Lecture 11: Generative Models

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Lecture 11 - 1 May 14, 2020

Administrative

- A3 is out. Due May 27.
- Milestone is due $May 18 \rightarrow May 20$
 - Read website page for milestone requirements.
 - Need to Finish data preprocessing and initial results by then.

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- Don't discuss exam yet since people might be taking make-ups.
- Anonymous midterm survey: Link will be posted on Piazza today

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Supervised Learning

Data: (x, y) x is data, y is label

Goal: Learn a *function* to map x -> y

Examples: Classification, regression, object detection, semantic segmentation, image captioning, etc.

Supervised Learning

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Classification

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Supervised Learning

Data: (x, y) x is data, y is label

Goal: Learn a *function* to map x -> y

Examples: Classification, regression, object detection, semantic segmentation, image captioning, etc.



DOG, DOG, CAT

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Object Detection

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Supervised Learning

Data: (x, y) x is data, y is label

Goal: Learn a *function* to map x -> y

Examples: Classification, regression, object detection, semantic segmentation, image captioning, etc.



TREE, SKY

Semantic Segmentation

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Supervised Learning

Data: (x, y) x is data, y is label

Goal: Learn a *function* to map x -> y

Examples: Classification, regression, object detection, semantic segmentation, image captioning, etc.



A cat sitting on a suitcase on the floor

Image captioning

Caption generated using <u>neuraltalk2</u> <u>Image</u> is <u>CC0 Public domain</u>.

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Unsupervised Learning

Data: x Just data, **no labels!**

Goal: Learn some underlying hidden *structure* of the data

Examples: Clustering, dimensionality reduction, feature learning, density estimation, etc.

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Unsupervised Learning

Data: x Just data, no labels!

Goal: Learn some underlying hidden *structure* of the data

Examples: Clustering, dimensionality reduction, density estimation, etc.



K-means clustering

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Unsupervised Learning

Data: x Just data, no labels!

Goal: Learn some underlying hidden *structure* of the data

Examples: Clustering, dimensionality reduction, density estimation, etc.



Principal Component Analysis (Dimensionality reduction)

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Unsupervised Learning

Data: x Just data, no labels!

Goal: Learn some underlying hidden *structure* of the data

Examples: Clustering, dimensionality reduction, density estimation, etc.



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1-d density estimation



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Supervised Learning

Data: (x, y) x is data, y is label

Goal: Learn a *function* to map x -> y

Examples: Classification, regression, object detection, semantic segmentation, image captioning, etc. **Unsupervised Learning**

Data: x Just data, no labels!

Goal: Learn some underlying hidden *structure* of the data

Examples: Clustering, dimensionality reduction, density estimation, etc.

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Generative Modeling

Given training data, generate new samples from same distribution



Objectives:

Learn p_{model}(x) that approximates p_{data}(x)
Sampling new x from p_{model}(x)

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Generative Modeling

Given training data, generate new samples from same distribution



Formulate as density estimation problems:

- Explicit density estimation: explicitly define and solve for p_{model}(x)
- Implicit density estimation: learn model that can sample from p_{model}(x) without explicitly defining it.

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Why Generative Models?



- Realistic samples for artwork, super-resolution, colorization, etc.
- Learn useful features for downstream tasks such as classification.
- Getting insights from high-dimensional data (physics, medical imaging, etc.)

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- Modeling physical world for simulation and planning (robotics and reinforcement learning applications)
- Many more ...

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- Glow

- Ffjord

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- Glow
- Ffjord

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PixelRNN and PixelCNN

(A very brief overview)

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Fully visible belief network (FVBN)

Explicit density model

Use chain rule to decompose likelihood of an image x into product of 1-d distributions:

$$p(x) = \prod_{i=1}^{n} p(x_i | x_1, \dots, x_{i-1})$$

Likelihood of image x Probability of i'th pixel value given all previous pixels

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Then maximize likelihood of training data

Fully visible belief network (FVBN)

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Explicit density model

Use chain rule to decompose likelihood of an image x into product of 1-d distributions:

$$p(x) = \prod_{i=1}^{n} p(x_i | x_1, \dots, x_{i-1})$$

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Likelihood of image x

Probability of i'th pixel value given all previous pixels

Complex distribution over pixel values => Express using a neural network!

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Then maximize likelihood of training data

Recurrent Neural Network



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Generate image pixels starting from corner

Dependency on previous pixels modeled using an RNN (LSTM)



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Generate image pixels starting from corner

Dependency on previous pixels modeled using an RNN (LSTM)



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Generate image pixels starting from corner

Dependency on previous pixels modeled using an RNN (LSTM)



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Generate image pixels starting from corner

Dependency on previous pixels modeled using an RNN (LSTM)

Drawback: sequential generation is slow in both training and inference!



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Still generate image pixels starting from corner

Dependency on previous pixels now modeled using a CNN over context region (masked convolution)



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Still generate image pixels starting from corner

Dependency on previous pixels now modeled using a CNN over context region (masked convolution) Training is faster than PixelRNN (can parallelize convolutions since context region values known from training images)

Generation is still slow: For a 32x32 image, we need to do forward passes of the network 1024 times for a single image

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Generation Samples



32x32 CIFAR-10



32x32 ImageNet

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PixelRNN and **PixelCNN**

Pros:

- Can explicitly compute likelihood p(x)
- Easy to optimize
- Good samples

Con:

- Sequential generation => slow

Improving PixelCNN performance

- Gated convolutional layers
- Short-cut connections
- Discretized logistic loss
- Multi-scale
- Training tricks
- Etc...

See

- Van der Oord et al. NIPS 2016
- Salimans et al. 2017 (PixelCNN++)

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Ffjord

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Variational Autoencoders (VAE)

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So far...

PixelRNN/CNNs define tractable density function, optimize likelihood of training data: $p_{\theta}(x) = \prod_{i=1}^{n} p_{\theta}(x_i | x_1, ..., x_{i-1})$

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So far...

PixelCNNs define tractable density function, optimize likelihood of training data: $p_{\theta}(x) = \prod_{i=1}^{n} p_{\theta}(x_i | x_1, ..., x_{i-1})$

Variational Autoencoders (VAEs) define intractable density function with latent **z**: $p_{\theta}(x) = \int p_{\theta}(z)p_{\theta}(x|z)dz$

Cannot optimize directly, derive and optimize lower bound on likelihood instead

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So far...

PixelCNNs define tractable density function, optimize likelihood of training data: $p_{\theta}(x) = \prod_{i=1}^{n} p_{\theta}(x_i | x_1, ..., x_{i-1})$

Variational Autoencoders (VAEs) define intractable density function with latent **z**: $p_{\theta}(x) = \int p_{\theta}(z) p_{\theta}(x|z) dz$

Cannot optimize directly, derive and optimize lower bound on likelihood instead

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Why latent z?

Some background first: Autoencoders

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





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Some background first: Autoencoders

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





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





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Reconstructed

input data

Reconstructed data



Encoder: 4-layer conv Decoder: 4-layer upconv

Input data



How to learn this feature

representation?

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Train such that features can be used to reconstruct original data



Doesn't use labels!



Reconstructed data

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

Features capture factors of variation in training data.

But we can't generate new images from an autoencoder because we don't know the space of z.

How do we make autoencoder a generative model?

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

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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 the distribution of unobserved (latent) representation **z**



Kingma and Welling, "Auto-Encoding Variational Bayes", ICLR 2014

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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 the distribution of unobserved (latent) representation **z**



Intuition (remember from autoencoders!):x is an image, z is latent factors used to generate x: attributes, orientation, etc.

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We want to estimate the true parameters θ^* of this generative model given training data x.



Kingma and Welling, "Auto-Encoding Variational Bayes", ICLR 2014

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We want to estimate the true parameters θ^* of this generative model given training data x.



How should we represent this model?

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We want to estimate the true parameters θ^* of this generative model given training data x.



How should we represent this model?

Choose prior p(z) to be simple, e.g. Gaussian. Reasonable for latent attributes, e.g. pose, how much smile.

Kingma and Welling, "Auto-Encoding Variational Bayes", ICLR 2014

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We want to estimate the true parameters θ^* of this generative model given training data x.

Sample from
true conditional \boldsymbol{x} $p_{\theta^*}(x \mid z^{(i)})$ Decoder
networkSample from
true prior
 $z^{(i)} \sim p_{\theta^*}(z)$ \boldsymbol{z}

How should we represent this model?

Choose prior p(z) to be simple, e.g. Gaussian. Reasonable for latent attributes, e.g. pose, how much smile.

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

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We want to estimate the true parameters θ^* of this generative model given training data x.

How to train the model?

xtrue conditional $p_{\theta^*}(x \mid z^{(i)})$ Sample from true prior z $z^{(i)} \sim p_{ heta^*}(z)$

Sample from

Decoder network

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We want to estimate the true parameters θ^* of this generative model given training data x.

How to train the model?

Learn model parameters to maximize likelihood of training data

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

Kingma and Welling, "Auto-Encoding Variational Bayes", ICLR 2014

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We want to estimate the true parameters θ^* of this generative model given training data x.

How to train the model?

Learn model parameters to maximize likelihood of training data

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

Q: What is the problem with this?

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We want to estimate the true parameters θ^* of this generative model given training data x.

How to train the model?

Learn model parameters to maximize likelihood of training data

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

Q: What is the problem with this?

Intractable!

Kingma and Welling, "Auto-Encoding Variational Bayes", ICLR 2014

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

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

Simple Gaussian prior

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

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Data likelihood: $p_{\theta}(x) = \int p_{\theta}(z) p_{\theta}(x|z) dz$ Intractable to compute p(x|z) for every z!

Kingma and Welling, "Auto-Encoding Variational Bayes", ICLR 2014

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

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

$$\log p(x) pprox \log rac{1}{k} \sum_{i=1}^k p(x|z^{(i)}),$$
 where $z^{(i)} \sim p(z)$

Monte Carlo estimation is too high variance

Kingma and Welling, "Auto-Encoding Variational Bayes", ICLR 2014

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

Posterior density: $p_{\theta}(z|x) = p_{\theta}(x|z)p_{\theta}(z)/p_{\theta}(x)$

Intractable data likelihood

Kingma and Welling, "Auto-Encoding Variational Bayes", ICLR 2014

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

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

Solution: In addition to modeling $p_{\theta}(x|z)$, learn $q_{\phi}(z|x)$ that approximates the true posterior $p_{\theta}(z|x)$.

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

Variational inference is to approximate the unknown posterior distribution from only the observed data x

Kingma and Welling, "Auto-Encoding Variational Bayes", ICLR 2014

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 $\log p_{\theta}(x^{(i)}) = \mathbf{E}_{z \sim q_{\phi}(z|x^{(i)})} \left[\log p_{\theta}(x^{(i)})\right] \quad (p_{\theta}(x^{(i)}) \text{ Does not depend on } z)$

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$$\log p_{\theta}(x^{(i)}) = \mathbf{E}_{z \sim q_{\phi}(z|x^{(i)})} \left[\log p_{\theta}(x^{(i)}) \right] \quad (p_{\theta}(x^{(i)}) \text{ Does not depend on } z)$$

Taking expectation wrt. z
(using encoder network) will
come in handy later

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$$\log p_{\theta}(x^{(i)}) = \mathbf{E}_{z \sim q_{\phi}(z|x^{(i)})} \left[\log p_{\theta}(x^{(i)})\right] \quad (p_{\theta}(x^{(i)}) \text{ Does not depend on } z)$$
$$= \mathbf{E}_{z} \left[\log \frac{p_{\theta}(x^{(i)} \mid z)p_{\theta}(z)}{p_{\theta}(z \mid x^{(i)})}\right] \quad (\text{Bayes' Rule})$$

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$$\log p_{\theta}(x^{(i)}) = \mathbf{E}_{z \sim q_{\phi}(z|x^{(i)})} \left[\log p_{\theta}(x^{(i)}) \right] \quad (p_{\theta}(x^{(i)}) \text{ Does not depend on } z)$$
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$$= \mathbf{E}_{z} \left[\log \frac{p_{\theta}(x^{(i)} \mid z)p_{\theta}(z)}{p_{\theta}(z \mid x^{(i)})} \frac{q_{\phi}(z \mid x^{(i)})}{q_{\phi}(z \mid x^{(i)})} \right] \quad (\text{Multiply by constant})$$

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$$\begin{split} \log p_{\theta}(x^{(i)}) &= \mathbf{E}_{z \sim q_{\phi}(z|x^{(i)})} \left[\log p_{\theta}(x^{(i)}) \right] \quad (p_{\theta}(x^{(i)}) \text{ Does not depend on } z) \\ &= \mathbf{E}_{z} \left[\log \frac{p_{\theta}(x^{(i)} \mid z)p_{\theta}(z)}{p_{\theta}(z \mid x^{(i)})} \right] \quad (\text{Bayes' Rule}) \\ &= \mathbf{E}_{z} \left[\log \frac{p_{\theta}(x^{(i)} \mid z)p_{\theta}(z)}{p_{\theta}(z \mid x^{(i)})} \frac{q_{\phi}(z \mid x^{(i)})}{q_{\phi}(z \mid x^{(i)})} \right] \quad (\text{Multiply by constant}) \\ &= \mathbf{E}_{z} \left[\log p_{\theta}(x^{(i)} \mid z) \right] - \mathbf{E}_{z} \left[\log \frac{q_{\phi}(z \mid x^{(i)})}{p_{\theta}(z)} \right] + \mathbf{E}_{z} \left[\log \frac{q_{\phi}(z \mid x^{(i)})}{p_{\theta}(z \mid x^{(i)})} \right] \quad (\text{Logarithms}) \end{split}$$

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$$\begin{split} \log p_{\theta}(x^{(i)}) &= \mathbf{E}_{z \sim q_{\phi}(z|x^{(i)})} \left[\log p_{\theta}(x^{(i)}) \right] \quad (p_{\theta}(x^{(i)}) \text{ Does not depend on } z) \\ &= \mathbf{E}_{z} \left[\log \frac{p_{\theta}(x^{(i)} \mid z) p_{\theta}(z)}{p_{\theta}(z \mid x^{(i)})} \right] \quad (\text{Bayes' Rule}) \\ &= \mathbf{E}_{z} \left[\log \frac{p_{\theta}(x^{(i)} \mid z) p_{\theta}(z)}{p_{\theta}(z \mid x^{(i)})} \frac{q_{\phi}(z \mid x^{(i)})}{q_{\phi}(z \mid x^{(i)})} \right] \quad (\text{Multiply by constant}) \\ &= \mathbf{E}_{z} \left[\log p_{\theta}(x^{(i)} \mid z) \right] - \mathbf{E}_{z} \left[\log \frac{q_{\phi}(z \mid x^{(i)})}{p_{\theta}(z)} \right] + \mathbf{E}_{z} \left[\log \frac{q_{\phi}(z \mid x^{(i)})}{p_{\theta}(z \mid x^{(i)})} \right] \quad (\text{Logarithms}) \\ &= \mathbf{E}_{z} \left[\log p_{\theta}(x^{(i)} \mid z) \right] - D_{KL}(q_{\phi}(z \mid x^{(i)}) \mid p_{\theta}(z)) + D_{KL}(q_{\phi}(z \mid x^{(i)}) \mid p_{\theta}(z \mid x^{(i)})) \right] \\ &\uparrow \\ \text{Decoder network gives } p_{\theta}(x|z), \text{ can} \\ \text{compute estimate of this term through} \\ \text{sampling (need some trick to} \\ \text{differentiate through sampling).} & \text{This KL term (between \\ \text{Gaussians for encoder and } z \\ \text{prior) has nice closed-form } \\ \text{solution!} \\ \text{Decoder network KL divergence always } >= 0. \end{split}$$

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$$\log p_{\theta}(x^{(i)}) = \mathbf{E}_{z \sim q_{\phi}(z|x^{(i)})} \left[\log p_{\theta}(x^{(i)})\right] \quad (p_{\theta}(x^{(i)}) \text{ Does not depend on } z)$$

$$= \mathbf{E}_{z} \left[\log \frac{p_{\theta}(x^{(i)} \mid z)p_{\theta}(z)}{p_{\theta}(z \mid x^{(i)})}\right] \quad (Bayes' \text{ Rule})$$
We want to
maximize the
data
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$$= \mathbf{E}_{z} \left[\log \frac{p_{\theta}(x^{(i)} \mid z)p_{\theta}(z)}{p_{\theta}(z \mid x^{(i)})} \frac{q_{\phi}(z \mid x^{(i)})}{q_{\phi}(z \mid x^{(i)})}\right] \quad (Multiply \text{ by constant})$$

$$= \mathbf{E}_{z} \left[\log p_{\theta}(x^{(i)} \mid z)\right] - \mathbf{E}_{z} \left[\log \frac{q_{\phi}(z \mid x^{(i)})}{p_{\theta}(z)}\right] + \mathbf{E}_{z} \left[\log \frac{q_{\phi}(z \mid x^{(i)})}{p_{\theta}(z \mid x^{(i)})}\right] \quad (Logarithms)$$

$$= \mathbf{E}_{z} \left[\log p_{\theta}(x^{(i)} \mid z)\right] - D_{KL}(q_{\phi}(z \mid x^{(i)}) \mid p_{\theta}(z)) + D_{KL}(q_{\phi}(z \mid x^{(i)}) \mid p_{\theta}(z \mid x^{(i)}))\right]$$

$$= \mathbf{E}_{z} \left[\log p_{\theta}(x^{(i)} \mid z)\right] - D_{KL}(q_{\phi}(z \mid x^{(i)}) \mid p_{\theta}(z)) + D_{KL}(q_{\phi}(z \mid x^{(i)}) \mid p_{\theta}(z \mid x^{(i)}))\right]$$

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$$= \mathbf{E}_{z} \left[\log p_{\theta}(x^{(i)} \mid z)\right] - D_{KL}(q_{\phi}(z \mid x^{(i)}) \mid p_{\theta}(z)) + D_{KL}(q_{\phi}(z \mid x^{(i)}) \mid p_{\theta}(z \mid x^{(i)}))\right]$$

$$= \mathbf{E}_{z} \left[\log p_{\theta}(x^{(i)} \mid z)\right] - D_{KL}(q_{\phi}(z \mid x^{(i)}) \mid p_{\theta}(z)) + D_{KL}(q_{\phi}(z \mid x^{(i)}) \mid p_{\theta}(z \mid x^{(i)}))\right]$$

$$= \mathbf{E}_{z} \left[\log p_{\theta}(x^{(i)} \mid z)\right] - D_{KL}(q_{\phi}(z \mid x^{(i)}) \mid p_{\theta}(z)) + D_{KL}(q_{\phi}(z \mid x^{(i)}) \mid p_{\theta}(z \mid x^{(i)}))\right]$$

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$$\log p_{\theta}(x^{(i)}) = \mathbf{E}_{z \sim q_{\phi}(z|x^{(i)})} \left[\log p_{\theta}(x^{(i)})\right] \quad (p_{\theta}(x^{(i)}) \text{ Does not depend on } z)$$

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data
likelihood
$$= \mathbf{E}_{z} \left[\log \frac{p_{\theta}(x^{(i)} \mid z)p_{\theta}(z)}{p_{\theta}(z \mid x^{(i)})} \frac{q_{\phi}(z \mid x^{(i)})}{q_{\phi}(z \mid x^{(i)})}\right] \quad (\text{Multiply by constant})$$

$$= \mathbf{E}_{z} \left[\log p_{\theta}(x^{(i)} \mid z)\right] - \mathbf{E}_{z} \left[\log \frac{q_{\phi}(z \mid x^{(i)})}{p_{\theta}(z)}\right] + \mathbf{E}_{z} \left[\log \frac{q_{\phi}(z \mid x^{(i)})}{p_{\theta}(z \mid x^{(i)})}\right] \quad (\text{Logarithms})$$

$$= \underbrace{\mathbf{E}_{z} \left[\log p_{\theta}(x^{(i)} \mid z)\right] - D_{KL}(q_{\phi}(z \mid x^{(i)}) || p_{\theta}(z))}_{\mathcal{L}(x^{(i)}, \theta, \phi)} + \underbrace{D_{KL}(q_{\phi}(z \mid x^{(i)}) || p_{\theta}(z \mid x^{(i)}))}_{\geq 0}\right]$$

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

$$\log p_{\theta}(x^{(i)}) = \mathbf{E}_{z \sim q_{\phi}(z|x^{(i)})} \left[\log p_{\theta}(x^{(i)})\right] \quad (p_{\theta}(x^{(i)}) \text{ Does not depend on } z)$$

$$= \mathbf{E}_{z} \left[\log \frac{p_{\theta}(x^{(i)} \mid z)p_{\theta}(z)}{p_{\theta}(z \mid x^{(i)})}\right] \quad (\text{Bayes' Rule}) \qquad \text{Make approximate posterior distribution the input data} = \mathbf{E}_{z} \left[\log \frac{p_{\theta}(x^{(i)} \mid z)p_{\theta}(z)}{p_{\theta}(z \mid x^{(i)})} \frac{q_{\phi}(z \mid x^{(i)})}{q_{\phi}(z \mid x^{(i)})}\right] \quad (\text{Multiply by constant}) \quad \text{close to prior}$$

$$= \mathbf{E}_{z} \left[\log p_{\theta}(x^{(i)} \mid z)\right] - \mathbf{E}_{z} \left[\log \frac{q_{\phi}(z \mid x^{(i)})}{p_{\theta}(z)}\right] + \mathbf{E}_{z} \left[\log \frac{q_{\phi}(z \mid x^{(i)})}{p_{\theta}(z \mid x^{(i)})}\right] \quad (\text{Logarithms})$$

$$= \underbrace{\mathbf{E}_{z} \left[\log p_{\theta}(x^{(i)} \mid z)\right] - D_{KL}(q_{\phi}(z \mid x^{(i)}) || p_{\theta}(z))}_{\mathcal{L}(x^{(i)}, \theta, \phi)} + \underbrace{D_{KL}(q_{\phi}(z \mid x^{(i)}) || p_{\theta}(z \mid x^{(i)}))}_{\geq 0}\right]$$

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

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



Kingma and Welling, "Auto-Encoding Variational Bayes", ICLR 2014

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Putting it all together: maximizing the likelihood lower bound

$$\underbrace{\mathbf{E}_{z}\left[\log p_{\theta}(x^{(i)} \mid z)\right] - D_{KL}(q_{\phi}(z \mid x^{(i)}) \mid\mid p_{\theta}(z))}_{\mathcal{L}(x^{(i)}, \theta, \phi)}$$

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Putting it all together: maximizing the likelihood lower bound

$$\underbrace{\mathbf{E}_{z}\left[\log p_{\theta}(x^{(i)} \mid z)\right] - D_{KL}(q_{\phi}(z \mid x^{(i)}) \mid\mid p_{\theta}(z))}_{\mathcal{L}(x^{(i)}, \theta, \phi)}$$

Let's look at computing the KL divergence between the estimated posterior and the prior given some data



Putting it all together: maximizing the likelihood lower bound

$$\underbrace{\mathbf{E}_{z}\left[\log p_{\theta}(x^{(i)} \mid z)\right] - D_{KL}(q_{\phi}(z \mid x^{(i)}) \mid\mid p_{\theta}(z))}_{\mathcal{L}(x^{(i)}, \theta, \phi)}$$



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Putting it all together: maximizing the likelihood lower bound



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Putting it all together: maximizing the likelihood lower bound



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Putting it all together: maximizing the likelihood lower bound

 $z=\mu_{z|x}+\epsilon\sigma_{z|x}$ $\log p_{\theta}(x^{(i)} \mid z)$ $-D_{KL}(q_{\phi}(z \mid x^{(i)}) \mid\mid p_{\theta}(z)))$ \mathbf{E}_z $\mathcal{L}(x^{(i)}, \theta, \phi)$ zSample z from $\overline{z|x} \sim \overline{\mathcal{N}}(\mu_{z|x}, \Sigma_{z|x})$ Make approximate posterior distribution $\Sigma_{z|x}$ $\mu_{z|x}$ close to prior Encoder network $q_{\phi}(z|x)$ x**Input Data**

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Reparameterization trick to make

sampling differentiable:

Sample $\epsilon \sim \mathcal{N}(0,I)$

Putting it all together: maximizing the likelihood lower bound



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Reparameterization trick to make sampling differentiable:

Input to

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Sample $\epsilon \sim \mathcal{N}(0, I)$

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Putting it all together: maximizing the likelihood lower bound



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Our assumption about data generation process

Sample from
true conditional \boldsymbol{x} $p_{\theta^*}(x \mid z^{(i)})$ $\boldsymbol{p}_{\text{Decoder}}$ Sample from
true prior
 $z^{(i)} \sim p_{\theta^*}(z)$ \boldsymbol{z}

Kingma and Welling, "Auto-Encoding Variational Bayes", ICLR 2014

Our assumption about data generation process

Now given a trained VAE: use decoder network & sample z from prior!



Kingma and Welling, "Auto-Encoding Variational Bayes", ICLR 2014

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Use decoder network. Now sample z from prior!



Sample z from $\, z \sim \mathcal{N}(0, I) \,$

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Kingma and Welling, "Auto-Encoding Variational Bayes", ICLR 2014

Use decoder network. Now sample z from prior!

Data manifold for 2-d z



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Labeled Faces in the Wild

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Probabilistic spin to traditional autoencoders => allows generating data Defines an intractable density => derive and optimize a (variational) lower bound

Pros:

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

Cons:

- Maximizes lower bound of likelihood: okay, but not as good evaluation as PixelRNN/PixelCNN
- 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, e.g., Gaussian Mixture Models (GMMs), Categorical Distributions.

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- Learning disentangled representations.



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Generative Adversarial Networks (GANs)

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So far...

PixelCNNs define tractable density function, optimize likelihood of training data: $p_{\theta}(x) = \prod_{i=1}^{n} p_{\theta}(x_i | x_1, ..., x_{i-1})$

VAEs define intractable density function with latent z:

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

Cannot optimize directly, derive and optimize lower bound on likelihood instead

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So far...

PixelCNNs define tractable density function, optimize likelihood of training data: $p_{\theta}(x) = \prod_{i=1}^{n} p_{\theta}(x_i | x_1, ..., x_{i-1})$

VAEs define intractable density function with latent z:

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

Cannot optimize directly, derive and optimize lower bound on likelihood instead

What if we give up on explicitly modeling density, and just want ability to sample?

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So far...

PixelCNNs define tractable density function, optimize likelihood of training data: $p_{\theta}(x) = \prod_{i=1}^{n} p_{\theta}(x_i | x_1, ..., x_{i-1})$

VAEs define intractable density function with latent z:

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

Cannot optimize directly, derive and optimize lower bound on likelihood instead

What if we give up on explicitly modeling density, and just want ability to sample?

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GANs: not modeling any explicit density function!

Ian Goodfellow et al., "Generative Adversarial Nets", NIPS 2014

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Problem: Want to sample from complex, high-dimensional training distribution. No direct way to do this!

Solution: Sample from a simple distribution we can easily sample from, e.g. random noise. Learn transformation to training distribution.

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Q: What can we use to represent this complex transformation?

Ian Goodfellow et al., "Generative Adversarial Nets", NIPS 2014

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Problem: Want to sample from complex, high-dimensional training distribution. No direct way to do this!

Solution: Sample from a simple distribution we can easily sample from, e.g. random noise. Learn transformation to training distribution.

Q: What can we use to represent this complex transformation?

A: A neural network!



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Ian Goodfellow et al., "Generative Adversarial Nets", NIPS 2014

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Problem: Want to sample from complex, high-dimensional training distribution. No direct way to do this!

Solution: Sample from a simple distribution we can easily sample from, e.g. random noise. Learn transformation to training distribution.

But we don't know which sample z maps to which training image -> can't learn by reconstructing training images



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Ian Goodfellow et al., "Generative Adversarial Nets", NIPS 2014

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Problem: Want to sample from complex, high-dimensional training distribution. No direct way to do this!

Solution: Sample from a simple distribution we can easily sample from, e.g. random noise. Learn transformation to training distribution.

But we don't know which sample z maps to which training image -> can't learn by reconstructing training images Solution: Use a discriminator network to tell whether the generate image is within data distribution or not

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Ian Goodfellow et al., "Generative Adversarial Nets", NIPS 2014

Discriminator network: try to distinguish between real and fake images **Generator network**: try to fool the discriminator by generating real-looking images

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Ian Goodfellow et al., "Generative Adversarial Nets", NIPS 2014

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Discriminator network: try to distinguish between real and fake images **Generator network**: try to fool the discriminator by generating real-looking images



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Ian Goodfellow et al., "Generative Adversarial Nets", NIPS 2014

Discriminator network: try to distinguish between real and fake images **Generator network**: try to fool the discriminator by generating real-looking images



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Discriminator network: try to distinguish between real and fake images **Generator network**: try to fool the discriminator by generating real-looking images

Train jointly in minimax game

Vinimax objective function:

$$\min_{\substack{\theta_g \\ \theta_d}} \max_{\substack{\theta_d \\ \theta_d}} \left[\mathbb{E}_{x \sim p_{data}} \log D_{\theta_d}(x) + \mathbb{E}_{z \sim p(z)} \log(1 - D_{\theta_d}(G_{\theta_g}(z))) \right]$$
Generator objective Discriminator objective

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Discriminator network: try to distinguish between real and fake images **Generator network**: try to fool the discriminator by generating real-looking images

Train jointly in **minimax game**

Minimax objective function:

Discriminator outputs likelihood in (0,1) of real image

$$\min_{\theta_g} \max_{\theta_d} \left[\mathbb{E}_{x \sim p_{data}} \log D_{\theta_d}(x) + \mathbb{E}_{z \sim p(z)} \log(1 - D_{\theta_d}(G_{\theta_g}(z))) \right]$$

Discriminator output for for real data x Discriminator output for generated fake data G(z)

Discriminator network: try to distinguish between real and fake images **Generator network**: try to fool the discriminator by generating real-looking images

Train jointly in **minimax game**

Minimax objective function:

$$\min_{\theta_g} \max_{\theta_d} \left[\mathbb{E}_{x \sim p_{data}} \log D_{\theta_d}(x) + \mathbb{E}_{z \sim p(z)} \log(1 - D_{\theta_d}(G_{\theta_g}(z))) \right]$$

Discriminator output for real data x Discriminator output for generated fake data G(z)

Discriminator outputs likelihood in (0,1) of real image

- Discriminator (θ_d) wants to **maximize objective** such that D(x) is close to 1 (real) and D(G(z)) is close to 0 (fake)
- Generator (θ_g) wants to **minimize objective** such that D(G(z)) is close to 1 (discriminator is fooled into thinking generated G(z) is real)

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Ian Goodfellow et al., "Generative Adversarial Nets", NIPS 2014

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Minimax objective function:

$$\min_{\theta_g} \max_{\theta_d} \left[\mathbb{E}_{x \sim p_{data}} \log D_{\theta_d}(x) + \mathbb{E}_{z \sim p(z)} \log(1 - D_{\theta_d}(G_{\theta_g}(z))) \right]$$

Alternate between:

1. Gradient ascent on discriminator

$$\max_{\theta_d} \left[\mathbb{E}_{x \sim p_{data}} \log D_{\theta_d}(x) + \mathbb{E}_{z \sim p(z)} \log(1 - D_{\theta_d}(G_{\theta_g}(z))) \right]$$

2. Gradient descent on generator

$$\min_{\theta_g} \mathbb{E}_{z \sim p(z)} \log(1 - D_{\theta_d}(G_{\theta_g}(z)))$$

Ian Goodfellow et al., "Generative Adversarial Nets", NIPS 2014

Minimax objective function:

$$\min_{\theta_g} \max_{\theta_d} \left[\mathbb{E}_{x \sim p_{data}} \log D_{\theta_d}(x) + \mathbb{E}_{z \sim p(z)} \log(1 - D_{\theta_d}(G_{\theta_g}(z))) \right]$$

Alternate between:

1. Gradient ascent on discriminator

$$\max_{\theta_d} \left[\mathbb{E}_{x \sim p_{data}} \log D_{\theta_d}(x) + \mathbb{E}_{z \sim p(z)} \log(1 - D_{\theta_d}(G_{\theta_g}(z))) \right]$$

2. Gradient descent on generator



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D(G(z))

Ian Goodfellow et al., "Generative Adversarial Nets", NIPS 2014

Minimax objective function:

$$\min_{\theta_g} \max_{\theta_d} \left[\mathbb{E}_{x \sim p_{data}} \log D_{\theta_d}(x) + \mathbb{E}_{z \sim p(z)} \log(1 - D_{\theta_d}(G_{\theta_g}(z))) \right]$$

Alternate between:

1. Gradient ascent on discriminator

$$\max_{\theta_d} \left[\mathbb{E}_{x \sim p_{data}} \log D_{\theta_d}(x) + \mathbb{E}_{z \sim p(z)} \log(1 - D_{\theta_d}(G_{\theta_g}(z))) \right]$$

2. Gradient descent on generator



region is relatively flat!

Gradient signal dominated by region where sample is already good

-D(G(z))

1.0

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D(G(z))

lan Goodfellow et al., "Generative Adversarial Nets", NIPS 2014

Minimax objective function:

$$\min_{\theta_g} \max_{\theta_d} \left[\mathbb{E}_{x \sim p_{data}} \log D_{\theta_d}(x) + \mathbb{E}_{z \sim p(z)} \log(1 - D_{\theta_d}(G_{\theta_g}(z))) \right]$$

Alternate between:

1. Gradient ascent on discriminator

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$$\max_{\theta_d} \left[\mathbb{E}_{x \sim p_{data}} \log D_{\theta_d}(x) + \mathbb{E}_{z \sim p(z)} \log(1 - D_{\theta_d}(G_{\theta_g}(z))) \right]$$

2. Instead: Gradient ascent on generator, different objective

$$\max_{\theta_g} \mathbb{E}_{z \sim p(z)} \log(D_{\theta_d}(G_{\theta_g}(z)))$$

Instead of minimizing likelihood of discriminator being correct, now maximize likelihood of discriminator being wrong. Same objective of fooling discriminator, but now higher gradient signal for bad samples => works much better! Standard in practice.



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Training GANs: Two-player game

Ian Goodfellow et al., "Generative Adversarial Nets", NIPS 2014

Putting it together: GAN training algorithm

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:

$$\nabla_{\theta_d} \frac{1}{m} \sum_{i=1}^m \left[\log D_{\theta_d}(x^{(i)}) + \log(1 - D_{\theta_d}(G_{\theta_g}(z^{(i)}))) \right]$$

end for

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

$$\nabla_{\theta_g} \frac{1}{m} \sum_{i=1}^m \log(D_{\theta_d}(G_{\theta_g}(z^{(i)})))$$

end for

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Training GANs: Two-player game

Ian Goodfellow et al., "Generative Adversarial Nets", NIPS 2014

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Putting it together: GAN training algorithm

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 $p_{\text{data}}(x)$.

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• Update the discriminator by ascending its stochastic gradient:

$$\nabla_{\theta_d} \frac{1}{m} \sum_{i=1}^m \left[\log D_{\theta_d}(x^{(i)}) + \log(1 - D_{\theta_d}(G_{\theta_g}(z^{(i)}))) \right]$$

end for

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

$$\nabla_{\theta_g} \frac{1}{m} \sum_{i=1}^m \log(D_{\theta_d}(G_{\theta_g}(z^{(i)})))$$

end for

Arjovsky et al. "Wasserstein gan." arXiv preprint arXiv:1701.07875 (2017) Berthelot, et al. "Began: Boundary equilibrium generative adversarial networks." arXiv preprint arXiv:1703.10717 (2017)

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Some find k=1 more stable, others use k > 1, no best rule.

Followup work (e.g. Wasserstein GAN, BEGAN) alleviates this problem, better stability!

Training GANs: Two-player game

Ian Goodfellow et al., "Generative Adversarial Nets", NIPS 2014

Generator network: try to fool the discriminator by generating real-looking images **Discriminator network**: try to distinguish between real and fake images



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Ian Goodfellow et al., "Generative Adversarial Nets", NIPS 2014

Generative Adversarial Nets

Generated samples



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Ian Goodfellow et al., "Generative Adversarial Nets", NIPS 2014

Generative Adversarial Nets

Generated samples (CIFAR-10)



Nearest neighbor from training set

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Generative Adversarial Nets: Convolutional Architectures

Generator is an upsampling network with fractionally-strided convolutions Discriminator is a convolutional network

Architecture guidelines for stable Deep Convolutional GANs

- Replace any pooling layers with strided convolutions (discriminator) and fractional-strided convolutions (generator).
- Use batchnorm in both the generator and the discriminator.
- Remove fully connected hidden layers for deeper architectures.
- Use ReLU activation in generator for all layers except for the output, which uses Tanh.

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• Use LeakyReLU activation in the discriminator for all layers.

Radford et al, "Unsupervised Representation Learning with Deep Convolutional Generative Adversarial Networks", ICLR 2016

Generative Adversarial Nets: Convolutional Architectures

Samples from the model look much better!

Radford et al, ICLR 2016



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Generative Adversarial Nets: Convolutional Architectures

Interpolating between random points in laten space

Radford et al, ICLR 2016



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Radford et al, ICLR 2016

Samples from the model







Neutral man

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Neutral man

Radford et al, ICLR 2016

Samples from the model



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Glasses man

No glasses man

No glasses woman

Radford et al, ICLR 2016

Woman with glasses



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2017: Explosion of GANs See also: <u>https://github.com/soumith/ganhacks</u> for tips and tricks for trainings GANs "The GAN Zoo"

- GAN Generative Adversarial Networks
- · 3D-GAN Learning a Probabilistic Latent Space of Object Shapes via 3D Generative-Adversarial Modeling
- acGAN Face Aging With Conditional Generative Adversarial Networks
- AC-GAN Conditional Image Synthesis With Auxiliary Classifier GANs
- AdaGAN AdaGAN: Boosting Generative Models
- AEGAN Learning Inverse Mapping by Autoencoder based Generative Adversarial Nets
- AffGAN Amortised MAP Inference for Image Super-resolution
- AL-CGAN Learning to Generate Images of Outdoor Scenes from Attributes and Semantic Layouts
- ALI Adversarially Learned Inference
- AM-GAN Generative Adversarial Nets with Labeled Data by Activation Maximization
- AnoGAN Unsupervised Anomaly Detection with Generative Adversarial Networks to Guide Marker Discovery
- ArtGAN ArtGAN: Artwork Synthesis with Conditional Categorial GANs
- b-GAN b-GAN: Unified Framework of Generative Adversarial Networks
- Bayesian GAN Deep and Hierarchical Implicit Models
- BEGAN BEGAN: Boundary Equilibrium Generative Adversarial Networks
- BiGAN Adversarial Feature Learning
- BS-GAN Boundary-Seeking Generative Adversarial Networks
- CGAN Conditional Generative Adversarial Nets
- CaloGAN CaloGAN: Simulating 3D High Energy Particle Showers in Multi-Layer Electromagnetic Calorimeters
 with Generative Adversarial Networks
- CCGAN Semi-Supervised Learning with Context-Conditional Generative Adversarial Networks
- CatGAN Unsupervised and Semi-supervised Learning with Categorical Generative Adversarial Networks
- CoGAN Coupled Generative Adversarial Networks

- Context-RNN-GAN Contextual RNN-GANs for Abstract Reasoning Diagram Generation
- · C-RNN-GAN C-RNN-GAN: Continuous recurrent neural networks with adversarial training
- CS-GAN Improving Neural Machine Translation with Conditional Sequence Generative Adversarial Nets
- CVAE-GAN CVAE-GAN: Fine-Grained Image Generation through Asymmetric Training
- CycleGAN Unpaired Image-to-Image Translation using Cycle-Consistent Adversarial Networks
- DTN Unsupervised Cross-Domain Image Generation
- DCGAN Unsupervised Representation Learning with Deep Convolutional Generative Adversarial Networks
- DiscoGAN Learning to Discover Cross-Domain Relations with Generative Adversarial Networks
- DR-GAN Disentangled Representation Learning GAN for Pose-Invariant Face Recognition
- DualGAN DualGAN: Unsupervised Dual Learning for Image-to-Image Translation
- EBGAN Energy-based Generative Adversarial Network
- f-GAN f-GAN: Training Generative Neural Samplers using Variational Divergence Minimization
- FF-GAN Towards Large-Pose Face Frontalization in the Wild
- GAWWN Learning What and Where to Draw
- GeneGAN GeneGAN: Learning Object Transfiguration and Attribute Subspace from Unpaired Data
- Geometric GAN Geometric GAN
- GoGAN Gang of GANs: Generative Adversarial Networks with Maximum Margin Ranking
- GP-GAN GP-GAN: Towards Realistic High-Resolution Image Blending
- IAN Neural Photo Editing with Introspective Adversarial Networks
- iGAN Generative Visual Manipulation on the Natural Image Manifold
- IcGAN Invertible Conditional GANs for image editing
- ID-CGAN Image De-raining Using a Conditional Generative Adversarial Network
- Improved GAN Improved Techniques for Training GANs
- InfoGAN InfoGAN: Interpretable Representation Learning by Information Maximizing Generative Adversarial Nets
- LAGAN Learning Particle Physics by Example: Location-Aware Generative Adversarial Networks for Physics
 Synthesis
- LAPGAN Deep Generative Image Models using a Laplacian Pyramid of Adversarial Networks

https://github.com/hindupuravinash/the-gan-zoo

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2017: Explosion of GANs

Better training and generation



LSGAN, Zhu 2017.



Wasserstein GAN, Arjovsky 2017. Improved Wasserstein GAN, Gulrajani 2017.





Progressive GAN, Karras 2018.

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2017: Explosion of GANs

Source->Target domain transfer



horse \rightarrow zebra



 $zebra \rightarrow horse$



apple \rightarrow orange









→ summer Yosemite



CycleGAN. Zhu et al. 2017.

Text -> Image Synthesis

this small bird has a pink breast and crown, and black almost all black with a red primaries and secondaries.

this magnificent fellow is crest, and white cheek patch.





Reed et al. 2017.

Many GAN applications





Pix2pix. Isola 2017. Many examples at https://phillipi.github.io/pix2pix/

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2019: BigGAN



Brock et al., 2019

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Scene graphs to GANs

Specifying exactly what kind of image you want to generate.

The explicit structure in scene graphs provides better image generation for complex scenes.

Scene Graph





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Johnson et al. Image Generation from Scene Graphs, CVPR 2019

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HYPE: Human eYe Perceptual Evaluations hype.stanford.edu



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GANs

Don't work with an explicit density function Take game-theoretic approach: learn to generate from training distribution through 2-player game

Pros:

- Beautiful, state-of-the-art samples!

Cons:

- Trickier / more unstable to train
- Can't solve inference queries such as p(x), p(z|x)

Active areas of research:

- Better loss functions, more stable training (Wasserstein GAN, LSGAN, many others)

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- Conditional GANs, GANs for all kinds of applications



- Glow
- Ffjord

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

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Useful Resources on Generative Models

CS 236: Deep Generative Models (Stanford)

CS 294-158 <u>Deep Unsupervised Learning</u> (Berkeley)

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Next: Detection and Segmentation

Classification

Semantic Segmentation

Object Detection

Instance Segmentation



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