Deep Generative Models

Ehsan Abbasnejad





Outline

- Generative models
- Why using Deep Generative models?
 - Generative vs. Discriminative models
- Existing Methods:
 - Autoregressive Methods
 - Latent Variable Models
 - Variational Autoencoders (VAEs)
 - Generative Adversarial Networks (GANs)
- Problems with existing GANs and our approaches
 - 3D Hand pose Estimation
 - Other divergences (Dudley GANs)
 - Uncertainty in Generation (Uncertainty-aware GAN)
 - Density Estimator Adversarial Network
 - Imitation Learning
 - Causality

Generative vs. Discriminative

Generative models leaps(x, y)
 Placing a joint distribution over all dimensions of the data

 $p_{ heta}(y|\mathbf{x})$

• Discriminative models learn

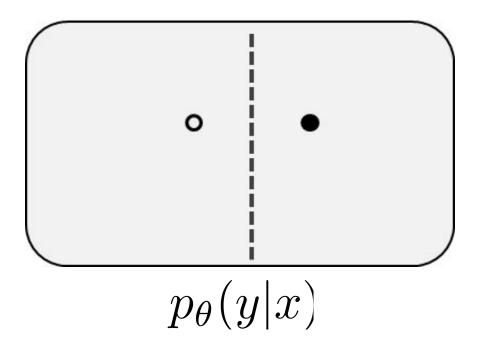
Remember:
$$\begin{array}{l} \min_{\theta} \ \mathbb{E}_{\mathbf{x},y}[\ell(h(\mathbf{x};\theta),y)] = \int \ell(h(\mathbf{x};\theta),y) dp(\mathbf{x},y) \\ \approx \frac{1}{n} \sum_{i=1}^{n} \ell(h(\mathbf{x}_{i};\theta),y_{i}) \quad (\mathbf{x}_{i},y_{i}) \sim p(\mathbf{x},y) \end{array}$$

$$p(\mathbf{x},y) = p(y|\mathbf{x})p(\mathbf{x})$$

and

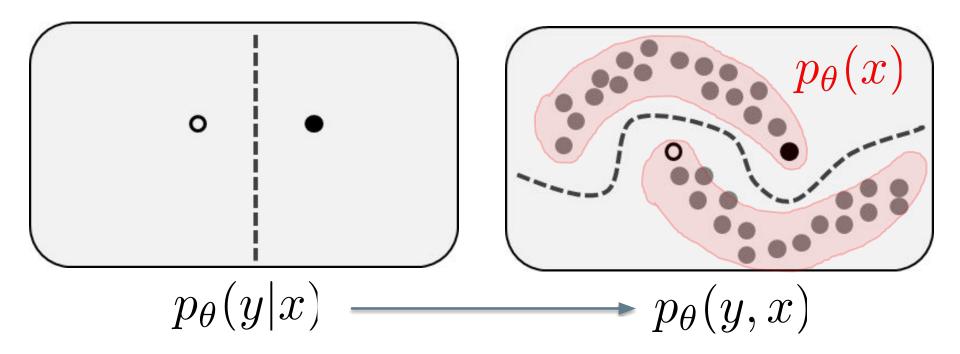
Generative models for

classification



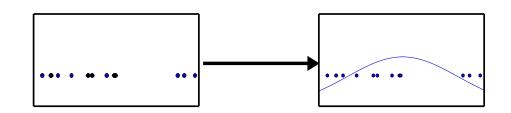
Generative models for

classification



Generative modeling

- Generative models allows to sample from some data distribution and learn a model that represents that distribution.
- Density estimation:
 - Probability for a sample (conditional or marginal)
 - Compare probability of examples
 - Dimensionality reduction and (latent) representation learning
 - Generate samples



Learning to generate

Images



redshank

ant

monastery



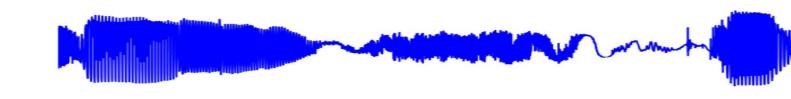
volcano

Anh et al. 2016





Speech



van der Oord et al. 2016

Learning to generate

Images

Speech

Handwriting

Stack more longers stuck more layers stack more layers stack more layers Stack more layers

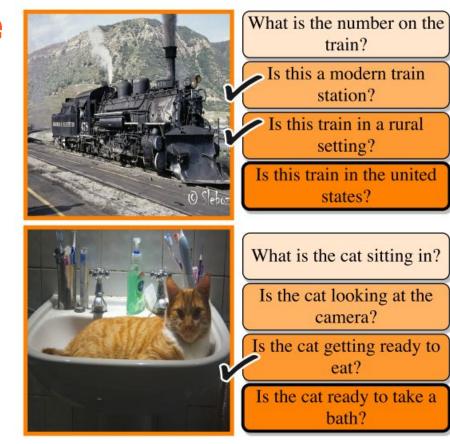
Graves 2013

Learning to generate

Images Speech

Handwriting

Language



Jain et al. 2017

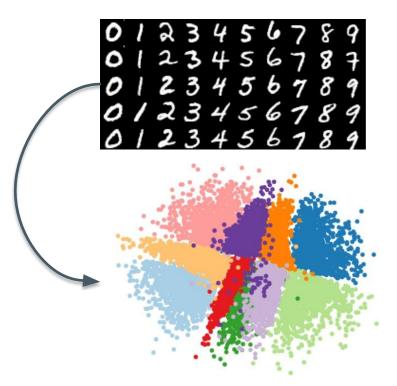


Images Speech

Handwriting

Language

Representation



Learning to generate

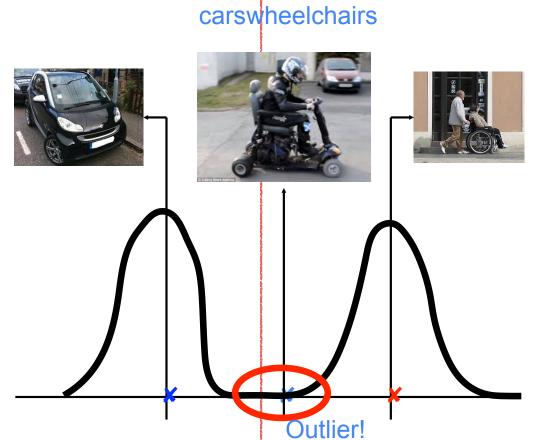
Images Speech

Handwriting

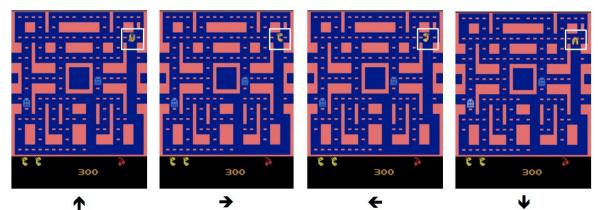
Language

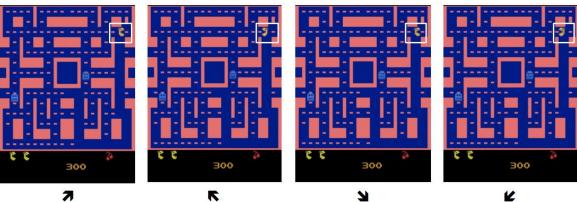
Representation

Outlier Detection



Simulation, planning, reasoning





Oh et al. 2015

Generation for Simulation

Supports Reinforcement Learning for Robotics: Make simulations sufficiently realistic that learned policies can readily transfer to real-world application



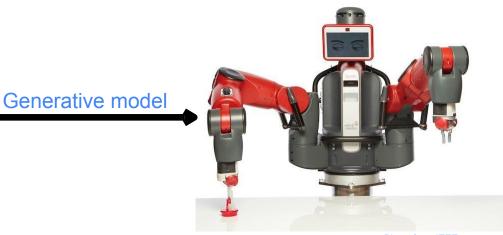


Photo from IEEE Spectrum

idea: learn to understand data through generation

Why generative models?

Many tasks requirestructured output for complex data

⁻ Eg. Machine translation

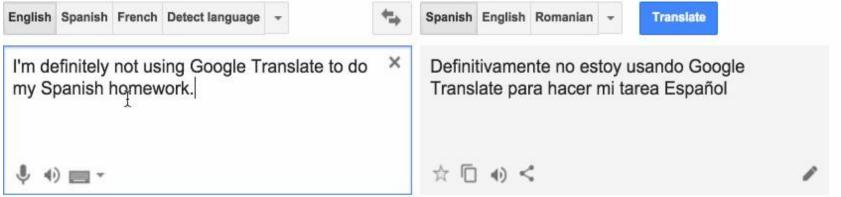


image credit: Adam Geitgey blog (2016) Machine Learning is Fun.

Generative Methods:

Autoregressive models

• Deep NADE, PixelRNN, PixelCNN, WaveNet, Video Pixel Network, etc.

Latent variable models

- Variational Auto encoders
- Generative Adversarial Networks

... and Beyond

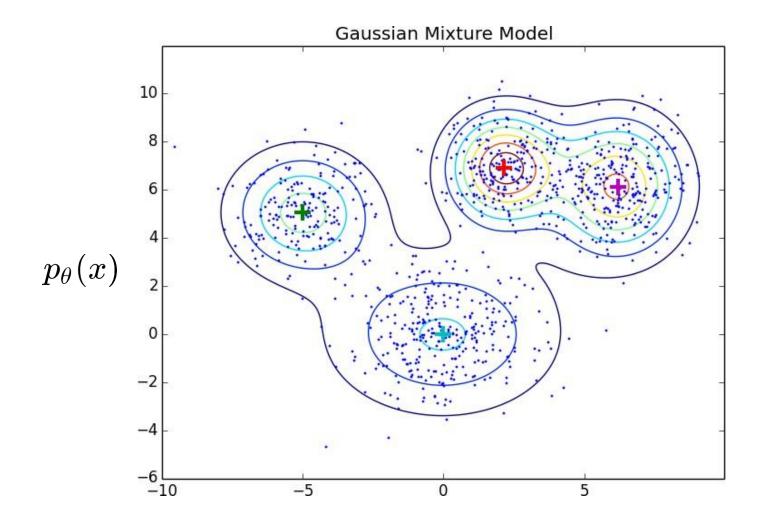


Discriminative model: given *n* examples $(x^{(i)}, y^{(i)})$ learn $h: X \to Y$

Generative model: given *n* examples $x^{(i)}$, recover p(x)

Maximum-likelihood objective: $\prod_{i} p_{\theta}(x) = \sum_{i} \log p_{\theta}(x)$ Generation: Sampling from $p_{\theta}(x)$

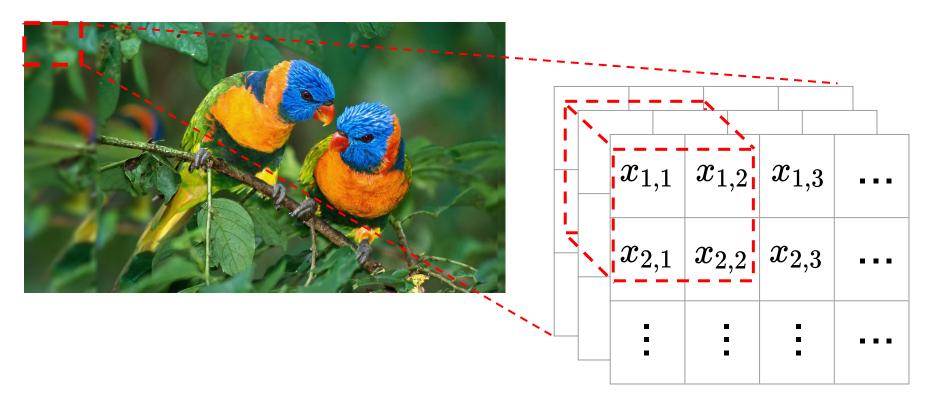
Attempt 1: learn $p_{\theta}(x)$ directly



Attempt 1: learn $p_{ heta}(x)$ directly Problem: We need to enforce that $\int\limits_{x} p_{ heta}(x) dx = 1$

For most models (i.e. neural networks) this integral is intractable.

Why Images are difficult?



Autoregressive Models

Factorize dimension-wise:

 $p(x) = p(x_1)p(x_2|x_1)\dots p(x_n|x_1,\dots,x_{n-1})$

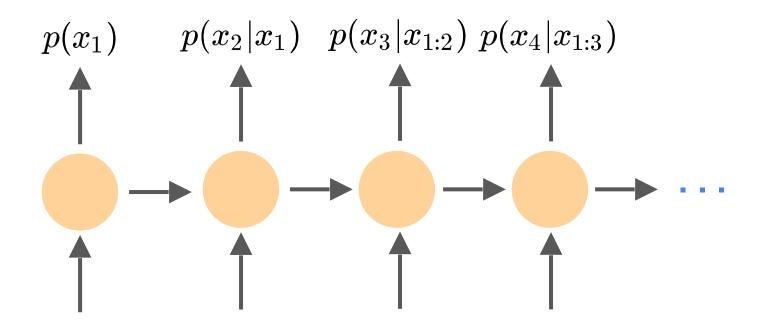
Build a "next-step prediction" model $p(x_n | x_1, \ldots, x_{n-1})$

If x is **discrete**, network outputs a probability for each possible value

If x is **continuous**, network outputs parameters of a simple distribution (e.g. Gaussian mean and variance)... *or just discretize!*

Generation: sample one step at a time, conditioned on all previous steps

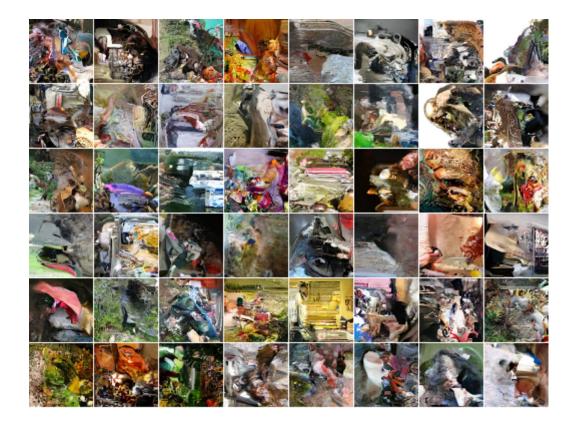
RNNs for Autoregressive Modeling



PixelRNN

Autoregressive RNN over pixels in an image

Models pixels as discrete-valued (256-way softmax at each step)

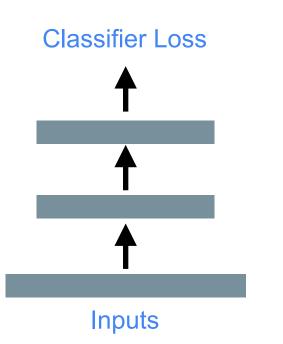


van der Oord et al. 2016

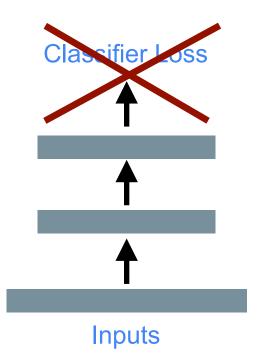
Autoregressive models

- Autoregressive models are powerful density estimators, but:
 - Sequential generation can be slow
 - Doesn't closely reflect the "true" generating process
 - Tends to emphasize details over global data
 - Not very good for learning representations



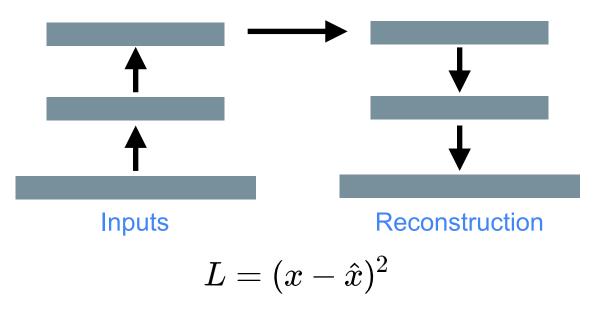




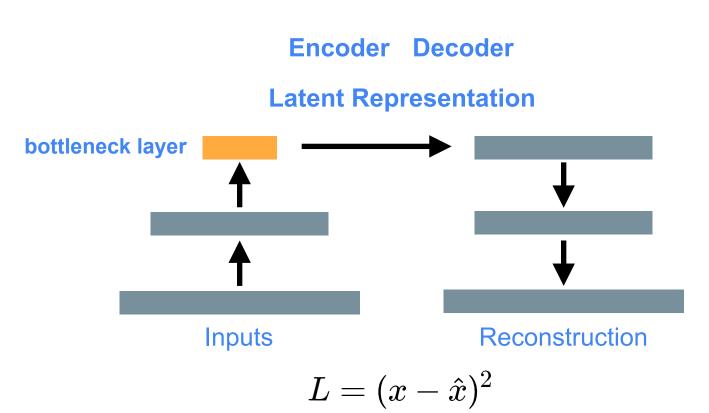














Reconstruction loss forces hidden layer to represent information about the input

Bottleneck hidden layer forces network to learn a compressed latent representation

Latent Variable Models: compression as implicit generative modeling

Variational Autoencoders (VAEs)

Generative extension of autoencoders which allow sampling and estimating probabilities

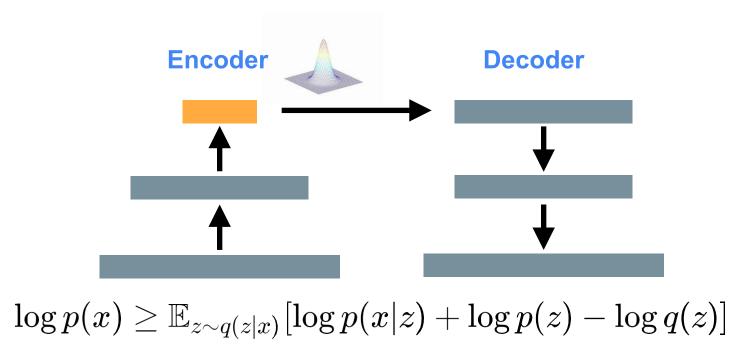
"Latent variables" with fixed prior distribution p(z)

Probabilistic encoder and decoder: q(z|x), p(x|z)

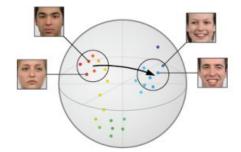
Trained to maximize a lower bound on log-probability:

$$\log p(x) \geq \mathbb{E}_{z \sim q(z|x)}[\log p(x|z) + \log p(z) - \log q(z)]$$

Variational Autoencoders



Interpolation in the Latent Space

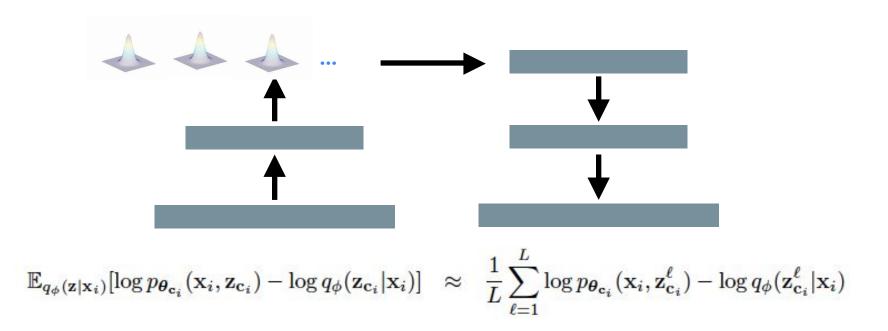




Tom White 2016

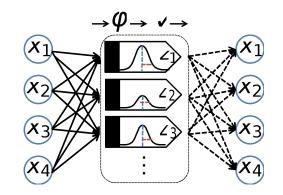
Infinite Variational Autoencoders

Encoder Decoder



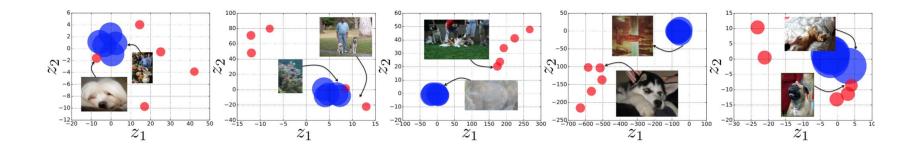
Infinite VAEs

- Infinite dimensional latent space
- Combine potentially infinite number of VAEs
- Infinite dimensional latent space
- Potential to capture all the diversity in the data



Mixture of Autoencoders

If we train our model with dogs, it is uncertain about other images Mapping the image to the hidden space



Problems with VAEs

• Encoder and decoder's output distributions are typically limited (diagonal-covariance Gaussian or similar)

• This prevents the model from capturing fine details and leads to blurry generations



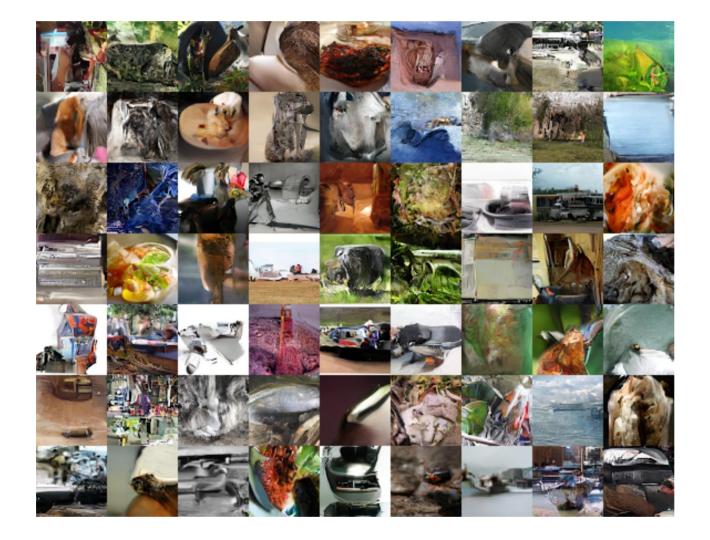
Andrej Karpathy 2015

Problems with VAEs

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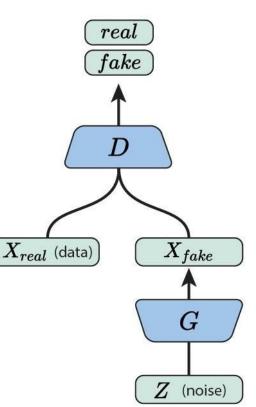
•Solution: use autoregressive networks in encoder and decoder



Generative Adversarial networks are a way to make a generative model by having two neural networks compete with each other

The **discriminator** tries to distinguish genuine data from forgeries created by the generator.

The **generator** turns random noise into imitations of the data, in an attempt to fool the discriminator

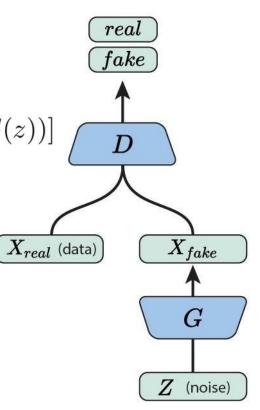


Problem setup:

$$\min_{G} \max_{D} \quad E_{x \sim p_X} \left[\log D(x) \right] + E_{z \sim p_Z} \left[\log(1 - D(G(z))) \right]$$

 P_X Data Distribution

 $P_G(z)$ Model Distribution



Algorithm 1 Minibatch stochastic gradient descent training of generative adversarial nets. The number of steps to apply to the discriminator, k, is a hyperparameter. We used k = 1, the least expensive option, in our experiments.

for number of training iterations do

for k steps do

- Sample minibatch of m noise samples $\{z^{(1)}, \ldots, z^{(m)}\}$ from noise prior $p_g(z)$.
- Sample minibatch of m examples $\{x^{(1)}, \ldots, x^{(m)}\}$ from data generating distribution $p_{\text{data}}(x)$.
- Update the discriminator by ascending its stochastic gradient:

$$abla_{ heta_d} rac{1}{m} \sum_{i=1}^m \left[\log D\left(oldsymbol{x}^{(i)}
ight) + \log \left(1 - D\left(G\left(oldsymbol{z}^{(i)}
ight)
ight)
ight)
ight].$$

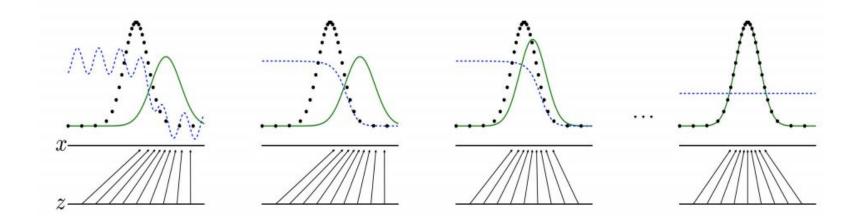
end for

- Sample minibatch of m noise samples $\{z^{(1)}, \ldots, z^{(m)}\}$ from noise prior $p_g(z)$.
- Update the generator by descending its stochastic gradient:

$$abla_{ heta_g} rac{1}{m} \sum_{i=1}^m \log\left(1 - D\left(G\left(oldsymbol{z}^{(i)}
ight)
ight)
ight).$$

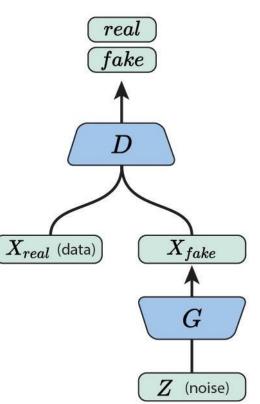
end for

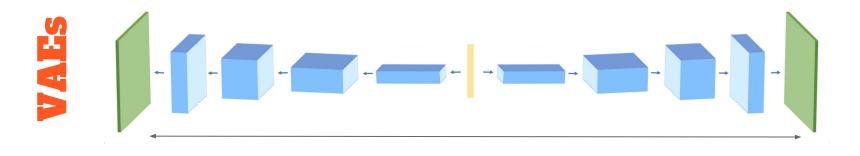
The gradient-based updates can use any standard gradient-based learning rule. We used momentum in our experiments.



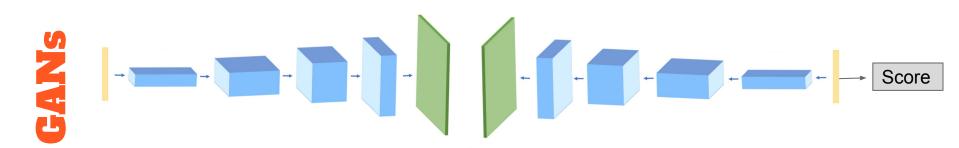
Why GANs?

- Sampling is straightforward
- Robust to overfitting since Generator never sees
 training data
- GANs are good at capturing the modes
- No need for Markov Chain
- No variational bound
- Produce better samples





S



VAES

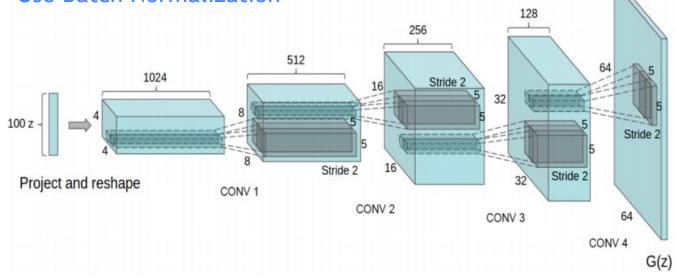
SD

GANS

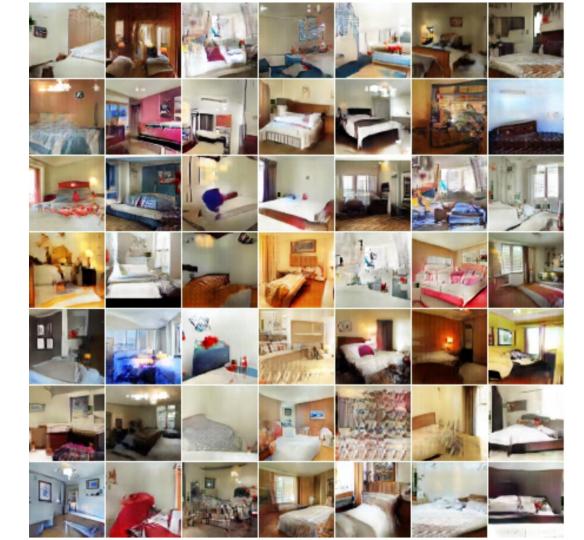
- VAEs maximize a lower bound on the likelihood of the data
- GANs maximize a "learned score" for the generated samples
- VAEs minimize the KL-divergence between the generated and real data
- GANs learn the loss based on the divergence between real/fake examples (will discuss)
 - VAEs generate data conditioned on the input
 - GANs' generator never sees real data
 - VAEs are trained as a single function (neural network)
 - GANs are trained as two individual network with their own loss
 - (Both follow a symmetric design)

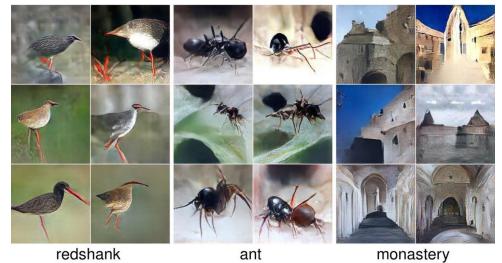
DCGAN

- Convolution for GANs
- Use Batch Normalization



3





redshank

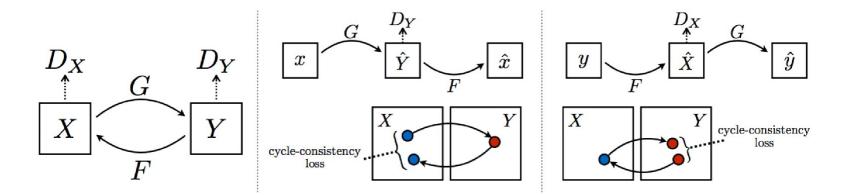
monastery



volcano

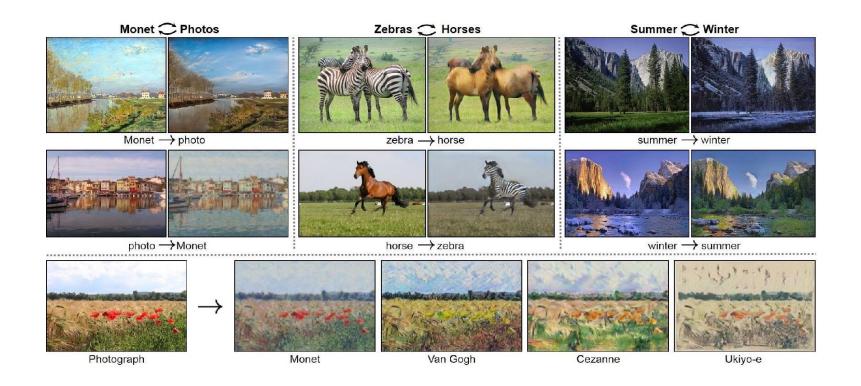
cycleGAN: Adversarial training of domain transformations

- CycleGAN learns transformations across domains with unpaired data.
- Combines GAN loss with "cycle-consistency loss": L1 reconstruction.

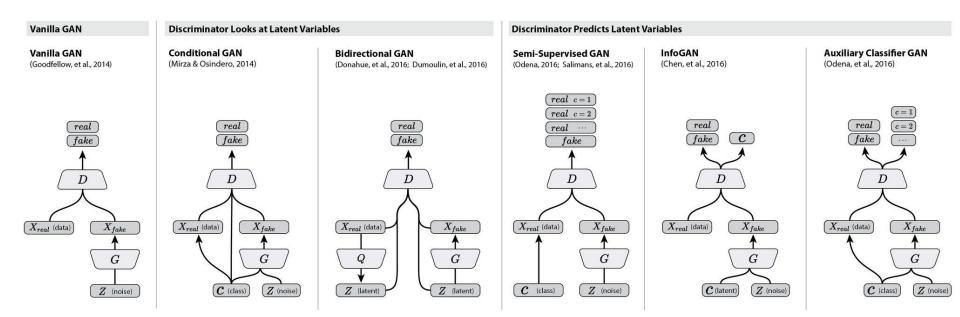


Zhu et al 2017.

CycleGAN for unpaired data

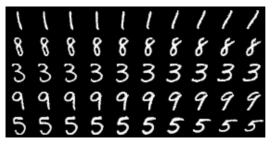


Various Architectures



Chris Olah, 2016

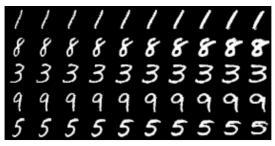
Representation learning



(c) Varying c_2 from -2 to 2 on InfoGAN (Rotation)

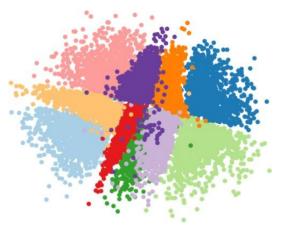


(a) Varying c_1 on InfoGAN (Digit type)



(d) Varying c_3 from -2 to 2 on InfoGAN (Width)

Chen et al. 2016



Sønderby et al. 2016

High dimensional faces using GANs

• Samples of 1024 * 1024





Fake videos







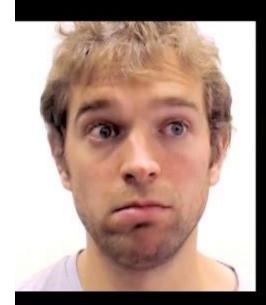
Fake videos







Fake videos









Text to Image





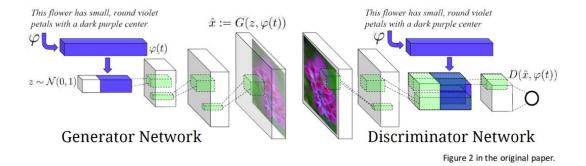
- a red and white bird with a small beak
- a yellow and black bird with long beak



a small yellow and black bird with red beak



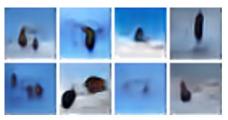
a small bird with blue crown, back and white belly



Generating Implausible Scenes from Captions



A stop sign is flying in blue skies.



A herd of elephants flying in the blue skies.



A toilet seat sits open in the grass field.



A person skiing on sand clad vast desert.

Mansimov et al. 2015

GANs for art: GANGogh

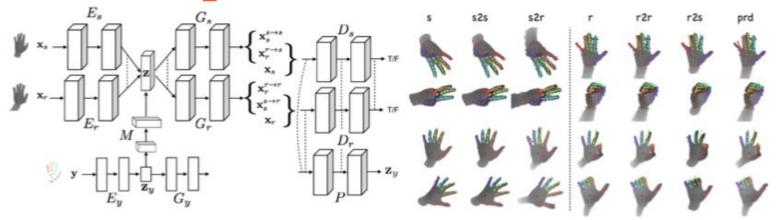


GANs for Games: Fully computer Generated Game



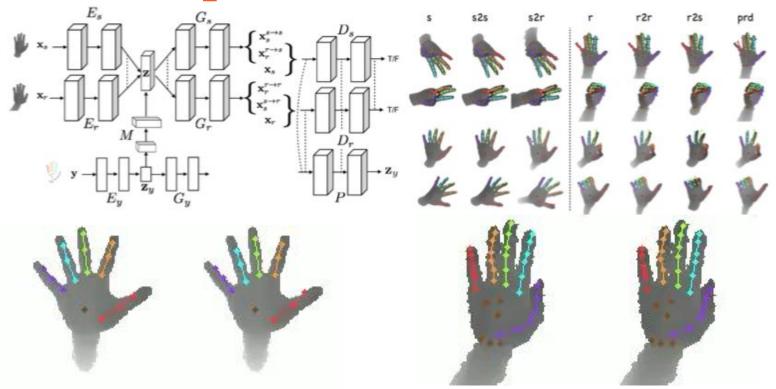
We have many orders of magnitude more data than labels; **unsupervised learning is important**.

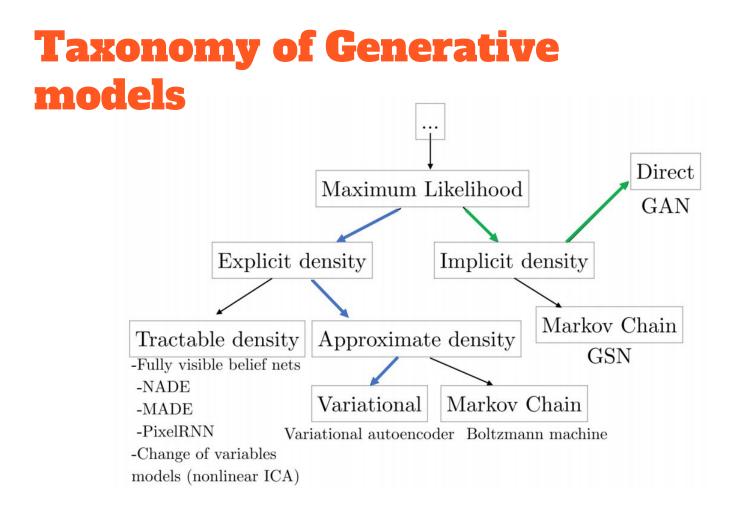
3D Hand pose estimation



- VAEs and GANs can be combined to learn a better latent space
- Hand pose from the depth images
- Combination of synthetic and real depth images
- From unpaired images

3D Hand pose estimation

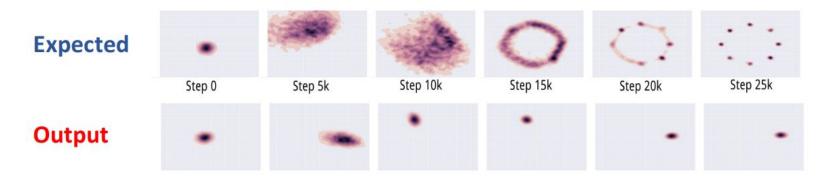




Problems with GANs

- non-convergence:
 - it might not converge to the Nash Equilibrium (e.g. minmax xy)
- Mode collapse





Problems with GANs

- In Vanilla GAN:
 - The divergence measure used is not always continuous
 - The discriminator may not provide sufficient gradients
 - For the optimal discriminator, the gradient is zero for generator
 - Generator collapses too many values to the same sample (modecollapse)

Divergences in GANs

Remember:

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

Then,

$$C(G) = \max_{D} V(G, D)$$

$$C(G) = -\log(4) + 2 \cdot JSD\left(p_{\text{data}} \| p_g\right)$$

In practice, however,

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

Divergences in GANs

Discriminator measures the divergence between the two distributions

A general class of divergences

$$D_f(P \| Q) = \int_{\mathcal{X}} q(x) f\left(\frac{p(x)}{q(x)}\right) \, \mathrm{d}x,$$

which is the upper bound for

$$\sup_{T \in \mathcal{T}} \left(\mathbb{E}_{x \sim P} \left[T(x) \right] - \mathbb{E}_{x \sim Q} \left[f^*(T(x)) \right] \right)$$

and

$$F(\theta,\omega) = \mathbb{E}_{x\sim P} \left[g_f(V_\omega(x)) \right] + \mathbb{E}_{x\sim Q_\theta} \left[-f^*(g_f(V_\omega(x))) \right]$$

Divergences in GANs

Name	Output activation g_f	dom_{f^*}	Conjugate $f^*(t)$	f'(1)
Total variation	$\frac{1}{2} \tanh(v)$	$-\frac{1}{2} \le t \le \frac{1}{2}$	t	0
Kullback-Leibler (KL)	v^2	R	$\exp(t-1)$	1
Reverse KL	$-\exp(v)$	\mathbb{R}_{-}	$-1 - \log(-t)$	-1
Pearson χ^2	v	R	$\frac{1}{4}t^2 + t$	0
Neyman χ^2	$1 - \exp(v)$	t < 1	$\overline{2} - 2\sqrt{1-t}$	0
Squared Hellinger	$1 - \exp(v)$	t < 1	$\frac{t}{1-t}$	0
Jeffrey	v	\mathbb{R}	$\hat{W}(e^{1-t}) + rac{1}{W(e^{1-t})} + t - 2$	0
Jensen-Shannon	$\log(2) - \log(1 + \exp(-v))$	$t < \log(2)$	$-\log(2-\exp(t))$	0
Jensen-Shannon-weighted	$-\pi\log\pi - \log(1 + \exp(-v))$	$t < -\pi \log \pi$	$(1-\pi)\lograc{1-\pi}{1-\pi e^{t/\pi}}$	0
GAN	$-\log(1+\exp(-v))$	R_	$-\log(1-\exp(t))$	$-\log(2)$
α -div. ($\alpha < 1, \alpha \neq 0$)	$rac{1}{1-lpha} - \log(1 + \exp(-v))$	$t < \frac{1}{1-\alpha}$	$rac{1}{lpha}(t(lpha-1)+1)^{rac{lpha}{lpha-1}}-rac{1}{lpha}$	0
α -div. ($\alpha > 1$)	v	\mathbb{R}	$rac{1}{lpha}(t(lpha-1)+1)^{rac{lpha}{lpha-1}}-rac{1}{lpha}$	0

Divergences in GANs

To solve vanishing gradient we use other divergences:

We use Integral Probability Measure (IPM):

$$ho(p,q_{m{ heta}}) \hspace{0.2cm} = \hspace{0.2cm} \sup_{f_{f{w}} \in \mathcal{F}} \left| \int_{\mathcal{X}} f_{f{w}} dp - \int_{\mathcal{X}} f_{f{w}} dq_{m{ heta}}
ight|$$

- Where f is the critic function (a deep neural net)
- Function f is chosen from a class of functions F
- Distribution of real data p
- Distribution of fake data q (it is learnt)

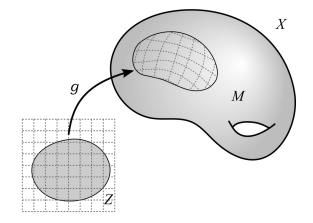
Dudley GAN

• We propose to use $||f_w||_{BL} \leq 1$ where

$$\|f_{\mathbf{w}}\|_{BL} = \|f_{\mathbf{w}}\|_{\infty} + \|f_{\mathbf{w}}\|_{L}$$

$$\begin{split} \|f\|_{L} &:= \sup \left\{ \frac{|f(\mathbf{x}_{1}) - f(\mathbf{x}_{2})|}{|\mathbf{x}_{1} - \mathbf{x}_{2}|} : \mathbf{x}_{1} \neq \mathbf{x}_{2} \forall \mathbf{x}_{1}, \mathbf{x}_{2} \in \mathcal{X} \right\} \\ \|f_{\mathbf{w}}\|_{\infty} &= \sup \left\{ |f_{\mathbf{w}}(\mathbf{x})| : \mathbf{x} \in \mathcal{X} \right\} \end{split}$$

- Bounded: Limits the critic's values
- Lipschitz: Limits the rate of change in the critic's compared to the change in the input
 - How to define Lipschitz neural networks?

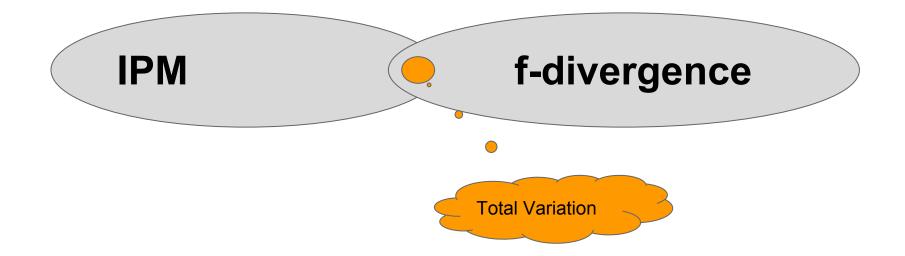


Lipschitz Neural Nets

- We can mathematically prove certain operations are Lipschitz:
 - Convolutional operations with normalized weights
 - Linear operations with normalized weights
 - Certain activation functions: sigmoid, relu, linear, tanh.

• We can then regularize the function to remain bounded

f-divergence vs IPM



What can we Do?

Generate Random real looking samples



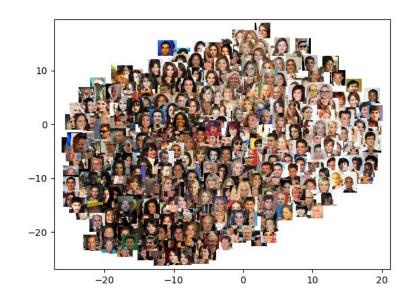






What can we Do?

Analyze latent space



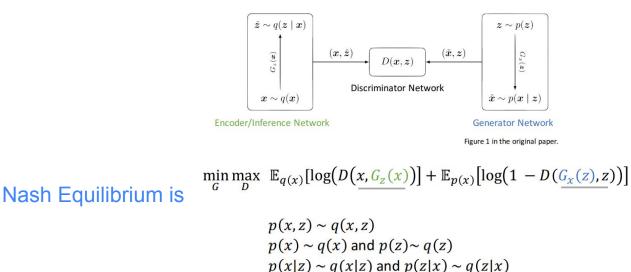
Adversarially Learned Inference

- Learn inference network
- Consider the following joint distribution

q(x,z) = q(x) q(z|x) encoder distribution p(x,z) = p(z) p(x|z) generator distribution

Adversarially Learned Inference

- Learn inference network
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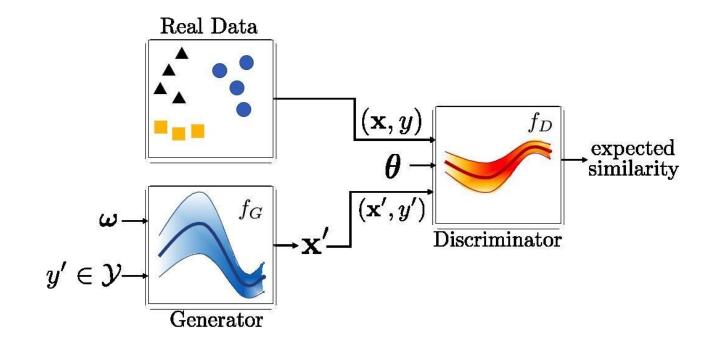


Uncertainty-aware GAN

- GANs are generated from a function evaluation
- We don't know if the sample generated
 - Is mapped to a good quality sample
 - Is from the dense region or not

• Let's treat generator and discriminator as "random functions"

Uncertainty-aware GAN



Uncertainty-aware GAN

• We perform a Monte Carlo estimate to the expected sample/score

• Training is more stable, due to averaging

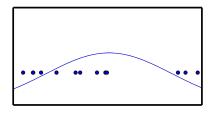
• We can compute the uncertainty in the discriminator score



- Generative models
- Why using Deep Generative models?
 - Generative vs. Discriminative models
- Existing Methods:
 - Autoregressive Methods
 - Latent Variable Models
 - Variational Autoencoders (VAEs)
 - Generative Adversarial Networks (GANs)
- Problems with existing GANs and our approaches
 - 3D Hand pose Estimation
 - Other divergences (Dudley GANs)
 - Uncertainty in Generation (Uncertainty-aware GAN)
 - Density Estimator Adversarial Network
 - Imitation Learning
 - Causality

Generative Adversarial Density estimator

- GANs are likelihood-free, we don't have a density function
- We can't evaluate probability of a sample in GANs



Let's consider a likelihood model

$$p(\mathbf{x}|\mathbf{w}) = \exp(\mathbf{w}^{\top}\phi(\mathbf{x}) - A(\mathbf{w})),$$

$$A(\mathbf{w}) = \log\left(\int \exp(\mathbf{w}^{\top}\phi(\mathbf{x}))d\mathbf{x}\right)$$

Generative Adversarial Density estimator

• We can find approximate this normalizer as

$$A_q(\mathbf{w}) = \sup_q \left\{ \int \mathbf{w}^\top \phi(\mathbf{x}) q(\mathbf{x}|\boldsymbol{\theta}) d\mathbf{x} + H_{\mathbf{x}}(q) \right\}$$

Introducing a generator, we have

$$A_q(\mathbf{w}) = \sup_q \left\{ \int \mathbf{w}^\top \phi(g_{\boldsymbol{\theta}_g}(\mathbf{z})) q(g_{\boldsymbol{\theta}_g}(\mathbf{z})) p_z(\mathbf{z}|\boldsymbol{\theta}_z) d\mathbf{z} + H_{\mathbf{z}}(q) \right\}$$

Generative Adversarial Density estimator $A_q(\mathbf{w}) = \sup_q \left\{ \int \mathbf{w}^\top \phi(g_{\theta_g}(\mathbf{z})) q(g_{\theta_g}(\mathbf{z})) p_z(\mathbf{z}|\boldsymbol{\theta}_z) d\mathbf{z} + H_{\mathbf{z}}(q) \right\} \frac{\text{Expectation of}}{\text{Generated samples}}$ $\int \mathbf{w}^{\top} \phi(\mathbf{x}) q(\mathbf{x}|\boldsymbol{\theta}) d\mathbf{x}$ Expectation of Real samples

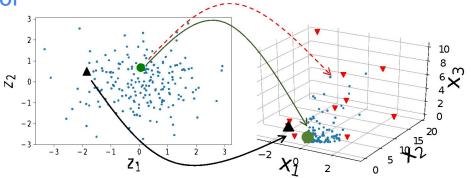
The expectation of the data and the generated samples should match in our density model (Moment matching property)

Generative Adversarial Density estimator

$$A_q(\mathbf{w}) = \sup_q \left\{ \int \mathbf{w}^\top \phi(g_{\theta_g}(\mathbf{z})) q(g_{\theta_g}(\mathbf{z})) p_z(\mathbf{z}|\boldsymbol{\theta}_z) d\mathbf{z} - H_{\mathbf{z}}(q) \right\}$$

Entropy of

- the latent space (e.g. larger variance),
- the curvature of the generator



Applications

Visual dialog: a sequence of question-answers about an image



Q: is the train old? A: i think so Sample A: yes (0.03 ± 0.2) Q: is the train moving? A: no but it does have some steam coming Sample A: no (0.02 ± 0.1)



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Q: is this in color ?
A: yes
Sample A: yes (0.1 \pm 0.05)
Q: how old does the boy look?
A: he is not facing me, but maybe
Sample A: \frac{3}{2}(0.1 \pm 0.4)
```



Q: what vegetables are there? A: carrots, cauliflower, broccoli Sample A: carrots, carrots, and cucumbers (0.1 ± 0.01) Q: what color is the table ? A: dark brown Sample A: white (0.1 ± 0.02)

Imitation learning and Inverse Reinforcement Learning

• Reinforcement learning requires a "reward function"



- An expert drives a car and an autonomous car imitates
- Sampling trajectories to simulate the expert's behavior

Imitation learning and Inverse Reinforcement Learning





Rather than p(y|x) is the conditional distribution We consider the causal expression p(y|do(x))p(y|do(x)) represents the *intervention* expression

$$\begin{array}{c} E_3 \rightarrow f_3 \rightarrow X_3 \\ \vdots E_1 \rightarrow f_1 \rightarrow X_1 \\ \vdots E_2 \rightarrow f_2 \rightarrow X_2 \end{array} \begin{array}{c} E_5 \\ f_5 \rightarrow X_5 \\ \vdots E_4 \rightarrow f_4 \rightarrow X_4 \end{array} \begin{array}{c} E_i & \sim \mathcal{E} \\ X_1 & = f_1(E_1) \\ X_2 & = f_2(X_1, E_2) \\ X_3 & = f_3(X_1, E_3) \\ X_4 & = f_4(E_4) \\ X_5 & = f_5(X_3, X_4, E_5) \end{array}$$

Goudet et al. 2018

Conclusion

- Generative models explain the data, likelihood of samples
- There is a simpler hidden space where complex data may be generated from
- If we create something, we understand it
- Capturing the uncertainty in the model and data
- Deep generative models can be used for
 - Data generation (generate various samples of road)
 - Human imitation (use them instead of real drivers)
 - Environment simulation
 - Use of unlabeled data (rather than expensive, often unavailable real one)