

Lecture Notes for **Neural Networks and Machine Learning**



Generative Networks
and
Auto-Encoding Generators

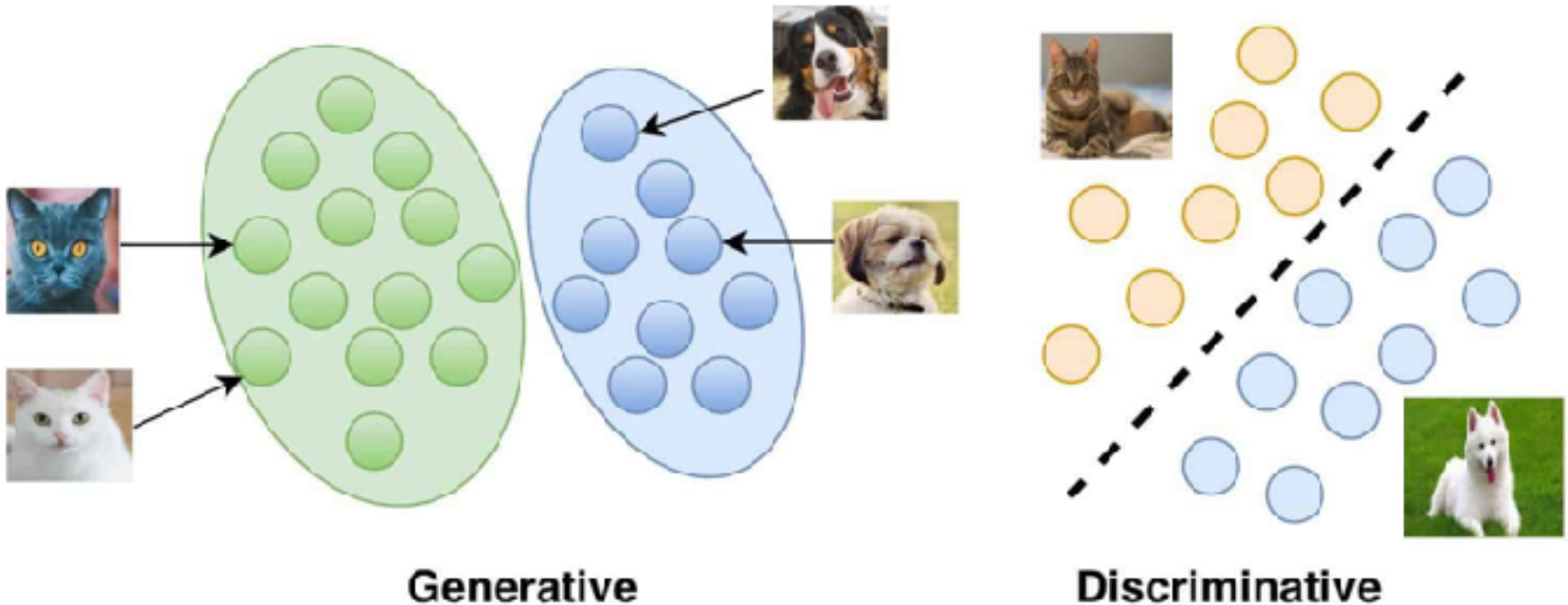


Logistics and Agenda

- Logistics
 - Office Hours, 12:30-1:30
 - Lab due date
 - Student paper presentation
- Agenda
 - A historical perspective of generative Neural Networks
 - Variational Auto-Encoding
 - VAE in Keras Demo (if time)
 - Adversarial Auto-Encoders (if time)



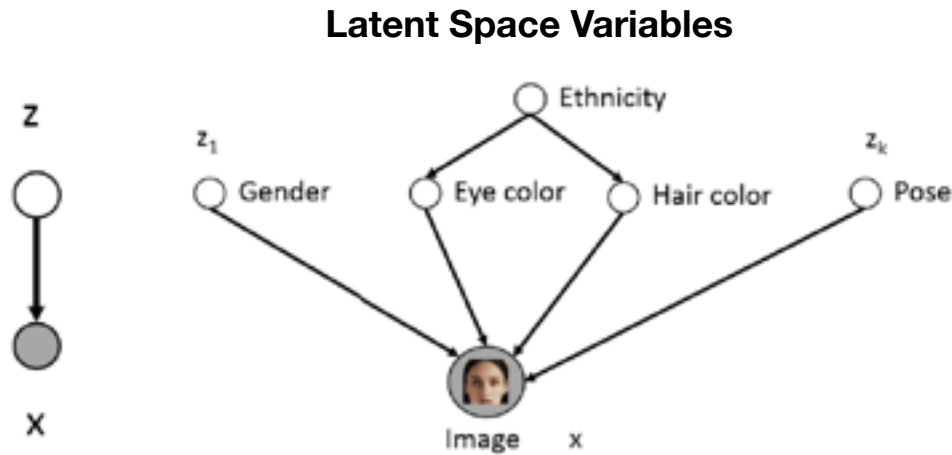
Generative versus Discriminative



<https://learnopencv.com/generative-and-discriminative-models/>



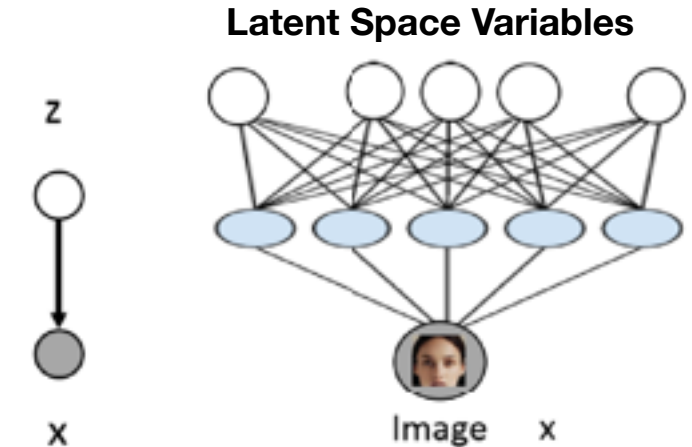
Motivations: Generative Latent Variables



$$p(\mathbf{x} | \mathbf{z})$$

Output Observation
(e.g., image)

Hard: \mathbf{z} is expertly chosen



$$p(\mathbf{x} | \mathbf{z})$$

Output Observation
(e.g., image)

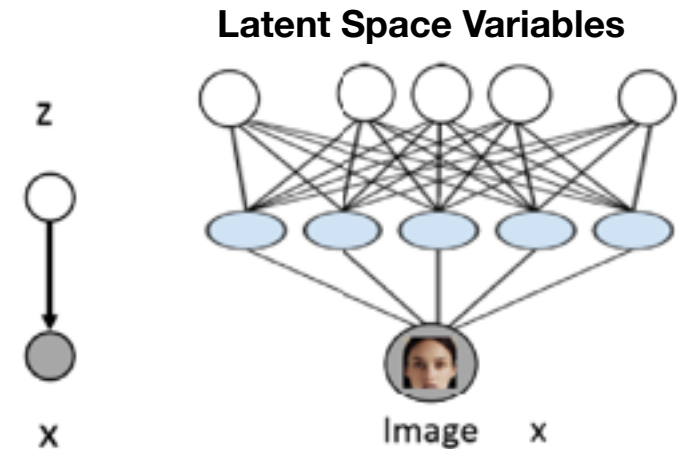
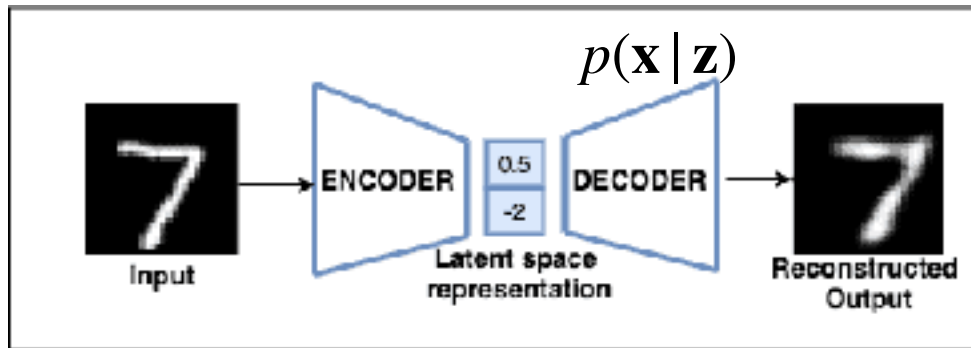
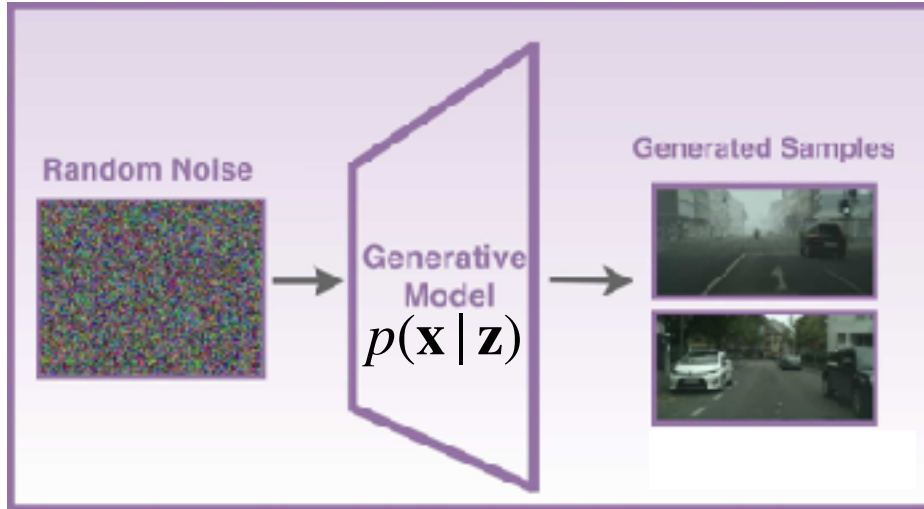
Not as Hard: \mathbf{z} is trained,
latent variables are uncontrolled

Want:

$$p(\mathbf{x}) \approx \sum_{\mathbf{z}} p(\mathbf{z}) p_{\theta}(\mathbf{x} | \mathbf{z})$$



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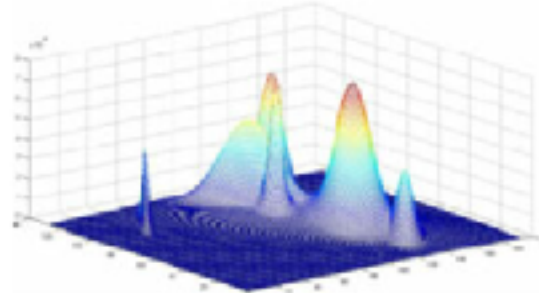
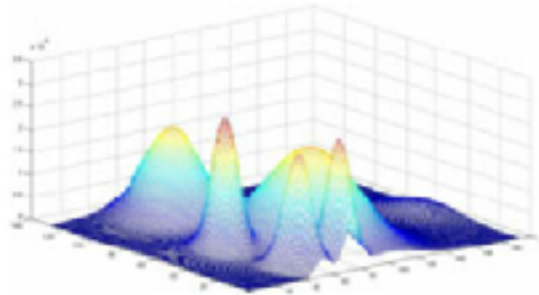
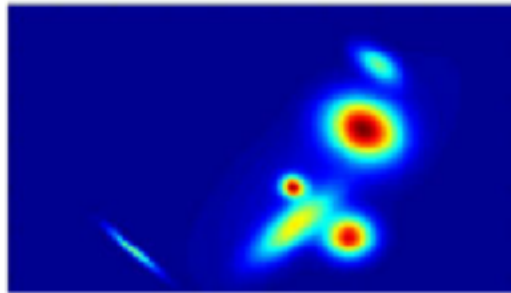
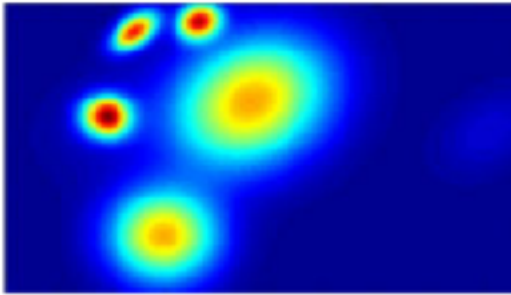
$$p(\mathbf{x}) \approx \sum_{\mathbf{z}} p(\mathbf{z}) p_{\theta}(\mathbf{x} | \mathbf{z})$$



Motivation: Mixtures for Simplicity

Want:
$$p(\mathbf{x}) \approx \sum_{\mathbf{z}} p(\mathbf{z}) p_{\theta}(\mathbf{x} | \mathbf{z})$$

- Each latent variable is mostly independent of other latent variables
- The sum of various mixtures can approximate most any distribution
- Good choice for conditional is Normal Distribution
- Can parameterize $p(\mathbf{x} | \mathbf{z})$ to be a Neural Network



$$p_{\theta}(\mathbf{x} | \mathbf{z} = k) = \mathcal{N}(\mathbf{x}, \mu_k, \Sigma_k)$$

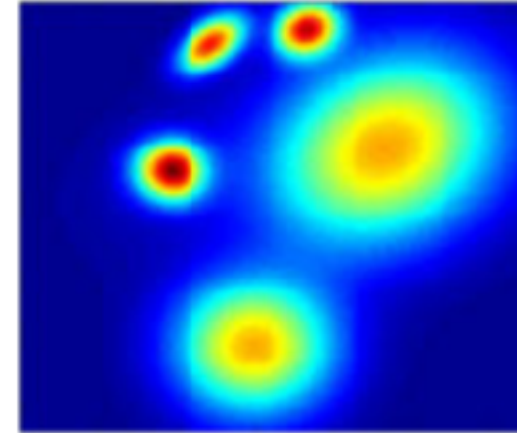
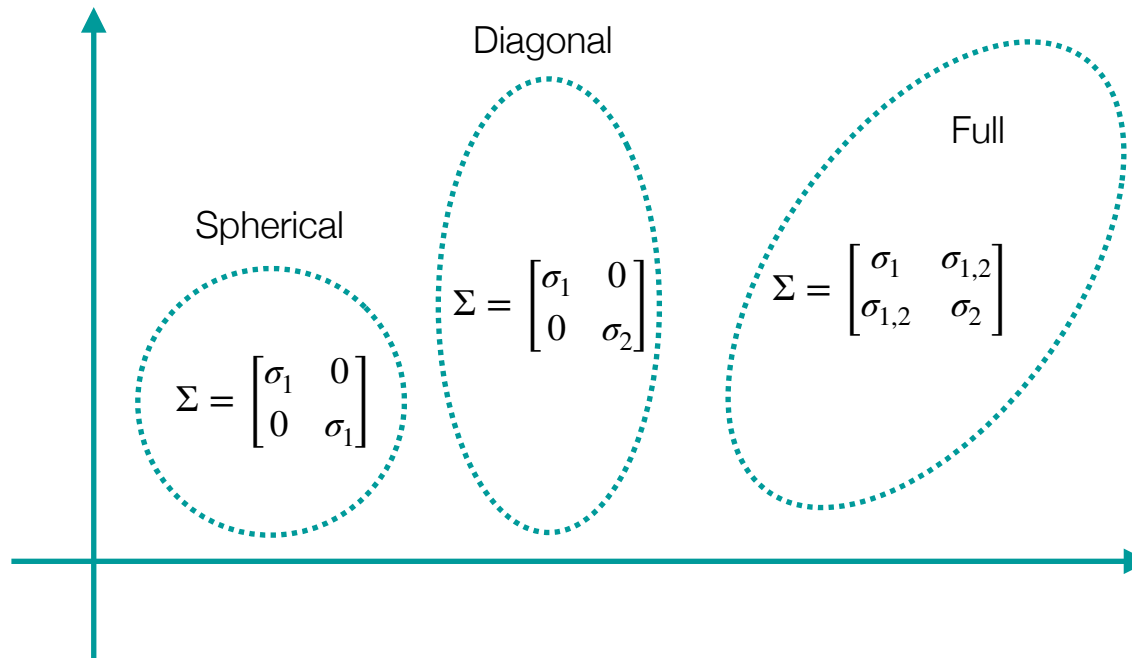
mean and covariance learned



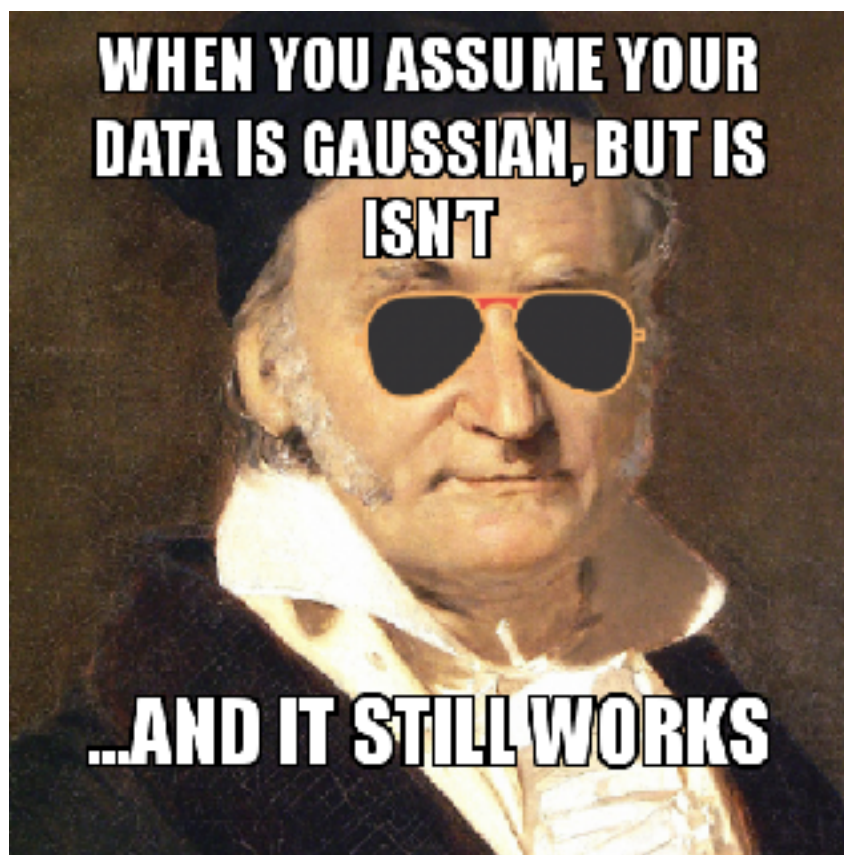
Motivation: Mixtures for Simplicity

$$= \mathcal{N}(\mathbf{x}, \mu_k, \Sigma_k)$$

mean and covariance learned



A History of Generative Networks



Taxonomy of Generative Models

Taxonomy of Generative Models

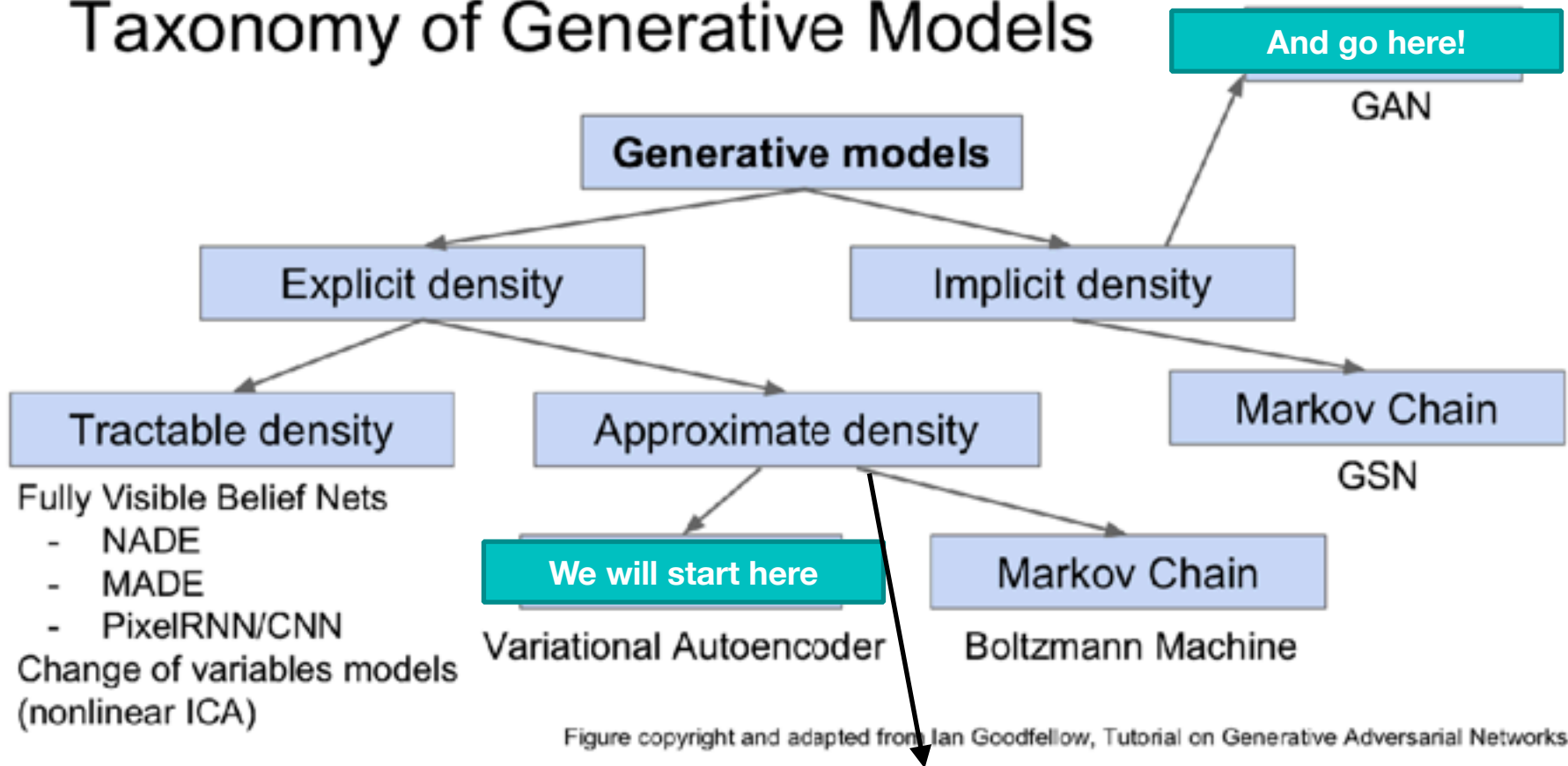


Figure copyright and adapted from Ian Goodfellow, Tutorial on Generative Adversarial Networks, 2017.

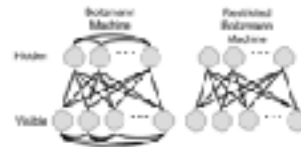
Stable Diffusion
And go here!



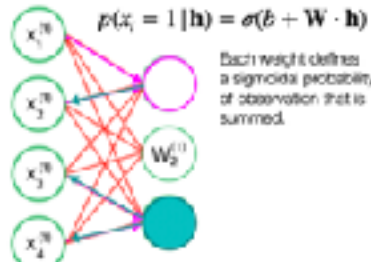
Abridged History of Generative Networks

- Restricted Boltzmann Machine

- Forward pass (visible to latent)
- Backward pass (latent to visible)
- Similar to an auto encoder



AUTODECODERS



RESULTS

<https://www.edureka.co/blog/machine-learning-machine-tutorial/>

2006 Restricted Boltzmann Machine

- Deep Boltzmann Machine

$$P(v, A^{(1)}, A^{(2)}, A^{(3)}) = \frac{1}{Z(\theta)} \exp \left(-L(v, A^{(1)}, A^{(2)}, A^{(3)}, \theta) \right), \quad (20.24)$$

To simplify our presentation, we omit the bias parameters below. The DFM energy function is then defined as follows:

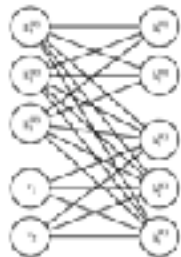
$$F(\mathbf{a}, E^{(1)}, E^{(2)}, \mathbf{A}^{(3)}, \partial) = -\mathbf{a}^T \mathbf{W}^{(1)} \mathbf{a}^{(1)} - E^{(1)} \mathbf{W}^{(2)} \mathbf{A}^{(2)} - E^{(2)} \mathbf{W}^{(3)} E^{(3)}. \quad (38.25)$$

We now develop the mean field approach for the example with two hidden layers. Let $\tilde{Q}(W^{(1)}, h^{(2)} | v)$ be the approximation of $P(h^{(2)} | v)$. The mean field assumption implies that

$$\mathcal{Q}A^{(1)}, A^{(2)}|\varphi\rangle = \prod_i \mathcal{Q}A_i^{(1)}|\varphi\rangle \prod_i Qb_i^{(2)}|\varphi\rangle, \quad (38.20)$$

Not tractable: Can only optimize the Evidence lower bound, ELBO

One can consider all many ways of measuring how well $Q(\mathbf{h}|\mathbf{w})$ fits $P(\mathbf{h}|\mathbf{w})$. The most field approach is to minimize



**Approximate via MCMC
like Gibbs Sampling**

$$\text{KL}(Q||P) = \sum_i Q(\mathbf{A}^{(i)}, \mathbf{b}^{(i)} | \mathbf{u}) \log \left(\frac{Q(\mathbf{A}^{(i)}, \mathbf{b}^{(i)} | \mathbf{u})}{P(\mathbf{A}^{(i)}, \mathbf{b}^{(i)} | \mathbf{u})} \right). \quad (20.30)$$

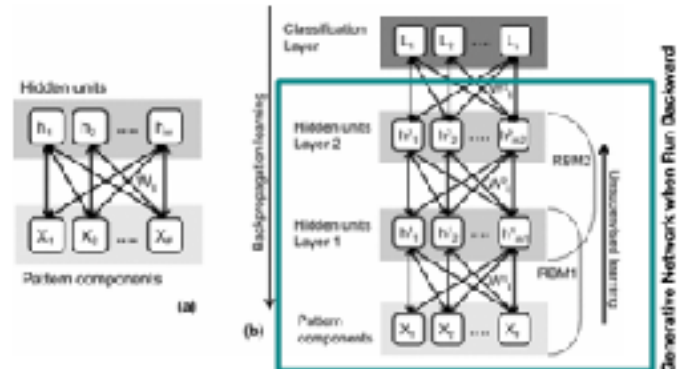
Copyright © 2004 by Harvard University. All rights reserved. Printed in the United States of America. This book is printed on acid-free paper.

2009 Deep Boltzmann Machine

Goodfellow, Bengio, Courville

- Deep Belief Network

- Many FBM blocks together!

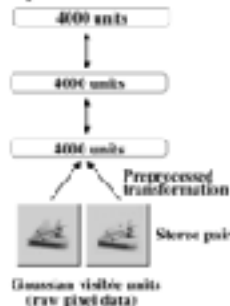


https://link.springer.com/chap/10.1007/978-3-319-58150-7_2

2007, Deep Belief Networks

RBM with many layers

Deep Reinforcement Machine



Training Samples



Figure 5: **Left:** The architecture of deep Boltzmann machine used for NCRB. **Right:** Random samples from the training set, and samples generated from the deep Boltzmann machines by running the Gibbs sampler for 10,000 steps.

2009, Practical Examples

Salakhutdinov and Hinton



Variational Auto Encoding

**“Mathematics is the
Khaleesi of sciences.”**



– Khal Friedrich Gauss



Aside: Remember These

$$p(z | x) = \frac{p(x | z)p(z)}{p(x)}$$

$$\overset{\text{some function}}{\mathbf{E}_{s \leftarrow q(s|x)}}[f(\cdot)] = \int q(s | x) \cdot f(x) \, dx \approx \overset{\text{could be neural networks}}{\sum_{\forall i} q(s | x^{(i)}) \cdot f(x^{(i)})}$$

Expected value of f under conditional distribution, q
 s is latent variable, $x^{(i)}$ is an observation

$$\therefore \mathbf{E}_{s \leftarrow q(s|x)}[\log f(\cdot)] = \sum_{\forall i} q(s | x^{(i)}) \cdot \log(f(x^{(i)}))$$

If function is a probability, this is just the negative of cross entropy of distributions:

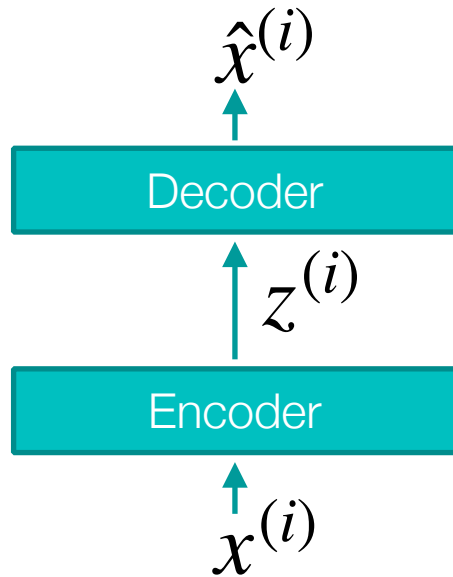
$$H(q, p) = - \sum_x q(x) \cdot \log(p(x))$$

Recall that KL divergence is a measure of difference in two distribution, and is just:

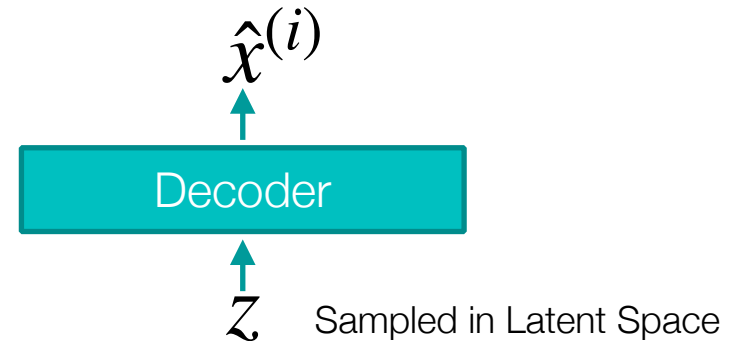
$$D(p \| q) = \sum_x p(x) \cdot \log \left(\frac{p(x)}{q(x)} \right) = \mathbf{E}_p \left[\log \left(\frac{p(x)}{q(x)} \right) \right]$$



Can Auto Encoding Generate Samples?



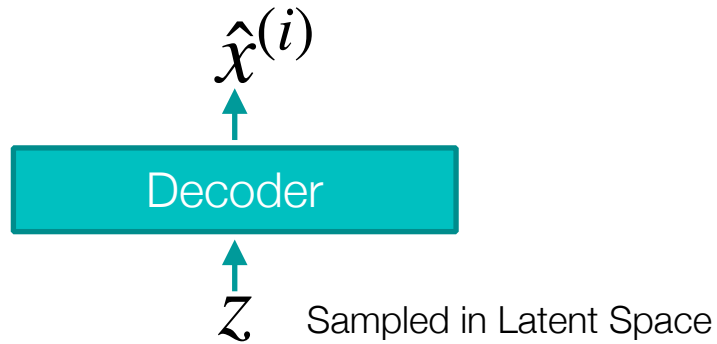
Once trained, is it possible to generate data?



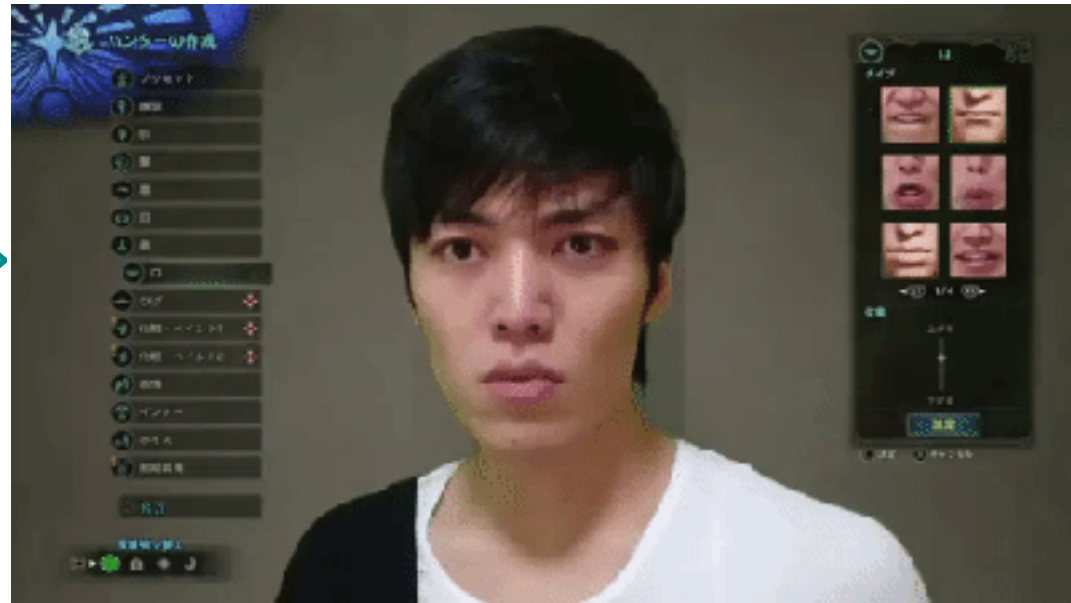
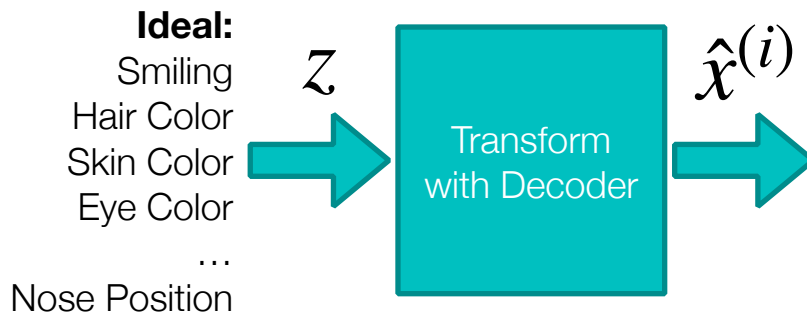
- Does this work for simple auto encoding?
 - Yes, but not satisfactory results
- Learned space is not continuous
- Features could be highly correlated, related in complex ways
 - So, how to sample from the latent space?
- Need to define constraints on latent space...



Reasonable constraints for $p(z)$?



- Should be simple, easy to sample from: **Normal**
- Each component should be independent and identically distributed (i.i.d.): **Diag. Covariance**
 - Encourages features that may be semantic, like expert might select



Mathematical Motivation

$$p(z | x) = \frac{p(x | z)p(z)}{p(x)}$$

We need this inference in order to compute latent variable

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

Denominator is of this form

- We can't compute! **Intractable computation** for all “ z ”
- So let's define this with **variational inference**:
 - AKA: Find the best approximation of desired distribution using a parametrized set of distributions (usually normal distributions)
 - Only needs to work for z **with observed** $x^{(i)}$
 - 1. **Encode** observed $x^{(i)}$ via network $q(z | x^{(i)})$ (with some constraints)
 - 2. Use $q(z | x^{(i)})$ to sample z appropriately, then **decode** with another neural network, $p(x^{(i)} | z^{(i)})$
 - 3. Make $q(z | x^{(i)})$ largest probability possible via Gaussian Distributions



KL Divergence

$$p(x) = \frac{p(z, x)}{p(z|x)} = \frac{p(x|z)p(z)}{p(z|x)}$$

$$\log p(x) = \log p(x) \cdot \int q(z) dz \quad \log p(x) \geq \int q(z) \cdot \log \left[\frac{p(x, z)}{q(z)} \right] dz$$

$$\log p(x) = \int \log p(x) \cdot q(z) dz$$

equal only if
 $p(z|x)$ and $q(z)$ are essentially
 the same distribution

$$\log p(x) = \int q(z) \log \left[\frac{p(x, z)}{p(z|x)} \right] dz$$

$$\therefore \min D_{KL} [q(z) \| p(z|x)]$$

$$\log p(x) = \int q(z) \log \left[\frac{p(x, z) \cdot q(z)}{p(z|x) \cdot q(z)} \right] dz$$

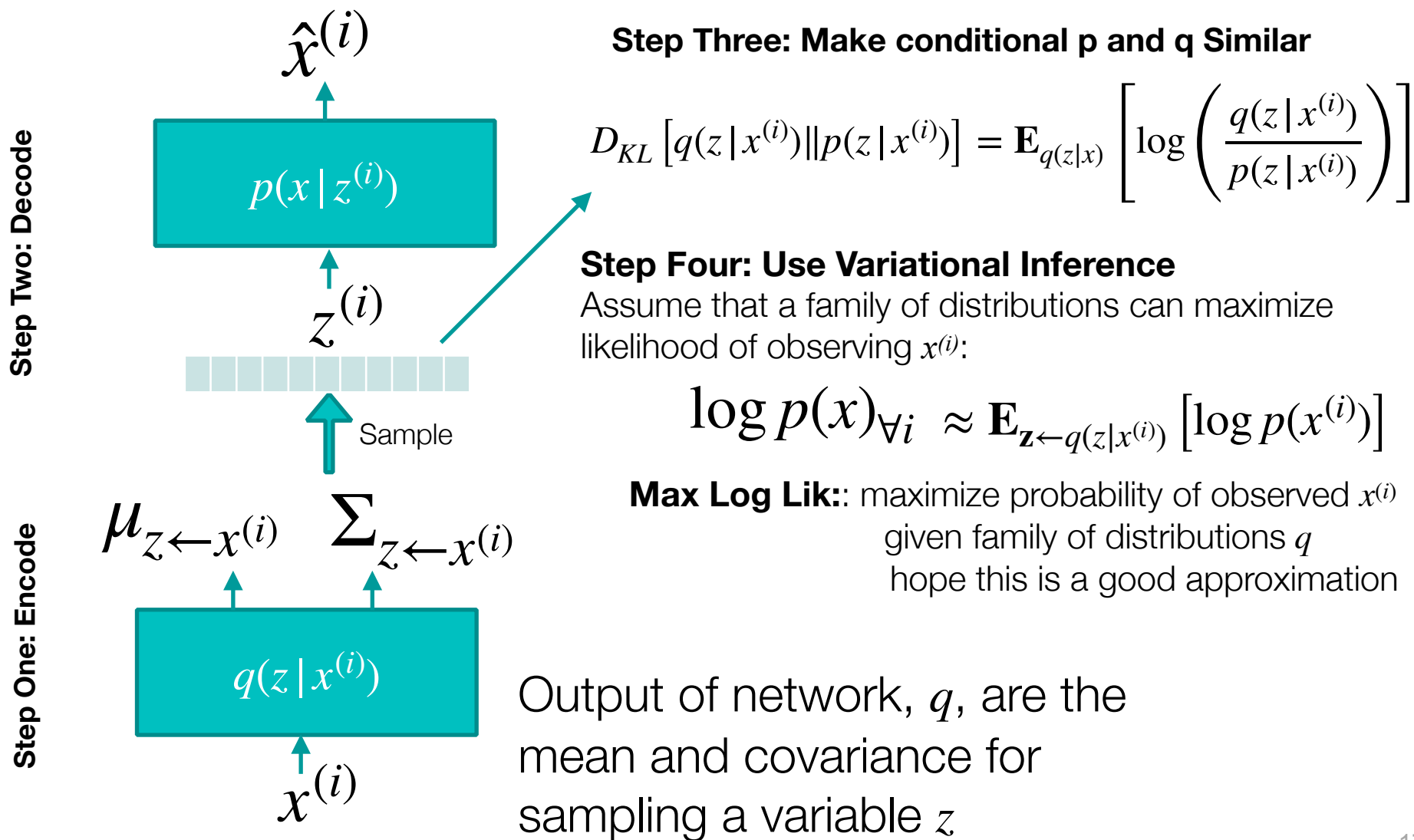
$$\log p(x) = \int q(z) \cdot \left(\log \left[\frac{p(x, z)}{q(z)} \right] + \log \left[\cdot \frac{q(z)}{p(z|x)} \right] \right) dz$$

$$\log p(x) = \int q(z) \cdot \log \left[\frac{p(x, z)}{q(z)} \right] dz + \boxed{\int q(z) \log \left[\frac{q(z)}{p(z|x)} \right] dz}$$

> 0



Need a new formulation



Need a new formulation

$$\log p(x)_{\forall i} \approx \mathbf{E}_{z \leftarrow q(z|x)} [\log p(x^{(i)})] \quad \text{Maximize!}$$

$$= \mathbf{E}_q \left[\log \frac{p(x^{(i)} | z) p(z)}{p(z | x^{(i)})} \frac{q(z | x^{(i)})}{q(z | x^{(i)})} \right] \quad \begin{array}{l} \text{Variational + multiply by one} \\ p(z | x^{(i)}) \text{ this is still a problem} \end{array}$$

$$= \mathbf{E}_q [\log p(x^{(i)} | z)] + \mathbf{E}_q \left[\log \frac{p(z)}{q(z | x^{(i)})} \right] + \mathbf{E}_q \left[\log \frac{q(z | x^{(i)})}{p(z | x^{(i)})} \right]$$

$$= \mathbf{E}_q [\log p(x^{(i)} | z)] - \mathbf{E}_q \left[\log \frac{q(z | x^{(i)})}{p(z)} \right] + \mathbf{E}_q \left[\log \frac{q(z | x^{(i)})}{p(z | x^{(i)})} \right]$$

$$= \mathbf{E}_q [\log p(x^{(i)} | z)] - D_{KL} [q(z | x^{(i)}) || p(z)] + D_{KL} [q(z | x^{(i)}) || p(z | x^{(i)})]$$

always non-negative

$$\log p(x)_{\forall i} \geq \mathbf{E}_q [\log p(x^{(i)} | z)] - D_{KL} [q(z | x^{(i)}) || p(z)] \quad \text{Will Maximize Lower Bound}$$

Can we motivate this in a different way?

