Introductory Overview Lecture The Deep Learning Revolution Part III: Learning Deep Generative Models

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Unsupervised Learning

Non-probabilistic Models

- > Sparse Coding
- > Autoencoders
- Others (e.g. k-means)

Probabilistic Generative)
Models

Tractable Models

- Mixture of Gaussians
- > Autoregressive Models
- Normalizing Flows
- Many others

Non-Tractable Models

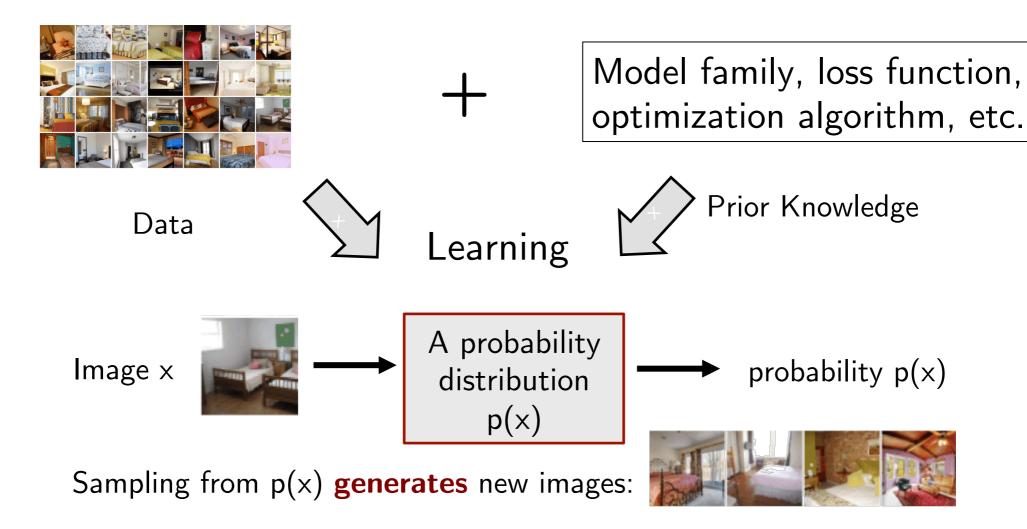
- ➤ Boltzmann Machines
- VariationalAutoencoders
- > Helmholtz Machines
- Many others...

- Generative Adversarial Networks
- Moment Matching Networks

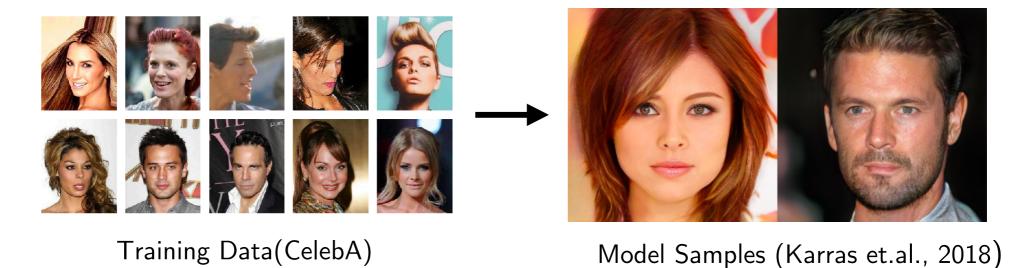
Explicit Density p(x)

Implicit Density

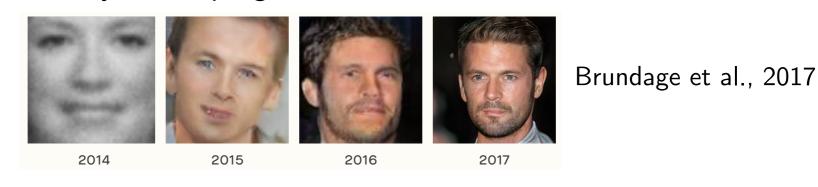
Statistical Generative Models



Statistical Generative Models



4 years of progression on Faces



Conditional Generation

► Conditional generative model P(zebra images| horse images)



▶ Style Transfer



Input Image



Monet



Van Gogh

Zhou el al., Cycle GAN 2017

Conditional Generation

► Conditional generative model P(zebra images| horse images)



► Failure Case



Talk Roadmap

- ► Fully Observed Models
- ▶ Undirected Deep Generative Models
 - Restricted Boltzmann Machines (RBMs),
 - Deep Boltzmann Machines (DBMs)
- ▶ Directed Deep Generative Models
 - Variational Autoencoders (VAEs)
 - Normalizing Flows
- ► Generative Adversarial Networks (GANs)

Fully Observed Models

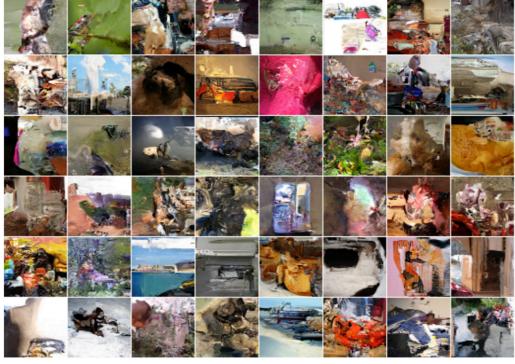
▶ Density Estimation by Autoregression

► Ordering of variables is crucial

NADE (Uria 2013), MADE (Germain 2017), MAF (Papamakarios 2017), PixelCNN (van den Oord, et al, 2016)

Fully Observed Models

▶ Density Estimation by Autoregression

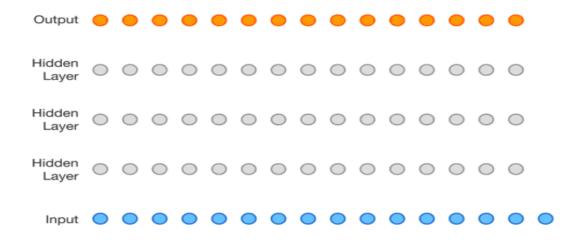


PixelCNN (van den Oord, et al, 2016)

NADE (Uria 2013), MADE (Germain 2017), MAF (Papamakarios 2017), PixelCNN (van den Oord, et al, 2016)

WaveNet

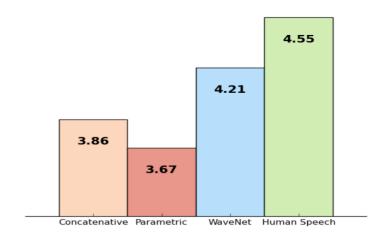
► Generative Model of Speech Signals





1 Second

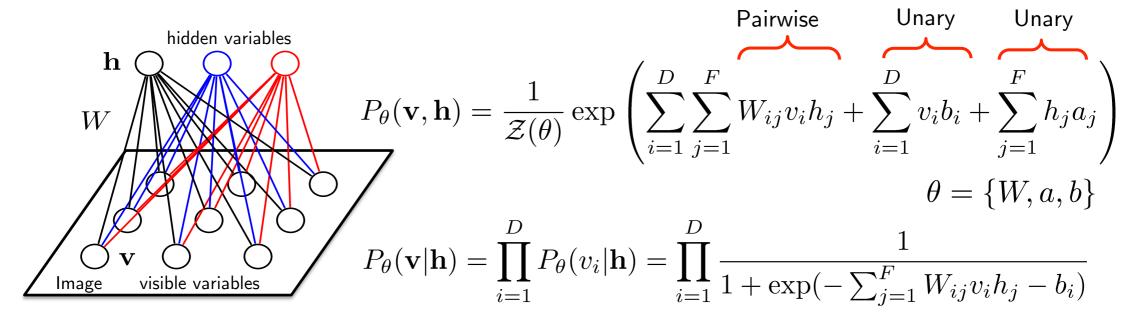
Quality: Mean Opinion Scores



Talk Roadmap

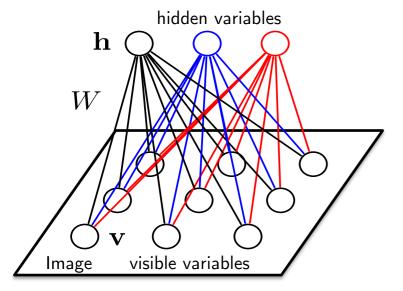
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Restricted Boltzmann Machines



- ▶ RBM is a Markov Random Field with
 - Stochastic binary visible variables $\mathbf{v} \in \{0,1\}^D$.
 - Stochastic binary hidden variables $\mathbf{h} \in \{0,1\}^F$.
 - ▶ Bipartite connections

Maximum Likelihood Learning



$$P_{\theta}(\mathbf{v}) = \frac{P^{*}(\mathbf{v})}{\mathcal{Z}(\theta)} = \frac{1}{\mathcal{Z}(\theta)} \sum_{\mathbf{h}} \exp \left[\mathbf{v}^{\top} W \mathbf{h} + \mathbf{a}^{\top} \mathbf{h} + \mathbf{b}^{\top} \mathbf{v} \right]$$

► Maximize log-likelihood objective:

$$L(\theta) = \frac{1}{N} \sum_{n=1}^{N} \log P_{\theta}(\mathbf{v}^{(n)})$$

▶ Derivative of the log-likelihood:

$$\frac{\partial L(\theta)}{\partial W_{ij}} = \frac{1}{N} \sum_{n=1}^{N} \frac{\partial}{\partial W_{ij}} \log \left(\sum_{\mathbf{h}} \exp \left[\mathbf{v}^{(n)\top} W \mathbf{h} + \mathbf{a}^{\top} \mathbf{h} + \mathbf{b}^{\top} \mathbf{v}^{(n)} \right] \right) - \frac{\partial}{\partial W_{ij}} \log \mathcal{Z}(\theta)$$

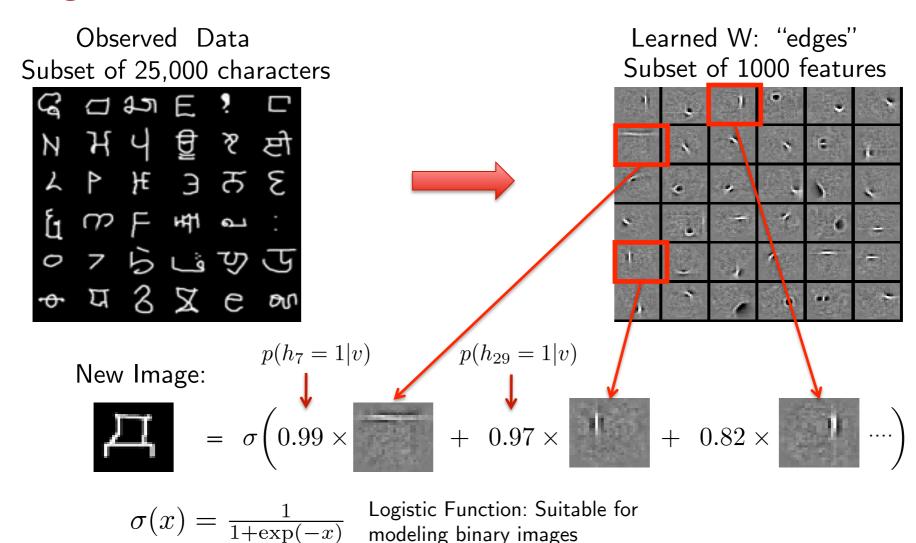
$$= \mathbf{E}_{P_{data}}[v_i h_j] - \mathbf{E}_{P_{\theta}}[v_i h_j]$$

$$P_{data}(\mathbf{v}, \mathbf{h}; \theta) = P(\mathbf{h}|\mathbf{v}; \theta)P_{data}(\mathbf{v})$$

$$P_{data}(\mathbf{v}) = \frac{1}{N} \sum \delta(\mathbf{v} - \mathbf{v}^{(n)})$$

Difficult to compute: exponentially many configurations

Learning Features



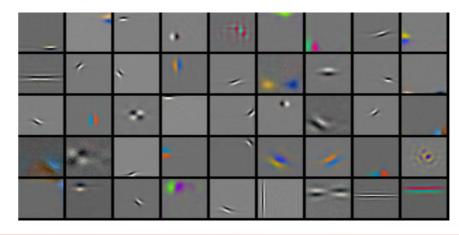
RBMs for Real-valued & Count Data

4 million unlabelled images





Learned features (out of 10,000)







Reuters dataset: 804,414 **unlabeled** newswire stories

Bag-of-Words

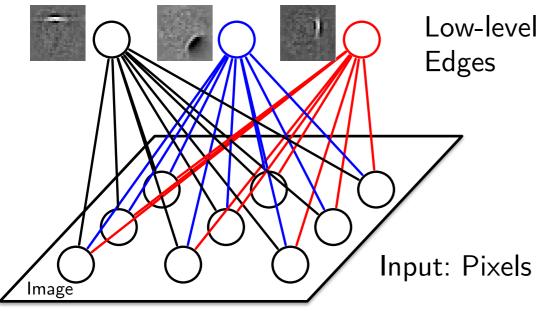


russian russia moscow yeltsin soviet clinton house president bill congress computer system product software develop

Learned features: ``topics''

trade country import world economy stock wall street point dow

Deep Boltzmann Machines

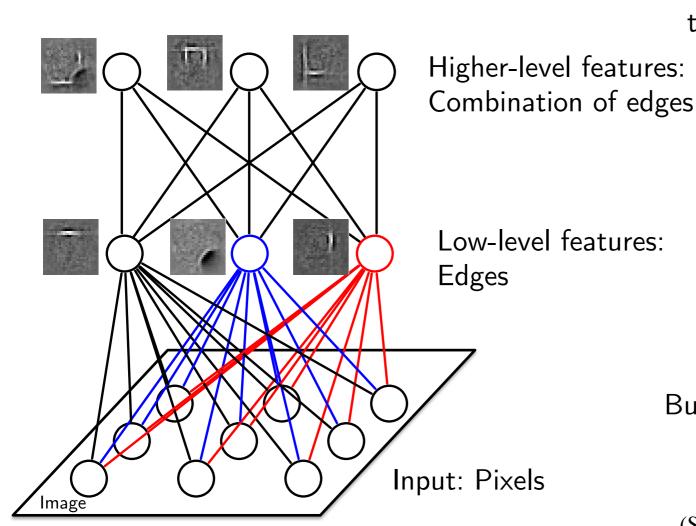


Low-level features:

Built from unlabeled inputs.

Deep Boltzmann Machines

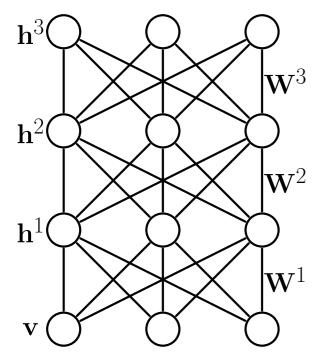
Learn simpler representations, then compose more complex ones



Built from unlabeled inputs.

Model Formation

$$P_{\theta}(\mathbf{v}, \mathbf{h}^{(1)}, \mathbf{h}^{(2)}, \mathbf{h}^{(3)}) = \frac{1}{\mathcal{Z}(\theta)} \exp \left[\mathbf{v}^{\top} W^{(1)} \mathbf{h}^{(1)} + \mathbf{h}^{(1)}^{\top} W^{(2)} \mathbf{h}^{(2)} + \mathbf{h}^{(2)}^{\top} W^{(3)} \mathbf{h}^{(3)} \right]$$



Same as RBMs

$$\theta = \{W^1, W^2, W^3\}$$
 model parameters

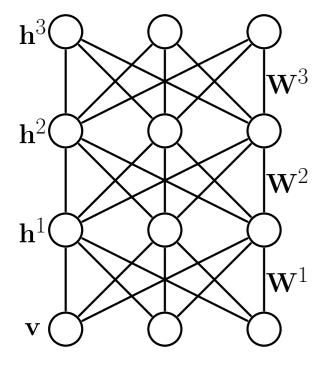
- Dependencies between hidden variables
- All connections are undirected
- ► Maximum Likelihood Learning:

$$\frac{\partial \log P_{\theta}(\mathbf{v})}{\partial W^{1}} = \mathbb{E}_{P_{data}}[\mathbf{vh^{1}}^{\top}] - \mathbb{E}_{P_{\theta}}[\mathbf{vh^{1}}^{\top}]$$

▶ Both expectations are intractable

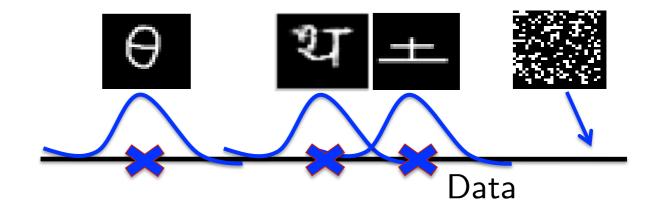
Approximate Learning

$$P_{\theta}(\mathbf{v}, \mathbf{h}^{(1)}, \mathbf{h}^{(2)}, \mathbf{h}^{(3)}) = \frac{1}{\mathcal{Z}(\theta)} \exp \left[\mathbf{v}^{\top} W^{(1)} \mathbf{h}^{(1)} + \mathbf{h}^{(1)}^{\top} W^{(2)} \mathbf{h}^{(2)} + \mathbf{h}^{(2)}^{\top} W^{(3)} \mathbf{h}^{(3)} \right]$$



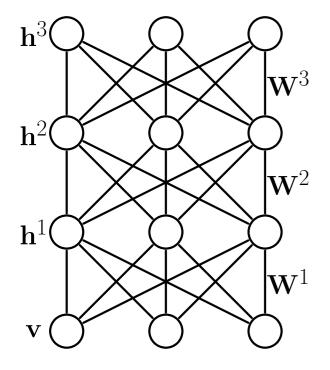
► Maximum Likelihood Learning:

$$\frac{\partial \log P_{\theta}(\mathbf{v})}{\partial W^{1}} = \mathbb{E}_{P_{data}}[\mathbf{vh^{1}}^{\top}] - \mathbb{E}_{P_{\theta}}[\mathbf{vh^{1}}^{\top}]$$

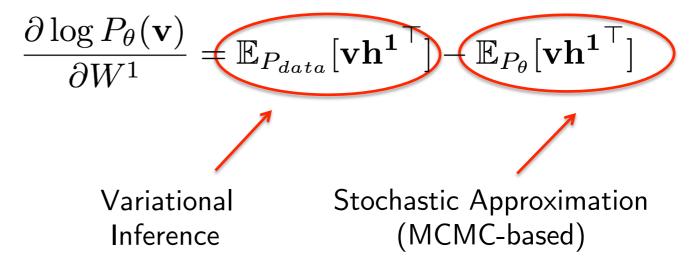


Approximate Learning

$$P_{\theta}(\mathbf{v}, \mathbf{h}^{(1)}, \mathbf{h}^{(2)}, \mathbf{h}^{(3)}) = \frac{1}{\mathcal{Z}(\theta)} \exp \left[\mathbf{v}^{\top} W^{(1)} \mathbf{h}^{(1)} + \mathbf{h}^{(1)}^{\top} W^{(2)} \mathbf{h}^{(2)} + \mathbf{h}^{(2)}^{\top} W^{(3)} \mathbf{h}^{(3)} \right]$$



► Maximum Likelihood Learning:



Good Generative Model?

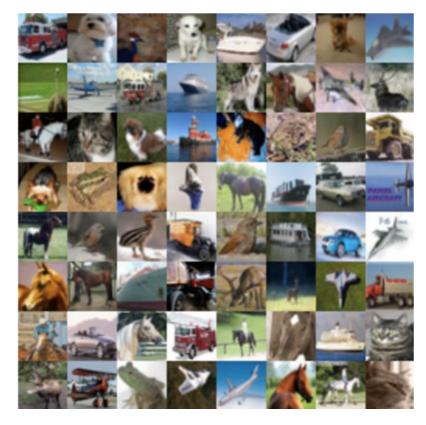
► Handwritten Characters

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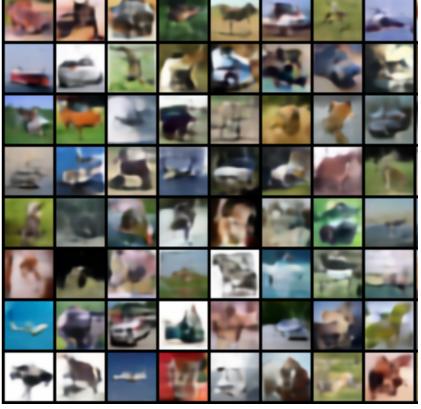
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Good Generative Model?

► CIFAR Dataset



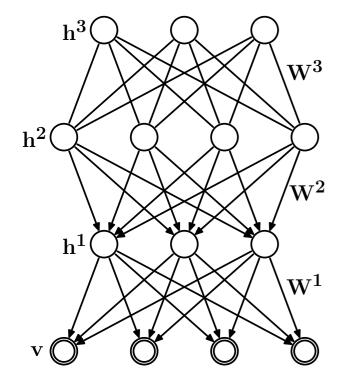
Training

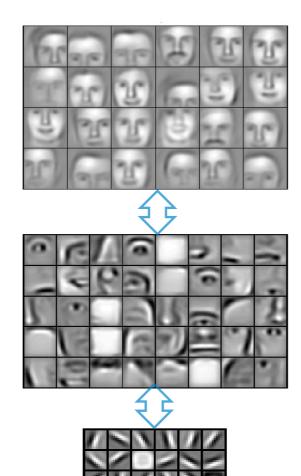


Samples

Learning Part-Based Representations

Deep Belief Network





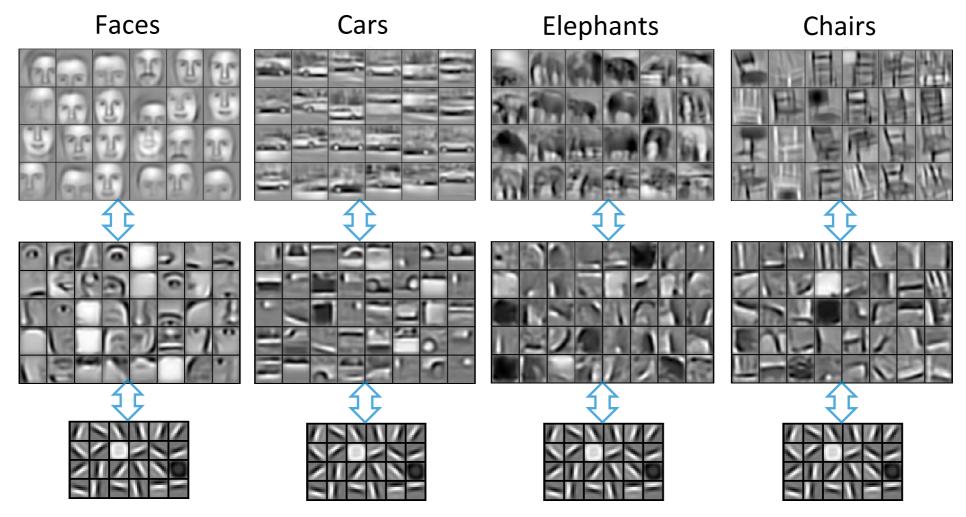
Groups of parts

Object Parts

Trained on face images.

Lee, Grosse, Ranganath, Ng, ICML 2009

Learning Part-Based Representations



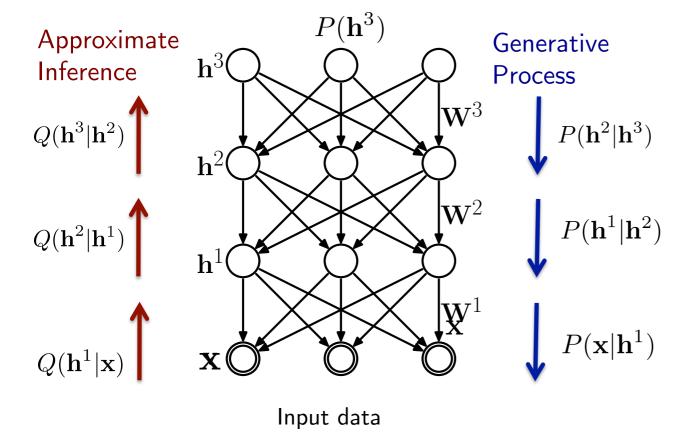
Lee, Grosse, Ranganath, Ng, ICML 2009

Talk Roadmap

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Helmholtz Machines

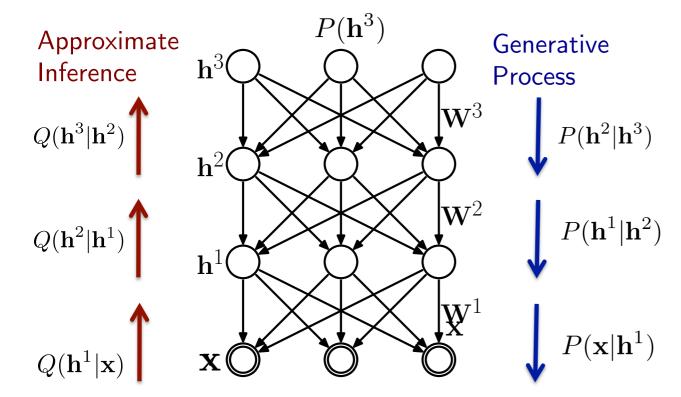
▶ Hinton, G. E., Dayan, P., Frey, B. J. and Neal, R., Science 1995



- ▶ Kingma & Welling, 2014
- ▶ Rezende, Mohamed, Daan, 2014
- ▶ Mnih & Gregor, 2014
- ▶ Bornschein & Bengio, 2015
- ► Tang & Salakhutdinov, 2013

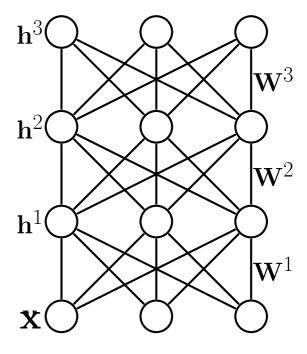
Helmholtz Machines

Helmholtz Machine

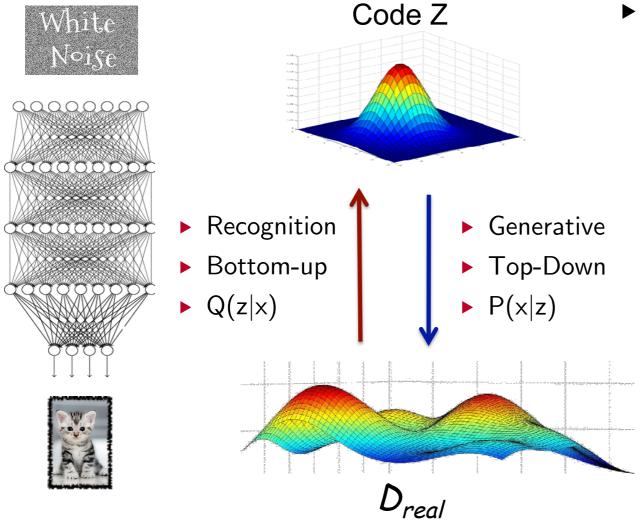


Input data

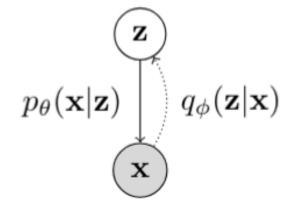
Deep Boltzmann Machine



Deep Directed Generative Models



► Latent Variable Models

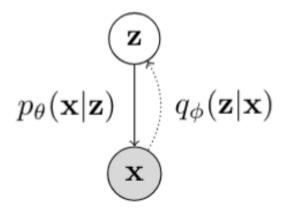


$$\log p_{\theta}(\mathbf{x}) = \log \int p_{\theta}(\mathbf{x}, \mathbf{z}) d\mathbf{z}$$

 Conditional distributions are parameterized by deep neural networks

Directed Deep Generative Models

► Directed Latent Variable Models with Inference Network



► Maximum log-likelihood objective

$$\max_{\theta} \sum_{\mathbf{x} \in \mathcal{D}} \log p_{\theta}(\mathbf{x})$$

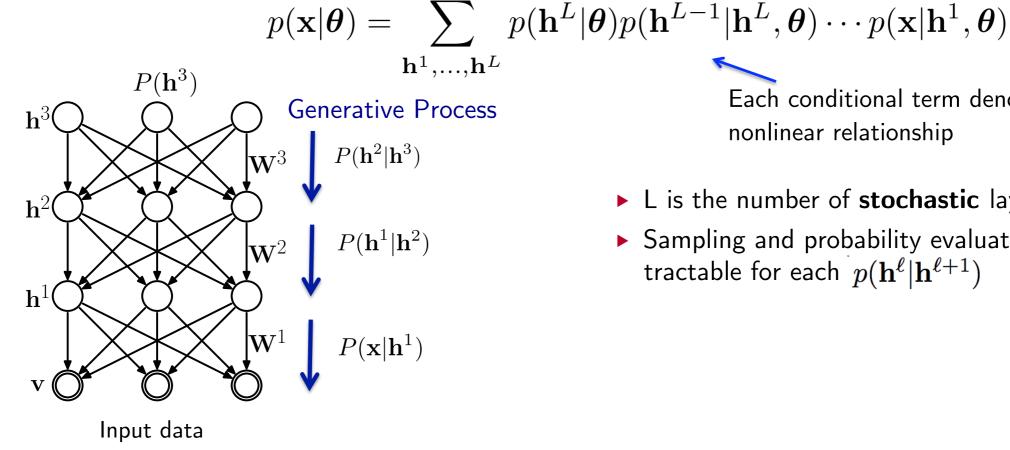
► Marginal log-likelihood is intractable:

$$\log p_{\theta}(\mathbf{x}) = \log \int p_{\theta}(\mathbf{x}, \mathbf{z}) d\mathbf{z}$$

▶ Key idea: Approximate true posterior p(z|x) with a simple, tractable distribution q(z|x) (inference/recognition network).

Variational Autoencoders (VAEs)

▶ The VAE defines a generative process in terms of ancestral sampling through a cascade of hidden stochastic layers:

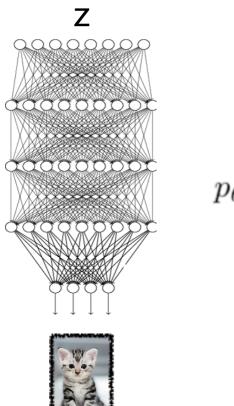


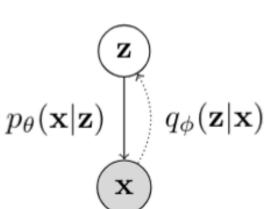
Each conditional term denotes a nonlinear relationship

- ▶ L is the number of **stochastic** layers
- Sampling and probability evaluation is tractable for each $p(\mathbf{h}^{\ell}|\mathbf{h}^{\ell+1})$

Variational Autoencoders (VAEs)

► Single stochastic (Gaussian) layer, followed by many deterministic layers





$$p(\mathbf{z}) = \mathcal{N}(0, I)$$

$$p_{\theta}(\mathbf{x}|\mathbf{z}) = \mathcal{N}(\mu(\mathbf{z}, \theta), \Sigma(\mathbf{z}, \theta))$$

Deep neural network parameterized by θ . (Can use different noise models)

$$q_{\phi}(\mathbf{z}|\mathbf{x}) = \mathcal{N}(\mu(\mathbf{x}, \phi), \Sigma(\mathbf{x}, \phi))$$

Deep neural network parameterized by ϕ .

Variational Bound

► VAE is trained to maximize the variational lower bound:

$$\log p_{\theta}(\mathbf{x}) = \log \int p_{\theta}(\mathbf{x}, \mathbf{z}) d\mathbf{z} = \log \int q_{\phi}(\mathbf{z}|\mathbf{x}) \frac{p_{\theta}(\mathbf{x}, \mathbf{z})}{q_{\phi}(\mathbf{z}|\mathbf{x})} d\mathbf{z}$$

$$= \log \mathbb{E}_{q_{\phi}(\mathbf{z}|\mathbf{x})} \left[\frac{p_{\theta}(\mathbf{x}, \mathbf{z})}{q_{\phi}(\mathbf{z}|\mathbf{x})} \right] \qquad \text{Tightness Condition:}$$

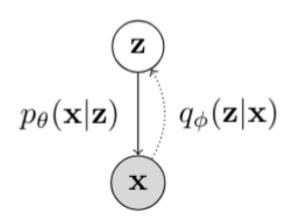
$$\geq \mathbb{E}_{q_{\phi}(\mathbf{z}|\mathbf{x})} \log \left[\frac{p_{\theta}(\mathbf{x}, \mathbf{z})}{q_{\phi}(\mathbf{z}|\mathbf{x})} \right]$$

$$= \log p_{\theta}(\mathbf{x}) - \text{KL}(q_{\phi}(\mathbf{z}|\mathbf{x})||p_{\theta}(\mathbf{z}|\mathbf{x})) = \mathcal{L}(\mathbf{x})$$

- ▶ Trading off the data log-likelihood and the KL divergence from the true posterior
- ▶ Hard to optimize the variational bound with respect to the q recognition network (high variance)
- ▶ Key idea of Kingma and Welling is to use reparameterization trick

Reparameterization

▶ Assume that the recognition distribution is Gaussian:



$$q_{\phi}(\mathbf{z}|\mathbf{x}) = \mathcal{N}(\mu(\mathbf{x}, \phi), \Sigma(\mathbf{x}, \phi))$$

 $p_{\theta}(\mathbf{x}|\mathbf{z})$ $q_{\phi}(\mathbf{z}|\mathbf{x})$ \blacktriangleright Alternatively, we can express this in term of auxiliary variable:

$$\mathbf{z}(\epsilon, \mathbf{x}, \phi) = \Sigma(\mathbf{x}, \phi)^{1/2} \epsilon + \mu(\mathbf{x}, \phi), \quad \epsilon \sim \mathcal{N}(0, I)$$

The recognition distribution can be expressed as a deterministic mapping

$$\mathbf{z}(\epsilon, \mathbf{x}, \phi)$$

 \blacktriangleright Distribution of ε does not depend on ϕ

Deterministic Encoder

Computing Gradients

► The gradients of the variational bound w.r.t the recognition (similar w.r.t the generative) parameters:

$$\nabla_{\phi} \mathcal{L}(\mathbf{x}) = \nabla_{\phi} \mathbb{E}_{\mathbf{z} \sim q_{\phi}(\mathbf{z}|\mathbf{x})} \left[\log \frac{p_{\theta}(\mathbf{x}, \mathbf{z})}{q_{\phi}(\mathbf{z}|\mathbf{x})} \right]$$

$$= \nabla_{\phi} \mathbb{E}_{\epsilon \sim \mathcal{N}(0, I)} \left[\log \frac{p_{\theta}(\mathbf{x}, \mathbf{z}(\epsilon, \mathbf{x}, \phi))}{q_{\phi}(\mathbf{z}(\epsilon, \mathbf{x}, \phi)|\mathbf{x})} \right]$$

$$= \mathbb{E}_{\epsilon \sim \mathcal{N}(0, I)} \left[\nabla_{\phi} \log \frac{p_{\theta}(\mathbf{x}, \mathbf{z}(\epsilon, \mathbf{x}, \phi))}{q_{\phi}(\mathbf{z}(\epsilon, \mathbf{x}, \phi)|\mathbf{x})} \right]$$

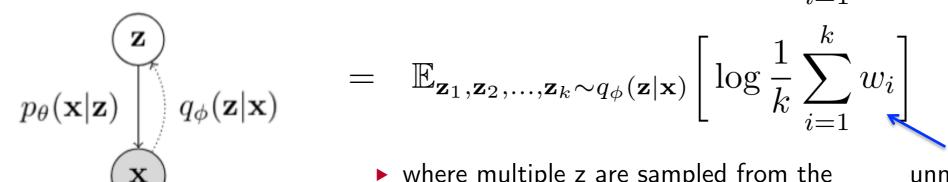
Gradients can be computed by backprop

The mapping ${\bf z}$ is a deterministic neural net for fixed ϵ

Importance Weighted Autoencoder

► Improve VAE by using the following k-sample importance weighting of the log-likelihood:

$$\mathcal{L}_k(\mathbf{x}) = \mathbb{E}_{\mathbf{z}_1, \mathbf{z}_2, \dots, \mathbf{z}_k \sim q_{\phi}(\mathbf{z}|\mathbf{x})} \left[\log \frac{1}{k} \sum_{i=1}^{\kappa} \frac{p_{\theta}(\mathbf{x}, \mathbf{z}_i)}{q_{\phi}(\mathbf{z}_i|\mathbf{x})} \right]$$



where multiple z are sampled from the recognition network.

unnormalized importance weights

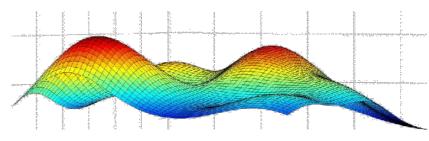
► Can improve the tightness of the bound.

Talk Roadmap

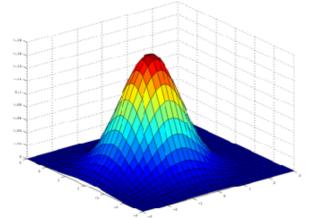
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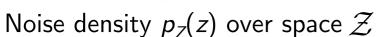
Generative Adversarial Networks (GAN)

- ▶ Implicit generative model for an unknown target density p(x)
- ► Converts sample from a known noise density $p_z(z)$ to the target p(x)



Unknown target density p(x) of data over domain \mathcal{X} , e.g. $\mathbb{R}^{32\times32}$







Distribution of generated samples should follow target density p(x)

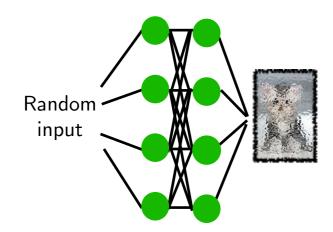
Goodfellow et al, 2014

GAN Formulation

► GAN consists of two components

Generator

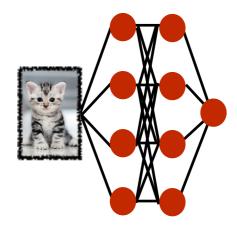
$$G: \mathcal{Z} \to \mathcal{X}$$



Goal: Produce samples indistinguishable from true data

Discriminator

$$D: \mathcal{X} \to \mathbb{R}$$



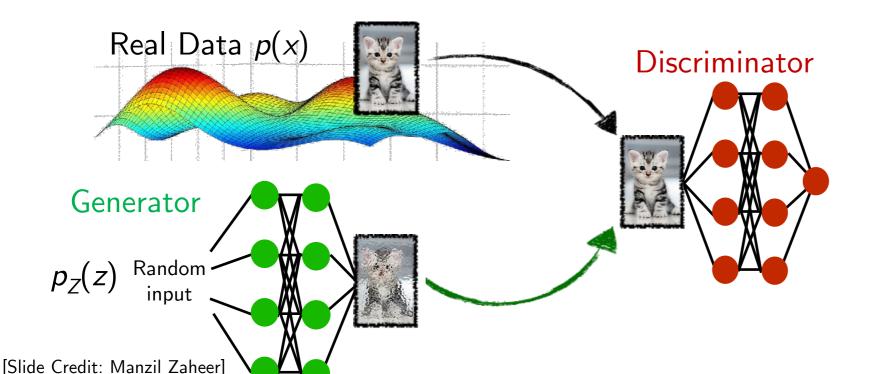
Goal: Distinguish true and generated data apart

Goodfellow et al, 2014

GAN Formulation: Discriminator

▶ Discriminator's objective: Tell real and generated data apart like a classifier

$$\max_{D} \mathbb{E}_{x \sim p} \left[\log D(x) \right] + \mathbb{E}_{z \sim p_{Z}} \left[\log \left(1 - D(G(z)) \right) \right]$$



D outputs:

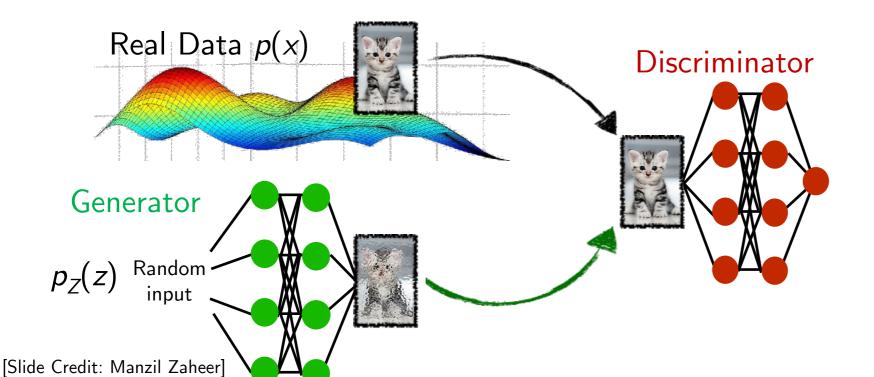
$$D(x) = 1$$
 real

$$D(x) = 0$$
 generated

GAN Formulation: Generator

► Generator's objective: Fool the best discriminator

$$\min_{G} \max_{D} \mathbb{E}_{x \sim p} \left[\log D(x) \right] + \mathbb{E}_{z \sim p_{Z}} \left[\log \left(1 - D(G(z)) \right) \right]$$



D outputs:

$$D(x) = 1$$
 real

$$D(x) = 0$$
 generated

GAN Formulation: Optimization

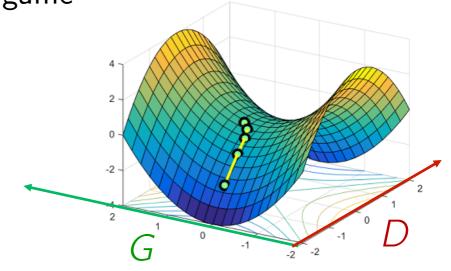
▶ Overall GAN optimization

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

► The generator-discriminator are iteratively updated using SGD to find "equilibrium" of a "min-max objective" like a game

$$G \leftarrow G - \eta_G \nabla_G V(G, D)$$

$$D \leftarrow D - \eta_D \nabla_D V(G, D)$$



[Slide Credit: Manzil Zaheer]

Wasserstein GAN

▶ WGAN optimization

$$\min_{G} \max_{D} W(G, D) = \mathbb{E}_{x \sim p} [D(x)] - \mathbb{E}_{z \sim p_{Z}} [D(G(z))]$$

- ▶ Difference in expected output on real vs. generated images
 - ► Generator attempts to drive objective ≈ 0
- ► More stable optimization

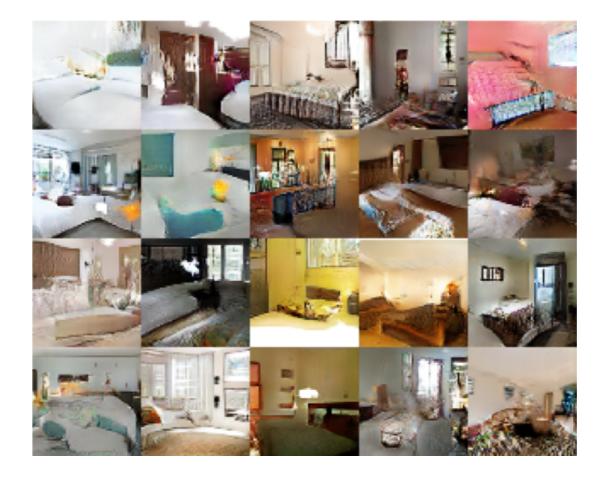
Compare to training DBMs
$$\frac{\partial \log P_{\theta}(\mathbf{v})}{\partial W^1} = \mathbb{E}_{P_{data}}[\mathbf{vh^1}^{\top}] - \mathbb{E}_{P_{\theta}}[\mathbf{vh^1}^{\top}]$$

D outputs:

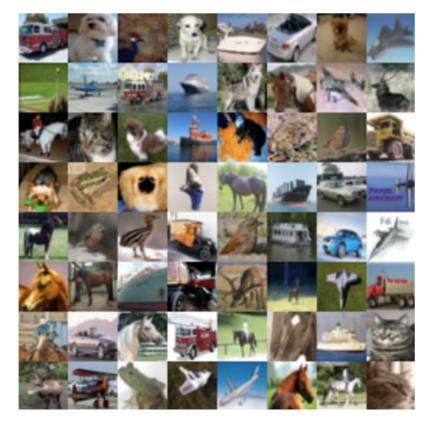
$$D(x) = 1$$
 real

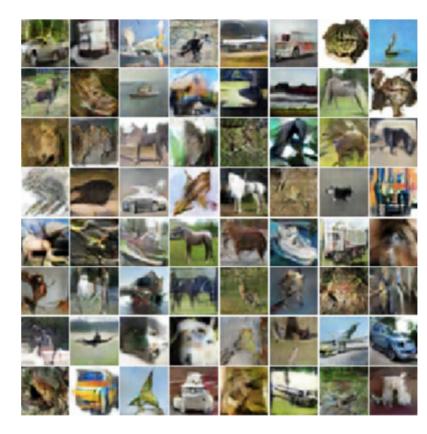
$$D(x) = 0$$
 generated

LSUN Bedroom: Samples



CIFAR Dataset





Training Samples

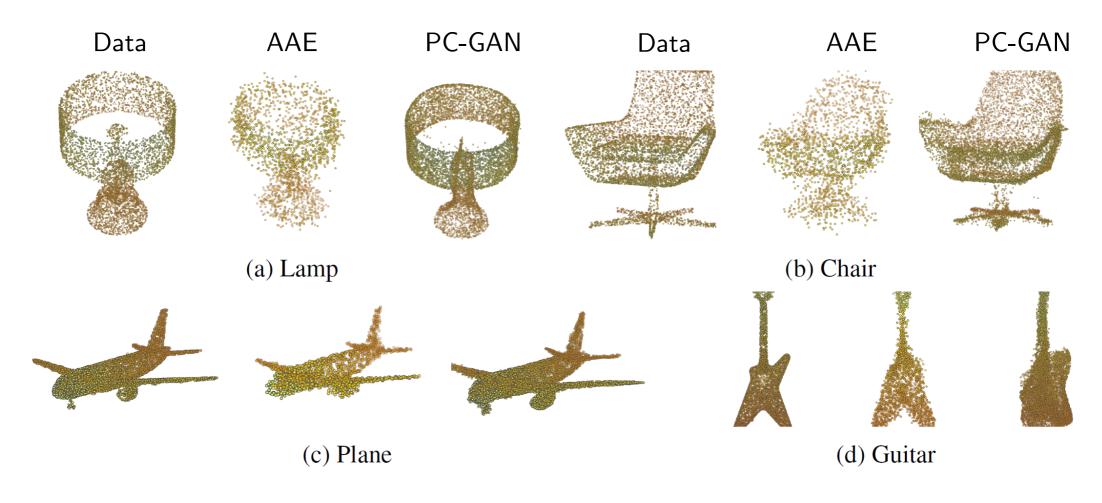
ImageNet: Cherry-Picked Samples



Open Question: How can we quantitatively evaluate these models!

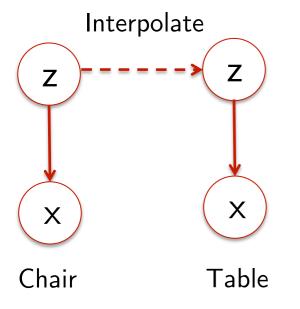
Slide Credit: Ian Goodfellow

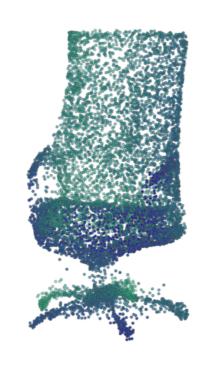
Modelling Point Cloud Data

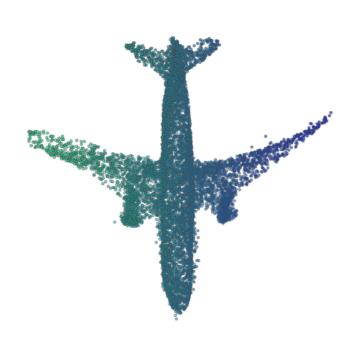


Zaheer et al. Point Cloud GAN 2018

Interpolation in Latent Space

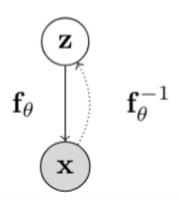






Normalizing Flows

► Directed Latent Variable Invertible models



► The mapping between x and z is deterministic and invertible:

$$\mathbf{x} = \mathbf{f}_{ heta}(\mathbf{z})$$
 $\mathbf{z} = \mathbf{f}_{ heta}^{-1}(\mathbf{x})$

► Use change-of-variables to relate densities between z and x

$$p_X(\mathbf{x}; \theta) = p_Z(\mathbf{z}) \left| \det \frac{\partial \mathbf{f}_{\theta}^{-1}(\mathbf{x})}{\partial X} \right|_{X=\mathbf{x}}$$

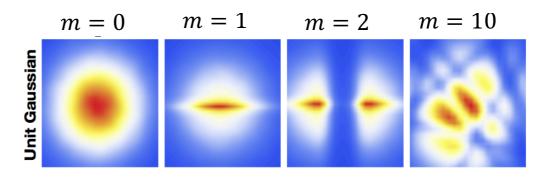
Normalizing Flows

▶ Invertible transformations can be composed:

$$\mathbf{x} = \mathbf{f}_{\theta}^{M} \circ \cdots \circ \mathbf{f}_{\theta}^{1}(\mathbf{z}^{0}); \quad p_{X}(\mathbf{x}; \theta) = p_{Z^{0}}(\mathbf{z}^{0}) \prod_{m=1}^{M} \left| \det \frac{\partial (\mathbf{f}_{\theta}^{m})^{-1}}{\partial Z^{m}} \right|_{Z^{m} = \mathbf{z}^{m}}$$

▶ Planar Flows

$$f(\mathbf{z}) = \mathbf{z} + \mathbf{u}g(\mathbf{w}^{\top}\mathbf{z} + b)$$



Rezendre and Mohamed, 2016

Normalizing Flows

► Maximum log-likelihood objective

$$\max_{\theta} \log p_X(\mathcal{D}; \theta) = \sum_{\mathbf{x} \in \mathcal{D}} \left(\log p_Z(\mathbf{z}) - \log \left| \det \frac{\partial (\mathbf{f}_{\theta})^{-1}}{\partial X} \right|_{X = \mathbf{x}} \right)$$

- ► Exact log-likelihood evaluation via inverse transformations
- ► Sampling from the model

$$\mathbf{z} \sim p_Z(\mathbf{z}), \quad \mathbf{x} = \mathbf{f}_{\theta}(\mathbf{z})$$

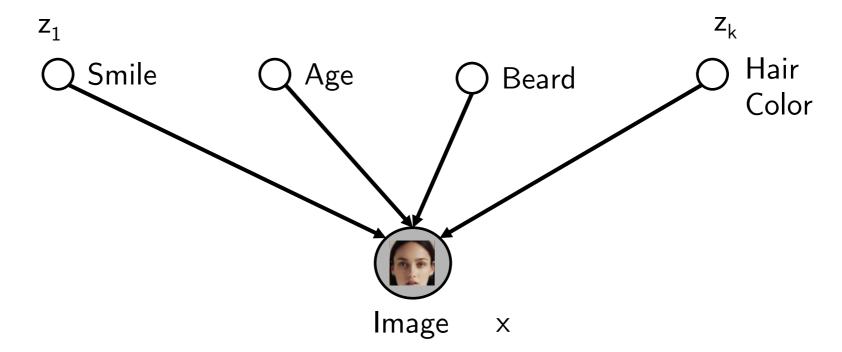
▶ Inference over the latent representations:

$$\mathbf{z} = \mathbf{f}_{\theta}^{-1}(\mathbf{x})$$

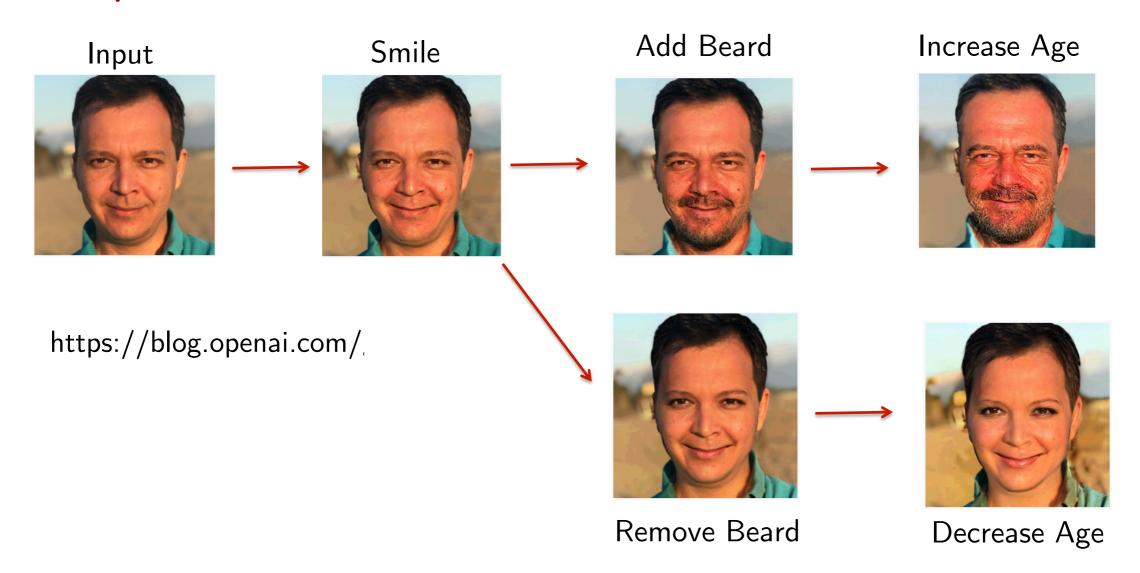
Example: GLOW

► Generative Flow with Invertible 1x1 Convolutions https://blog.openai.com/glow/

Latent factors of variation



Example: GLOW



Thank you