Generative Models

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Generative Modeling

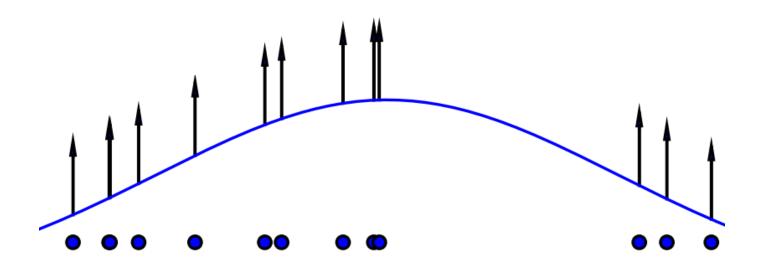
Density estimation



Sample generation

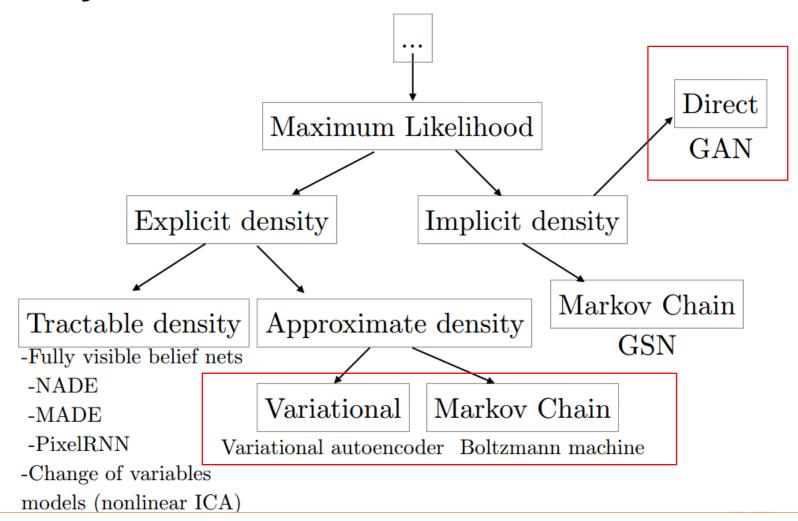


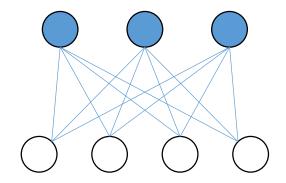
Maximum Likelihood



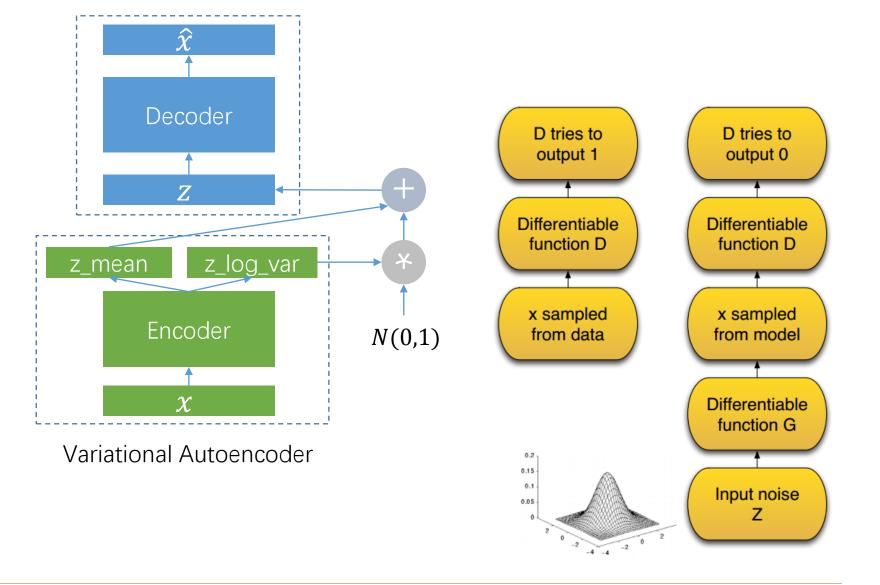
$$\boldsymbol{\theta}^* = \arg \max_{\boldsymbol{\theta}} \mathbb{E}_{\boldsymbol{x} \sim p_{data}} \log p(\boldsymbol{x}; \boldsymbol{\theta})$$

Taxonomy of Generative Models



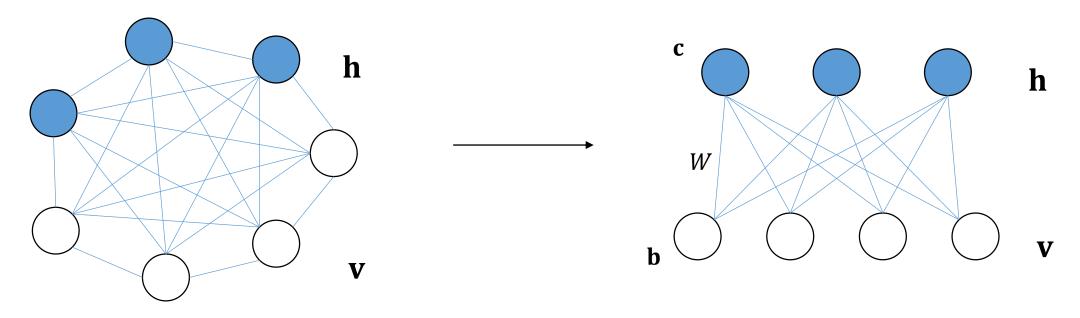


Restricted Boltzmann Machines



Boltzmann Machines

Boltzmann Machines



Restricted Boltzmann Machines

$$\theta = \{\mathbf{b}, \mathbf{c}, W\}$$

Energy Based Model (EBM)

Energy function: $E_{\theta}(\mathbf{v}, \mathbf{h}) = -\mathbf{b}^{\mathrm{T}}\mathbf{v} - \mathbf{c}^{\mathrm{T}}\mathbf{h} - \mathbf{v}^{\mathrm{T}}W\mathbf{h}$

Probability:
$$P_{\theta}(\mathbf{v}, \mathbf{h}) = \frac{1}{Z_{\theta}} e^{-E_{\theta}(\mathbf{v}, \mathbf{h})}$$

Partition function: $Z_{\theta} = \sum_{\mathbf{v},\mathbf{h}} e^{-E_{\theta}(\mathbf{v},\mathbf{h})}$



$$\ell(\theta) = \prod_{t=1}^{n} P(\mathbf{v}^{t}) \Rightarrow \ell(\theta) = \log \prod_{t=1}^{n} P(\mathbf{v}^{t})$$

$$\Rightarrow \ell(\theta) = \sum_{t=1}^{n} \log P(\mathbf{v}^{t}) = \sum_{t=1}^{n} \log \sum_{\mathbf{h}} P(\mathbf{v}^{t}, \mathbf{h})$$

$$\ell(\theta) = \sum_{t=1}^{n} \log \sum_{\mathbf{h}} e^{-E_{\theta}(\mathbf{v}^{t}, \mathbf{h})} - n \log \sum_{\mathbf{v}, \mathbf{h}} e^{-E_{\theta}(\mathbf{v}, \mathbf{h})}$$

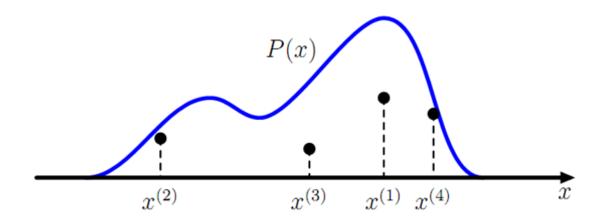
$$\ell(\theta) = \sum_{t=1}^{n} \log \sum_{\mathbf{h}} e^{-E_{\theta}(\mathbf{v}^{t}, \mathbf{h})} - n \log \sum_{\mathbf{v}, \mathbf{h}} e^{-E_{\theta}(\mathbf{v}, \mathbf{h})}$$

$$\nabla_{\theta} \ell(\theta) = \sum_{t=1}^{n} \nabla_{\theta} \log \sum_{\mathbf{h}} e^{-E_{\theta}(\mathbf{v}^{t}, \mathbf{h})} - n \nabla_{\theta} \log \sum_{\mathbf{v}, \mathbf{h}} e^{-E_{\theta}(\mathbf{v}, \mathbf{h})}$$

$$= \sum_{t=1}^{n} \mathbb{E}_{P(\mathbf{h}|\mathbf{v}^{t})} [\nabla_{\theta} - E_{\theta}(\mathbf{v}^{t}, \mathbf{h})] - n \mathbb{E}_{P(\mathbf{h}, \mathbf{v})} [\nabla_{\theta} - E_{\theta}(\mathbf{v}, \mathbf{h})]$$

it is impractical to compute the exact log-likelihood gradient

Markov Chain Monte Carlo



 $Z \sim N(0,1)$

Box–Muller transform



 $U_1, U_2, \dots U_n \sim Uniform(0,1)$

linear congruential generator



Gibbs Sampling



Metropolis-Hastings Sampling



detailed balance condition

Markov Chains - Stationary Distributions

$$\nabla_{\theta} \ell(\theta) = \sum_{t=1}^{n} \mathbb{E}_{P(\mathbf{h}|\mathbf{v}^{t})} [\nabla_{\theta} - E_{\theta}(\mathbf{v}^{t}, \mathbf{h})] - n \mathbb{E}_{P(\mathbf{h}, \mathbf{v})} [\nabla_{\theta} - E_{\theta}(\mathbf{v}, \mathbf{h})]$$

Gibbs Sampling



Contrastive Divergence

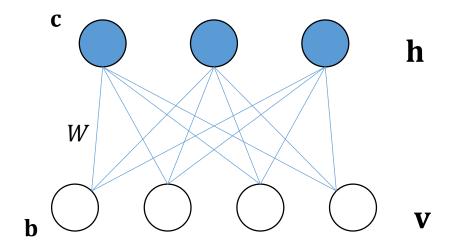
 $\mathbb{E}_{P(\mathbf{h},\mathbf{v})}[\nabla_{\theta} - E_{\theta}(\mathbf{v},\mathbf{h})]$

$$\mathbf{h}^t \sim P(\mathbf{h}|\mathbf{v}^t)$$
$$\mathbf{v}^{t+1} \sim P(\mathbf{v}|\mathbf{h}^t)$$

 $pprox \nabla_{\theta} - E_{\theta}(\mathbf{v}, \mathbf{h})|_{\mathbf{v} = \tilde{\mathbf{v}}, \mathbf{h} = \tilde{\mathbf{h}}}$

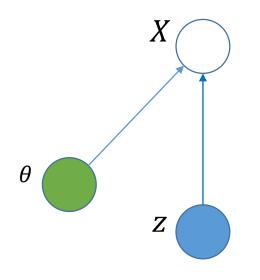
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Boltzmann Machines



Restricted Boltzmann Machines

- ✓ *Dimensionality reduction*
- ✓ Classification
- ✓ Feature learning
- ✓ Deep learning



$$f(z;\theta)$$
: $\mathcal{Z}\times\Theta\to\mathcal{X}$

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

$$Z$$
 $f(z;\theta)$ X

$$P(X|z; \theta) = \mathcal{N}(X|f(z;\theta), \sigma^2 * I)$$

Where is z from? $z \sim \mathcal{N}(0, I)$, Q(z|X)

Goal: $Q(z|X) \approx P(z|X)$

Kullback-Leibler divergence: $\mathcal{D}[Q(z|X)||P(z|X)]$

$$\mathcal{D}[Q(z|X)||P(z|X)] = \mathbb{E}_{z \sim Q} \left[\log Q(z|X) - \log P(z|X) \right]$$

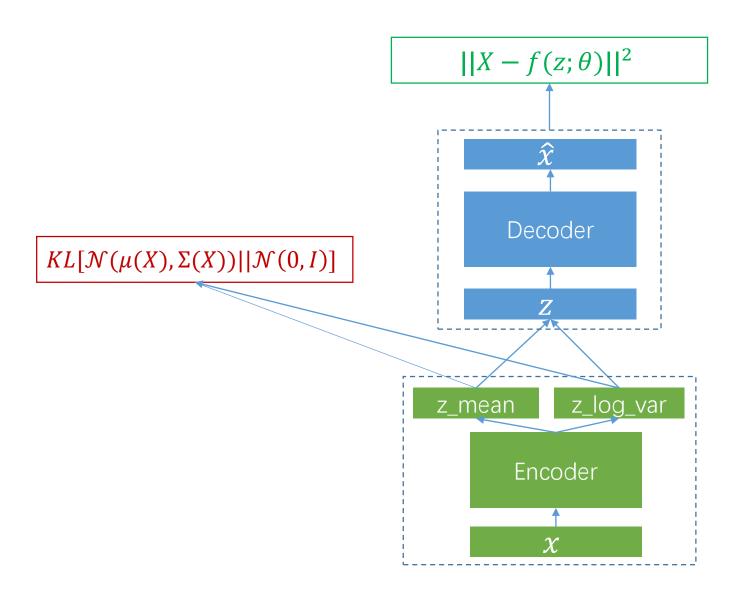


 $\log P(X) - \mathcal{D}[Q(z|X)||P(z|X)] = \mathbb{E}_{z \sim Q} \left[-\log Q(z|X) + \log P(z) + \log P(X|z) \right]$

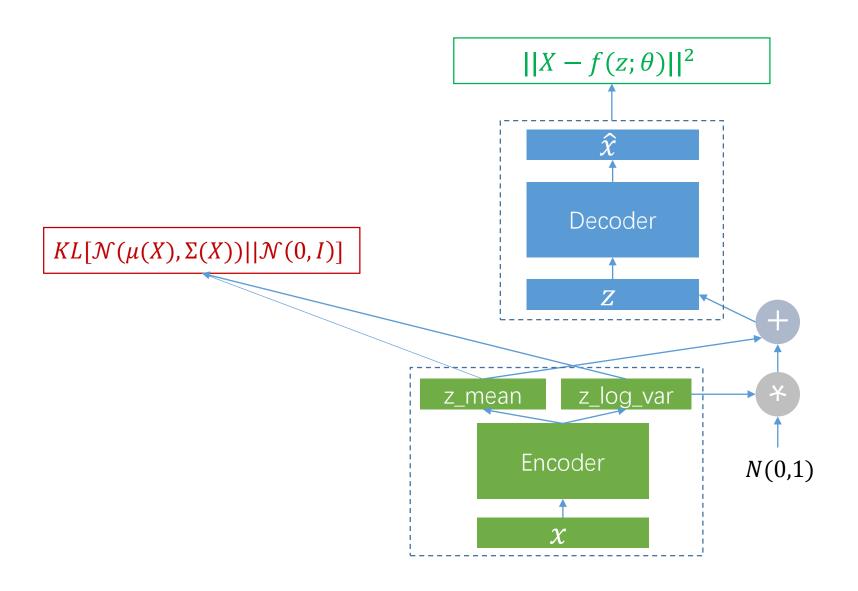
$$\log P(X) - \mathcal{D}[Q(z|X)||P(z|X)] = \mathbb{E}_{z \sim Q} \left[\log P(X|z)\right] - \mathcal{D}[Q(z|X)||P(z)]$$

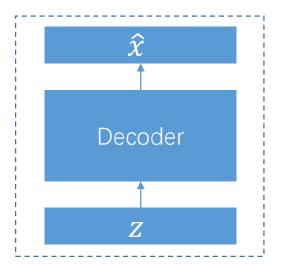
$$Q(z|X) \sim \mathcal{N}(z|\mu(X;\vartheta), \Sigma(X;\vartheta))$$

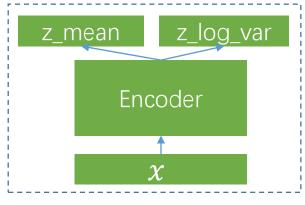
$\log P(X) - \mathcal{D}[Q(z|X)||P(z|X)] = \mathbb{E}_{z \sim Q} \left[\log P(X|z)\right] - \mathcal{D}[Q(z|X)||P(z)]$



$\log P(X) - \mathcal{D}[Q(z|X)||P(z|X)] = \mathbb{E}_{z \sim Q} \left[\log P(X|z)\right] - \mathcal{D}[Q(z|X)||P(z)]$







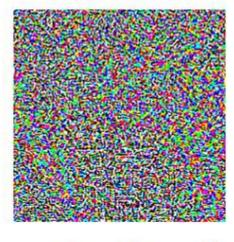
- ✓ Data generation
- ✓ *Dimensionality reduction*
- ✓ Hole filling
- ✓ Semi-supervised learning

Variational Autoencoder

adversarial examples



 $+.007 \times$



 $sign(\nabla_{\boldsymbol{x}}J(\boldsymbol{\theta},\boldsymbol{x},y))$ "nematode"

8.2% confidence



 $x + \epsilon sign(\nabla_x J(\theta, x, y))$ "gibbon"

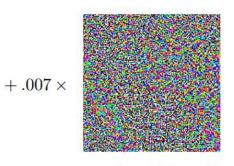
99.3 % confidence

x
"panda"
57.7% confidence

adversarial examples



x
"panda"
57.7% confidence



 $sign(\nabla_{\boldsymbol{x}} J(\boldsymbol{\theta}, \boldsymbol{x}, y))$ "nematode"
8.2% confidence



 $x + \epsilon sign(\nabla_x J(\theta, x, y))$ "gibbon"

99.3 % confidence

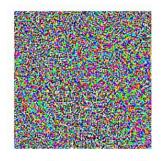
- Nonlinearity?
- Overfitting?

adversarial examples

+.007 ×



x
"panda"
57.7% confidence



 $sign(\nabla_{\boldsymbol{x}} J(\boldsymbol{\theta}, \boldsymbol{x}, y))$ "nematode"
8.2% confidence

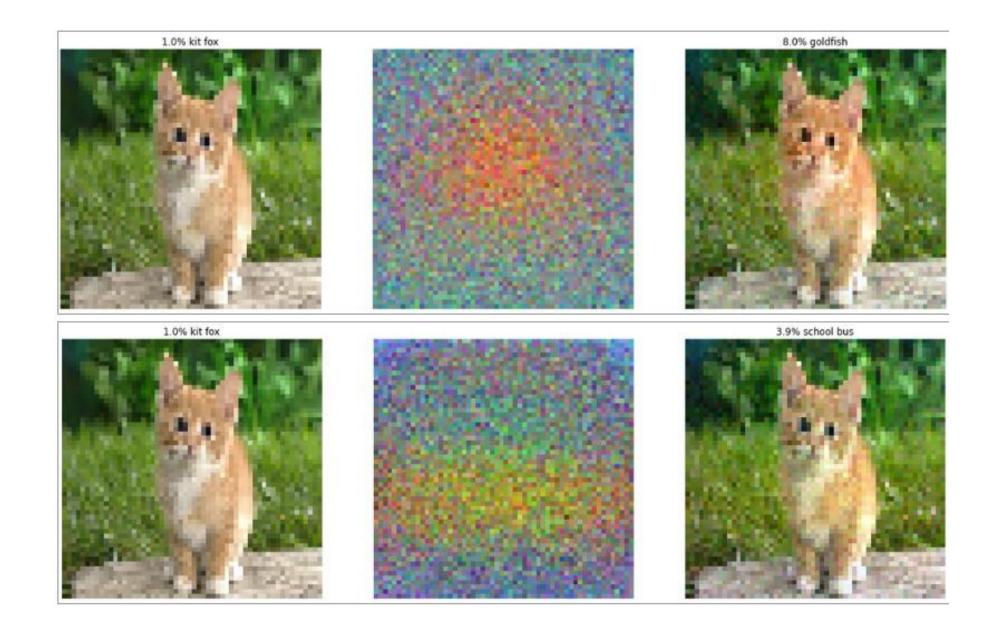


 $x + \epsilon sign(\nabla_x J(\theta, x, y))$ "gibbon"

99.3 % confidence

$$\boldsymbol{w}^{\mathrm{T}}\widetilde{\boldsymbol{x}} = \boldsymbol{w}^{\mathrm{T}}\boldsymbol{x} + \boldsymbol{w}^{\mathrm{T}}\boldsymbol{\eta}$$

$$\eta = \epsilon \operatorname{sign}(\nabla_{x} J(\boldsymbol{\theta}, \boldsymbol{x}, y))$$



adversarial examples (new objective function)

$$\tilde{J}(\boldsymbol{\theta}, \boldsymbol{x}, y) = \alpha J(\boldsymbol{\theta}, \boldsymbol{x}, y) + (1 - \alpha)J(\boldsymbol{\theta}, \boldsymbol{x} + \epsilon \operatorname{sign}(\nabla_{\boldsymbol{x}}J(\boldsymbol{\theta}, \boldsymbol{x}, y))$$

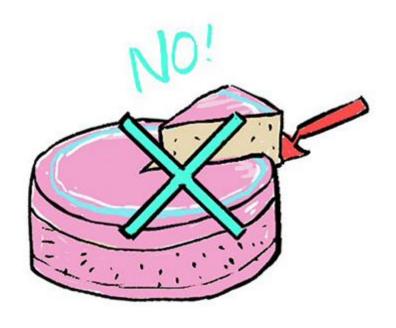
adversarial examples

modern machine learning techniques



Zero-Sum Game



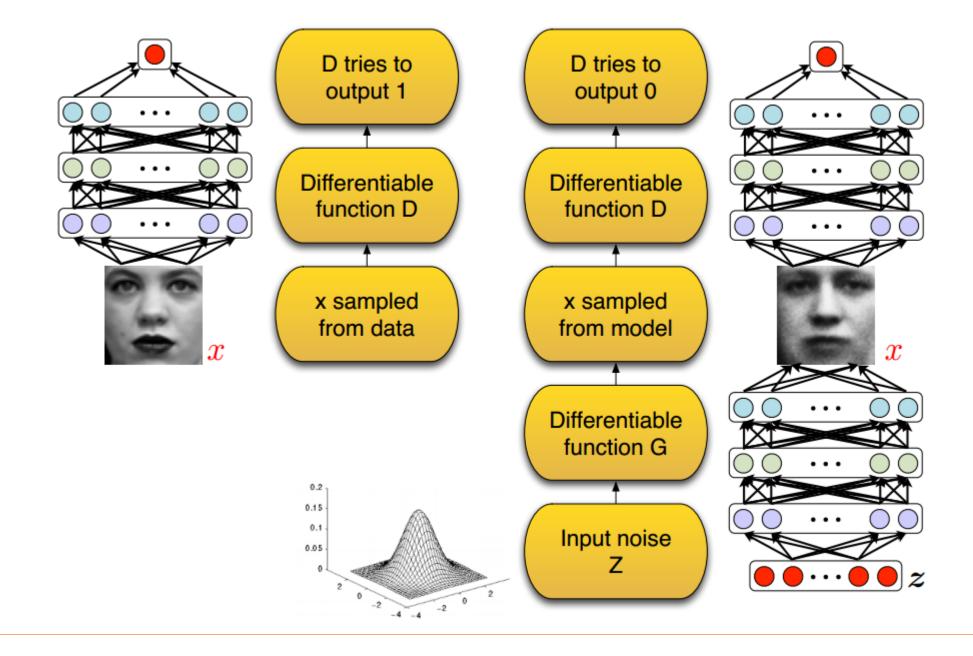


A game between two players:

- 1. Discriminator D
- 2. Generator G
- D tries to discriminate between:
 - A sample from the data distribution.
 - And a sample from the generator G.



G tries to "trick" D by generating samples that are hard for D to distinguish from data.



target function

$$\min_{G} \max_{D} V(G, D) = \mathbb{E}_{\boldsymbol{x} \sim p_{data}(\boldsymbol{x})}[\log D(\boldsymbol{x})] + \mathbb{E}_{\boldsymbol{z} \sim p_{\boldsymbol{z}}(\boldsymbol{z})}[\log(1 - D(G(\boldsymbol{z}))]$$

In practice:
$$\min_{G} \mathbb{E}_{\mathbf{z} \sim p_{\mathbf{z}}(\mathbf{z})} [\log(1 - D(G(\mathbf{x})))]$$

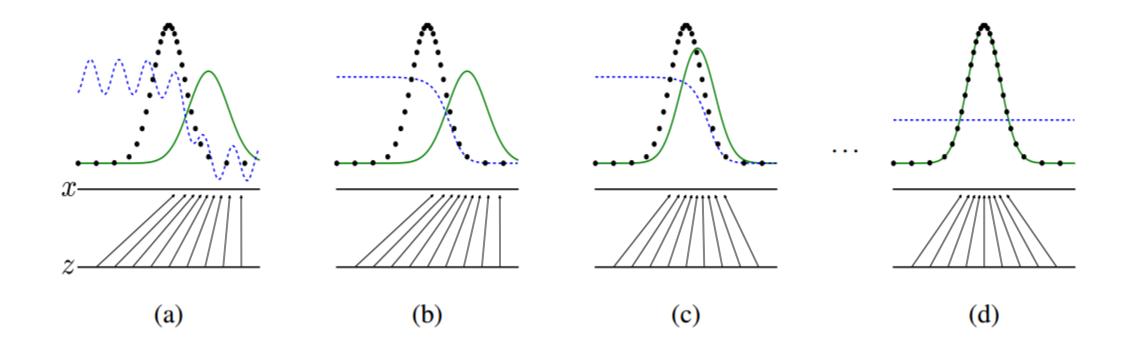
proof

For G fixed, the optimal discriminator D is

$$D(x) = \frac{p_{data}(x)}{p_{data}(x) + p_g(x)}$$

$$V(G, D) = \mathbb{E}_{\boldsymbol{x} \sim p_{data}(\boldsymbol{x})}[\log D(\boldsymbol{x})] + \mathbb{E}_{\boldsymbol{z} \sim p_{\boldsymbol{z}}(\boldsymbol{z})}[\log(1 - D(G(\boldsymbol{z})))]$$

$$V(G,D) = \int_{x} p_{data}(\mathbf{x}) \log D(\mathbf{x}) + p_{\mathbf{g}}(\mathbf{x}) \log(1 - D(\mathbf{x})) d\mathbf{x}$$



$$\min_{G} \max_{D} V(G, D) = \mathbb{E}_{\boldsymbol{x} \sim p_{data}(\boldsymbol{x})} [\log D(\boldsymbol{x})] + \mathbb{E}_{\boldsymbol{z} \sim p_{\boldsymbol{z}}(\boldsymbol{z})} [\log (1 - D(G(\boldsymbol{z})))]$$

$$D(x) = \frac{p_{data}(x)}{p_{data}(x) + p_g(x)}$$

$$\begin{split} C(G) &= \max_{D} V(G, D) \\ &= \mathbb{E}_{x \sim p_{data}(x)} [\log D(x)] + \mathbb{E}_{z \sim p_{z}(z)} [\log (1 - D(G(z))] \\ &= \mathbb{E}_{x \sim p_{data}(x)} [\log D(x)] + \mathbb{E}_{x \sim p_{g}(x)} [\log (1 - D(x))] \\ &= \mathbb{E}_{x \sim p_{data}(x)} \left[\log \frac{p_{data}(x)}{p_{data}(x) + p_{g}(x)} \right] + \mathbb{E}_{x \sim p_{g}(x)} \left[\log \frac{p_{g}(x)}{p_{data}(x) + p_{g}(x)} \right] \end{split}$$

$$C(G) = \mathbb{E}_{x \sim p_{data}(x)} \left[\log \frac{p_{data}(x)}{p_{data}(x) + p_g(x)} \right] + \mathbb{E}_{x \sim p_g(x)} \left[\log \frac{p_g(x)}{p_{data}(x) + p_g(x)} \right]$$

proof

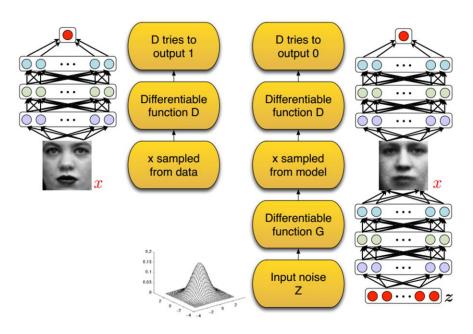
C(G) get its opt. at $p_{data}(x) = p_g(x)$, and the value is $-\log 4$

$$C(G) = \mathbb{E}_{x \sim p_{data}(x)} \left[\log \frac{p_{data}(x)}{p_{data}(x) + p_g(x)} \right] + \mathbb{E}_{x \sim p_g(x)} \left[\log \frac{p_g(x)}{p_{data}(x) + p_g(x)} \right]$$

$$C(G) = -\log 4 + KL[p_{data}(x)||\frac{p_{data}(x) + p_g(x)}{2}] + KL[p_g(x)||\frac{p_{data}(x) + p_g(x)}{2}]$$

$$C(G) = -\log 4 + 2 \cdot JSD[p_{data}(x)||p_g(x)]$$

If G and D have enough capacity, p_g converges to p_{data}



Generative Adversarial Nets

- ✓ Image generation
- ✓ Image Synthesis
- ✓ Super Resolution

Comparison (RBM, VAE, GAN)

RBM

- Have intractable likelihood functions and therefore require numerous approximations to the likelihood gradient;
- Markov chain

VAE

Not asymptotically consistent

GAN

- Asymptotically consistent
- No Markov chains needed

Reference

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