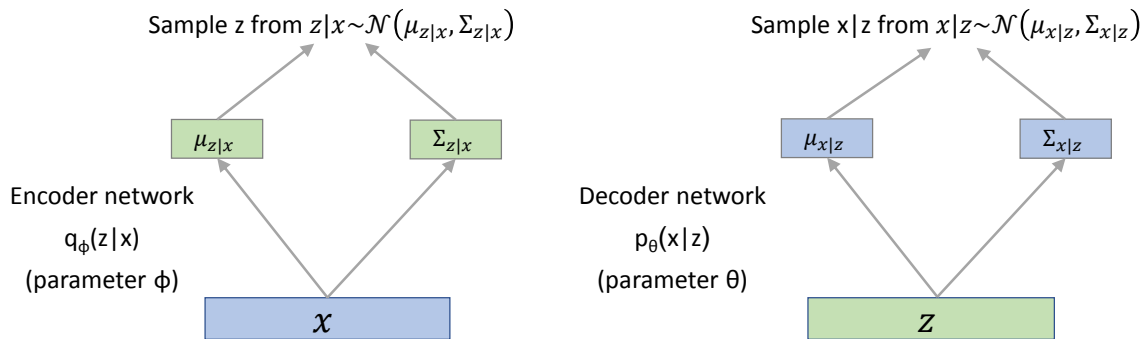


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Deep Generative Models

Variational Autoencoders

Since we're modeling probabilistic generation of data, encoder and decoder networks are probabilistic



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Deep Generative Models

Variational Autoencoders

Now equipped with our encoder and decoder networks, let's work out the (log) data likelihood:

$$\begin{aligned}
 \log p_\theta(x^{(i)}) &= \mathbb{E}_{z \sim q_\phi(z|x^{(i)})} [\log p_\theta(x^{(i)})] && (p_\theta(x^{(i)}) \text{ does not depend on } z) \\
 &= \mathbb{E}_z \left[\log \frac{p_\theta(x^{(i)}|z)p_\theta(z)}{p_\theta(z|x^{(i)})} \right] && (\text{Bayes' Rule}) \\
 &= \mathbb{E}_z \left[\log \frac{p_\theta(x^{(i)}|z)p_\theta(z)}{p_\theta(z|x^{(i)})} \frac{q_\phi(z|x^{(i)})}{q_\phi(z|x^{(i)})} \right] && (\text{Multiply by constant}) \\
 &= \mathbb{E}_z [\log p_\theta(x^{(i)}|z)] - \mathbb{E}_z \left[\log \frac{q_\phi(z|x^{(i)})}{p_\theta(z)} \right] + \mathbb{E}_z \left[\log \frac{q_\phi(z|x^{(i)})}{p_\theta(z|x^{(i)})} \right] && (\text{Logarithms}) \\
 &= \mathbb{E}_z [\log p_\theta(x^{(i)}|z)] - D_{KL}(q_\phi(z|x^{(i)}) || p_\theta(z)) + D_{KL}(q_\phi(z|x^{(i)}) || p_\theta(z|x^{(i)}))
 \end{aligned}$$

Decoder network gives $p_\theta(x|z)$, can compute estimate of this term through sampling

This KL term (between Gaussians for encoder and z prior) has nice closed-form solution!

$p_\theta(z|x)$ intractable (saw earlier), can't compute this KL term. But we know KL divergence always ≥ 0 .

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Deep Generative Models

Variational Autoencoders

Now equipped with our encoder and decoder networks, let's work out the (log) data likelihood:

$$\begin{aligned}
 \log p_{\theta}(x^{(i)}) &= \mathbb{E}_{z \sim q_{\phi}(z|x^{(i)})} [\log p_{\theta}(x^{(i)})] && (p_{\theta}(x^{(i)}) \text{ does not depend on } z) \\
 &= \mathbb{E}_z \left[\log \frac{p_{\theta}(x^{(i)}|z)p_{\theta}(z)}{p_{\theta}(z|x^{(i)})} \right] && (\text{Bayes' Rule}) \\
 &= \mathbb{E}_z \left[\log \frac{p_{\theta}(x^{(i)}|z)p_{\theta}(z)}{p_{\theta}(z|x^{(i)})} \frac{q_{\phi}(z|x^{(i)})}{q_{\phi}(z|x^{(i)})} \right] && (\text{Multiply by constant}) \\
 &= \mathbb{E}_z [\log p_{\theta}(x^{(i)}|z)] - \mathbb{E}_z \left[\log \frac{q_{\phi}(z|x^{(i)})}{p_{\theta}(z)} \right] + \mathbb{E}_z \left[\log \frac{q_{\phi}(z|x^{(i)})}{p_{\theta}(z|x^{(i)})} \right] && (\text{Logarithms}) \\
 &= \underbrace{\mathbb{E}_z [\log p_{\theta}(x^{(i)}|z)] - D_{KL}(q_{\phi}(z|x^{(i)}) || p_{\theta}(z))}_{\mathcal{L}(x^{(i)}, \theta, \phi)} + \underbrace{D_{KL}(q_{\phi}(z|x^{(i)}) || p_{\theta}(z|x^{(i)}))}_{\geq 0}
 \end{aligned}$$

Tractable lower bound which we can take gradient of and optimize! ($p_{\theta}(x|z)$ differentiable, KL term differentiable)

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Variational Autoencoders

Now equipped with our encoder and decoder networks, let's work out the (log) data likelihood:

$$\begin{aligned}
 \log p_{\theta}(x^{(i)}) &= \mathbb{E}_{z \sim q_{\phi}(z|x^{(i)})} [\log p_{\theta}(x^{(i)})] && (p_{\theta}(x^{(i)}) \text{ does not depend on } z) \\
 &= \mathbb{E}_z \left[\log \frac{p_{\theta}(x^{(i)}|z)p_{\theta}(z)}{p_{\theta}(z|x^{(i)})} \right] && (\text{Bayes' Rule}) \\
 &= \mathbb{E}_z \left[\log \frac{p_{\theta}(x^{(i)}|z)p_{\theta}(z)}{p_{\theta}(z|x^{(i)})} \frac{q_{\phi}(z|x^{(i)})}{q_{\phi}(z|x^{(i)})} \right] && (\text{Multiply by constant}) \\
 &= \mathbb{E}_z [\log p_{\theta}(x^{(i)}|z)] - \mathbb{E}_z \left[\log \frac{q_{\phi}(z|x^{(i)})}{p_{\theta}(z)} \right] + \mathbb{E}_z \left[\log \frac{q_{\phi}(z|x^{(i)})}{p_{\theta}(z|x^{(i)})} \right] && (\text{Logarithms}) \\
 &= \underbrace{\mathbb{E}_z [\log p_{\theta}(x^{(i)}|z)] - D_{KL}(q_{\phi}(z|x^{(i)}) || p_{\theta}(z))}_{\mathcal{L}(x^{(i)}, \theta, \phi)} + \underbrace{D_{KL}(q_{\phi}(z|x^{(i)}) || p_{\theta}(z|x^{(i)}))}_{\geq 0}
 \end{aligned}$$

$\log p_{\theta}(x^{(i)}) \geq \mathcal{L}(x^{(i)}, \theta, \phi)$
Variational lower bound ("ELBO")

$\theta^*, \phi^* = \arg \max_{\theta, \phi} \sum_{i=1}^N \mathcal{L}(x^{(i)}, \theta, \phi)$
Training: Maximize lower bound

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Deep Generative Models

Variational Autoencoders

Putting it all together: maximizing the likelihood lower bound

$$\underbrace{E_z[\log p_\theta(x^{(i)}|z)] - D_{KL}(q_\phi(z|x^{(i)})||p_\theta(z))}_{\mathcal{L}(x^{(i)}, \theta, \phi)}$$

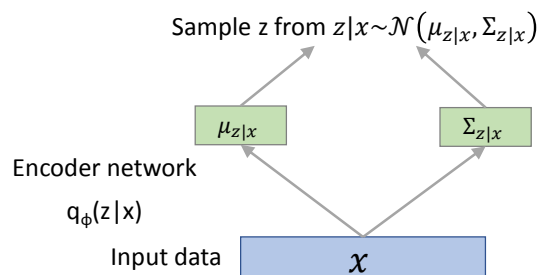
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Deep Generative Models

Variational Autoencoders

Putting it all together: maximizing the likelihood lower bound

$$\underbrace{E_z[\log p_\theta(x^{(i)}|z)] - D_{KL}(q_\phi(z|x^{(i)})||p_\theta(z))}_{\mathcal{L}(x^{(i)}, \theta, \phi)}$$



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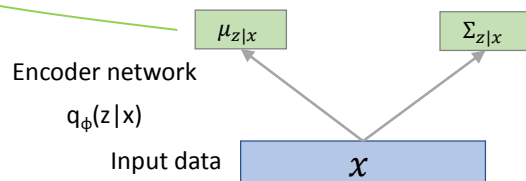
Deep Generative Models

Variational Autoencoders

Putting it all together: maximizing the likelihood lower bound

$$\underbrace{E_z[\log p_\theta(x^{(i)}|z)] - D_{KL}(q_\phi(z|x^{(i)})||p_\theta(z))}_{\mathcal{L}(x^{(i)}, \theta, \phi)}$$

Make approximate posterior distribution close to prior



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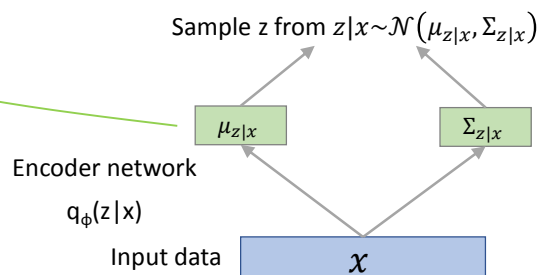
Deep Generative Models

Variational Autoencoders

Putting it all together: maximizing the likelihood lower bound

$$\underbrace{E_z[\log p_\theta(x^{(i)}|z)] - D_{KL}(q_\phi(z|x^{(i)})||p_\theta(z))}_{\mathcal{L}(x^{(i)}, \theta, \phi)}$$

Make approximate posterior distribution close to prior



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Deep Generative Models

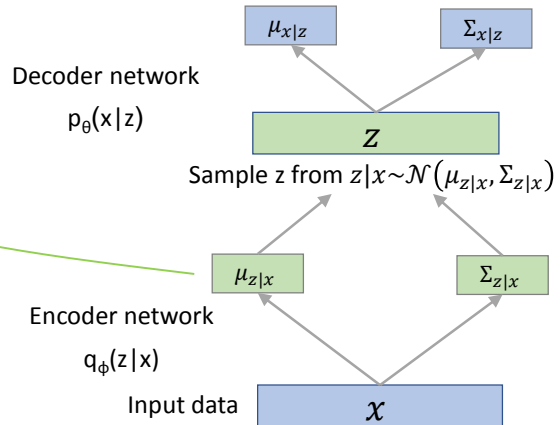
Variational Autoencoders

Putting it all together: maximizing the likelihood lower bound

$$E_z[\log p_\theta(x^{(i)}|z)] - D_{KL}(q_\phi(z|x^{(i)})||p_\theta(z))$$

$\mathcal{L}(x^{(i)}, \theta, \phi)$

Make approximate posterior distribution close to prior



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Deep Generative Models

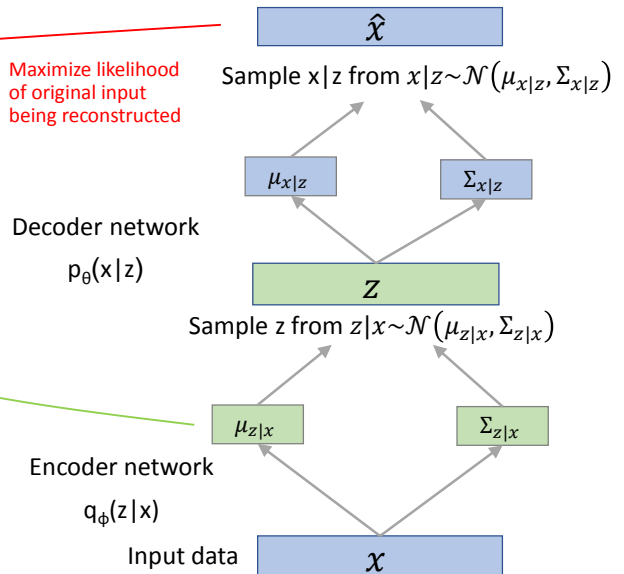
Variational Autoencoders

Putting it all together: maximizing the likelihood lower bound

$$E_z[\log p_\theta(x^{(i)}|z)] - D_{KL}(q_\phi(z|x^{(i)})||p_\theta(z))$$

$\mathcal{L}(x^{(i)}, \theta, \phi)$

Make approximate posterior distribution close to prior



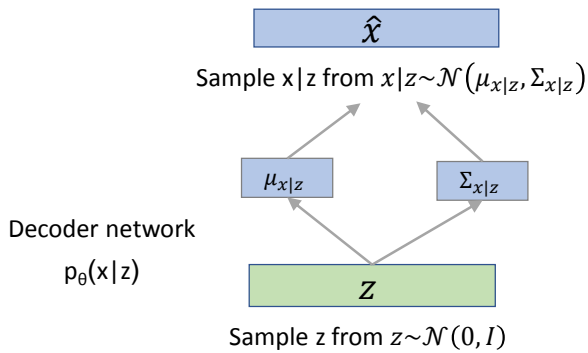
Maximize likelihood of original input being reconstructed

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Deep Generative Models

Variational Autoencoders

Use decoder network. Now sample z from prior!



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Deep Generative Models

Variational Autoencoders

Diagonal prior on z
=> independent
latent variables

Different dimensions
of z encode
interpretable factors
of variation

Degree of smile

Vary z_1



Vary z_2

Head pose

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Deep Generative Models

Variational Autoencoders

Diagonal prior on z
=> independent
latent variables

Different dimensions
of z encode
interpretable
factors
of variation

Also good feature representation that
can be computed using $q_{\phi}(z|x)$!

Degree of smile

Vary z_1



Vary z_2

Head pose

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Deep Generative Models

Variational Autoencoders: Generating Data



32x32 CIFAR-10



Labeled Faces in the Wild

Figures (L) from Dirk Kingma et al. 2016; (R) from Anders Larsen et al. 2017

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Deep Generative Models

Variational Autoencoders

Probabilistic spin to traditional autoencoders => allows generating data

Pros:

- Principled approach to generative models
- Allows inference of $q(z|x)$, can be useful feature representation for other tasks

Cons:

- Maximizes lower bound of likelihood: okay
- Samples blurrier and lower quality compared to state-of-the-art (GANs)

Active areas of research:

- More flexible approximations, e.g. richer approximate posterior instead of diagonal Gaussian
- Incorporating structure in latent variables

Tools

- Python library for Bernoulli Restricted Boltzmann Machines: `sklearn.neural_network.BernoulliRBM`
- Python Keras for Variational auto-encoder
- Generative models (including RBM and VAE): <https://github.com/wiseodd/generative-models>
- Variational Auto-encoder:
 - Tutorials: <http://pyro.ai/examples/vae.html>
 - Codes: <https://github.com/uber/pyro/tree/dev/examples/vae>

References and Resources

- Goodfellow, Ian, et al. Deep learning. Vol. 1. Cambridge: MIT press, 2016.
- Diederik P Kingma, Max Welling: *Auto-Encoding Variational Bayes*. ICLR 2014
- *Restricted Boltzmann machines Tutorial* - Chris Maddison:
https://www.cs.toronto.edu/~tijmen/csc321/documents/maddison_rbmtutorial.pdf
- Geoffrey E. Hinton: *Training products of experts by minimizing contrastive divergence*. Neural Computation (2002)
- Generative Models Lecture (Stanford University): http://cs231n.stanford.edu/slides/2017/cs231n_2017_lecture13.pdf
- Restricted Boltzmann Machines (CMU): <https://www.youtube.com/watch?v=JfpP9CY1EFo>
- Hugo Larochelle's class on Neural Networks: http://info.usherbrooke.ca/hlarochelle/neural_networks/content.html
- Image Generation (ICLR 2018): <https://www.youtube.com/watch?v=G06dEcZ-QTg>

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Deep Generative Models

THANK YOU!!!

Hung Kim Chau

University of Pittsburgh
School of Computing and Information
Department of Informatics and Networked Systems

135 N Bellefield Ave, Pittsburgh, PA, 15260
Phone: +1 (412) 552-3055