CS 1674: Generative Models

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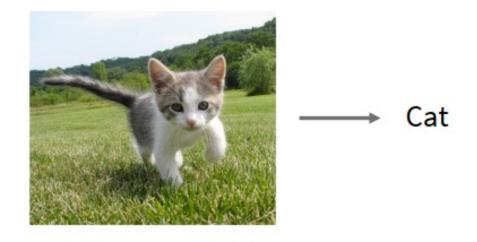
Supervised Learning

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.



Classification

This image is CC0 public domain

Supervised Learning

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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>

Supervised Learning

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Goal: Learn a function to map x -> y

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



DOG, DOG, CAT

Object Detection

This image is CC0 public domain

Supervised Learning

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



Semantic Segmentation

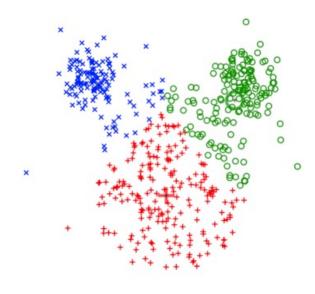
Unsupervised Learning

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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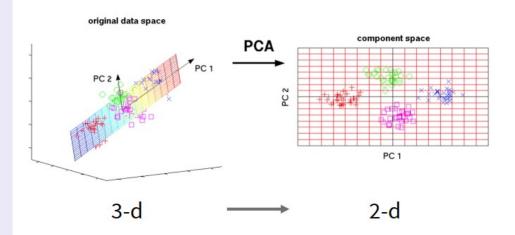
Unsupervised Learning

Data: x

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Goal: Learn some underlying hidden structure of the data

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



Principal Component Analysis (Dimensionality reduction)

This image from Matthias Scholz is CC0 public domain

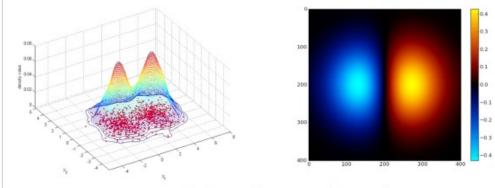
Unsupervised Learning

Data: x

Just data, no labels!

Goal: Learn some underlying hidden structure of the data

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



2-d density estimation

Modeling P(x)

2-d density images <u>left</u> and <u>right</u> are <u>CC0 public domain</u>

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.

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Just data, no labels!

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

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.

Self-Supervised Learning

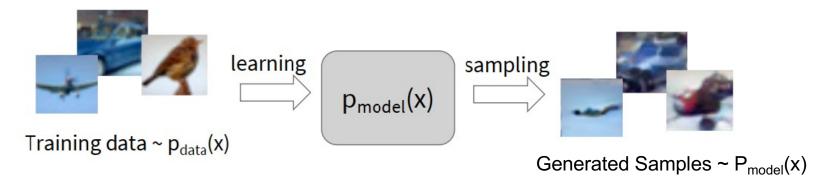
Data: (x, pseudo generated y) No manual labels!

Goal: Learn to generate good features (reduce the data to useful/generic features)

Example: Classification in downstream applications where we have limited data

Generative Modeling

Given training data, generate new samples from same distribution



Objectives:

- 1. Learn $p_{model}(x)$ that approximates $p_{data}(x)$
- 2. Sampling new x from $p_{model}(x)$

Why Generative Models? Debiasing

Capable of uncovering underlying features in a dataset

VS



Homogeneous skin color, pose



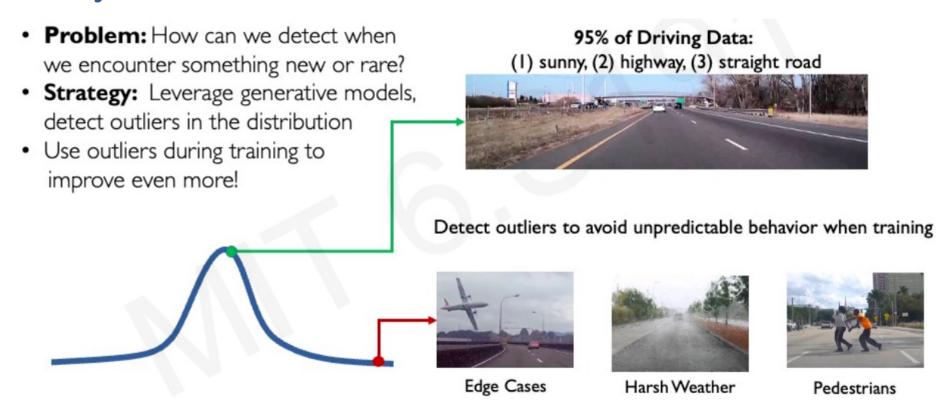
Diverse skin color, pose, illumination

How can we use this information to create fair and representative datasets?

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Why Generative Models? Outlier Detection

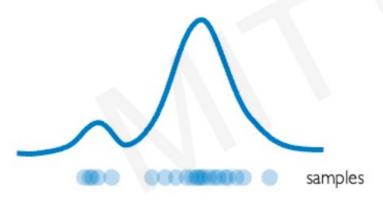


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Why Generative Models? Sample Generation

- Generative models learn probability distributions
- Sampling from that distribution → new data instances
- Backbone of Generative AI: generate language, images, and more















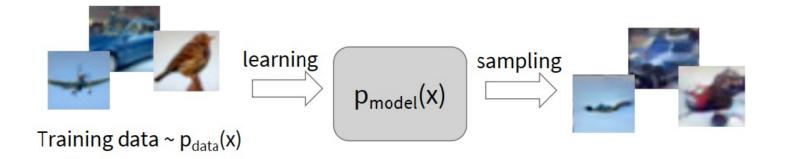


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Generative Modeling

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.

Generative Modeling: Applications







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

Taxonomy of Generative Models

Glow Ffjord

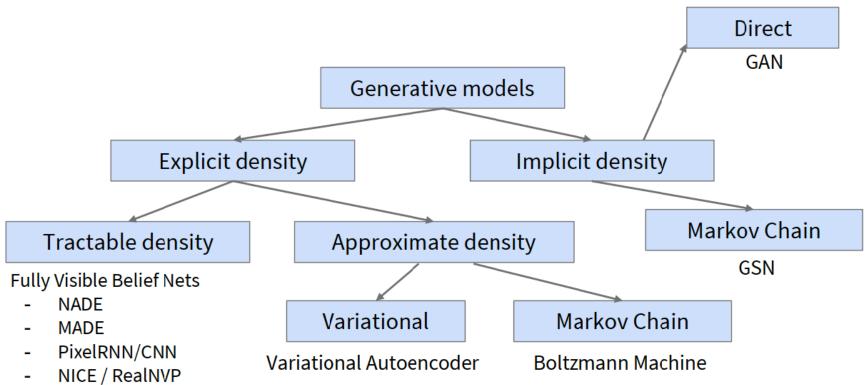
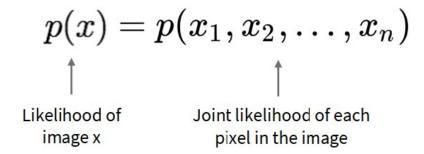


Figure copyright and adapted from Ian Goodfellow, Tutorial on Generative Adversarial Networks, 2017

PixelRNN and PixelCNN

Fully visible belief network (FVBN)

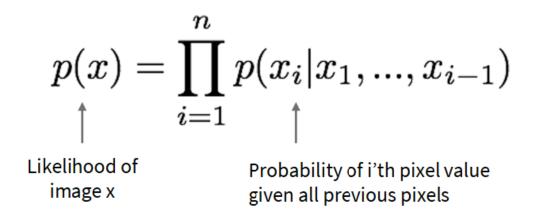
Explicit density model

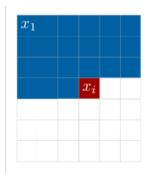


Fully visible belief network (FVBN)

Explicit density model

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



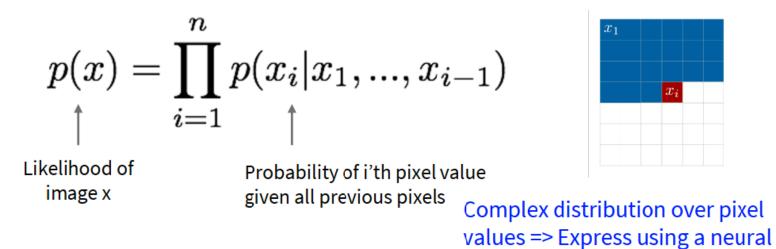


Then maximize likelihood of training data

Fully visible belief network (FVBN)

Explicit density model

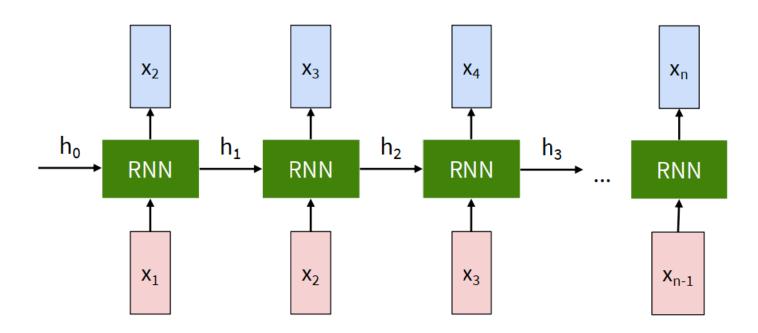
Use chain rule to decompose likelihood of an image x into product of 1-d distributions:



network!

Then maximize likelihood of training data

Another solution: Recurrent Neural Network



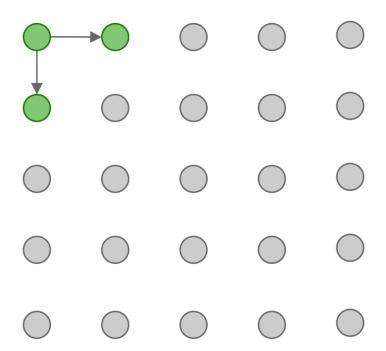
$$p(x_i|x_1,...,x_{i-1})$$

Generate image pixels starting from corner

Dependency on previous pixels modeled using an RNN (LSTM)

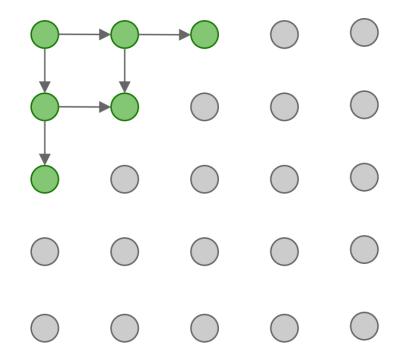
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Dependency on previous pixels modeled using an RNN (LSTM)



Generate image pixels starting from corner

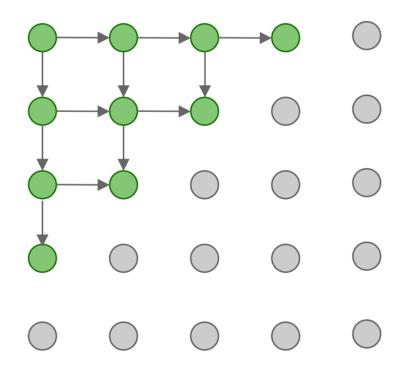
Dependency on previous pixels modeled using an RNN (LSTM)

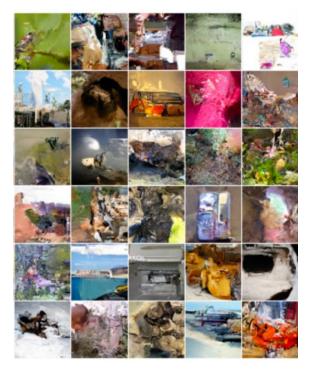


Generate image pixels starting from corner

Dependency on previous pixels modeled using an RNN (LSTM)

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





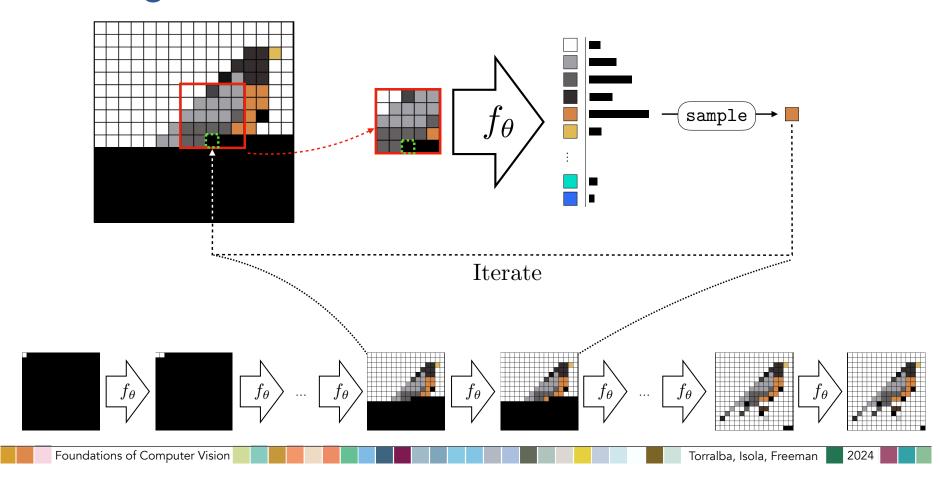
Samples from PixelRNN



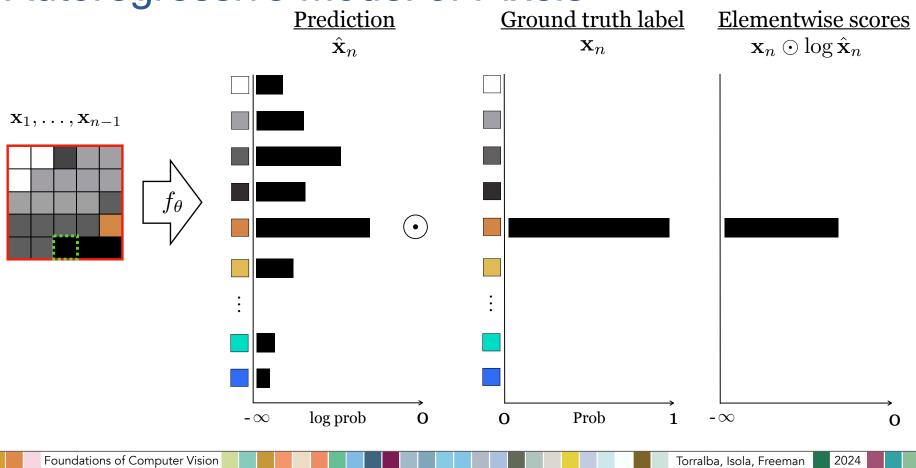
Image completions (conditional samples) from PixelRNN

[PixelRNN, van der Oord et al. 2016]

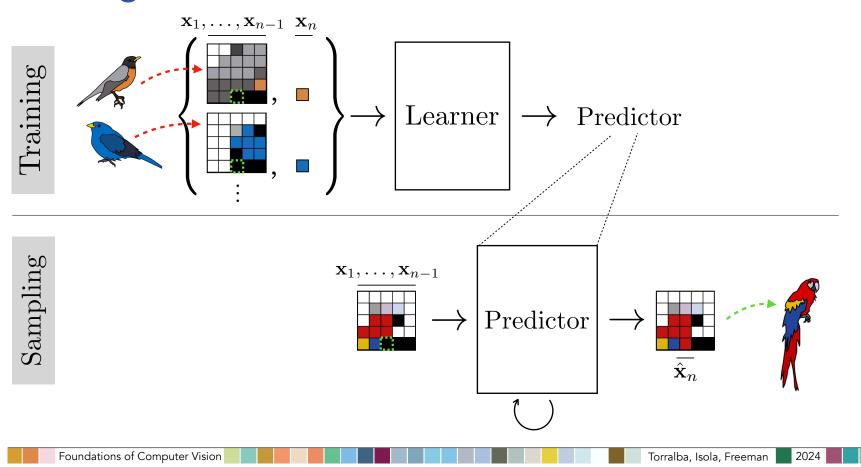
Autoregressive Model of Pixels



Autoregressive Model of Pixels



Autoregressive Model of Pixels



Taxonomy of Generative Models

Ffjord

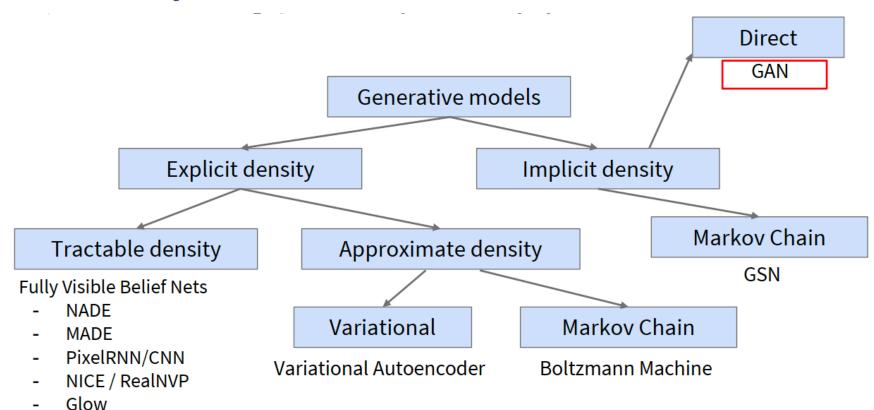


Figure copyright and adapted from Ian Goodfellow, Tutorial on Generative Adversarial Networks, 2017.

Generative Adversarial Networks (GANs)

PixelRNN/CNNs define tractable density function, optimize likelihood of training data:

$$p_{\theta}(x) = \prod_{i=1}^{n} p_{\theta}(x_i|x_1, ..., x_{i-1})$$

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

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

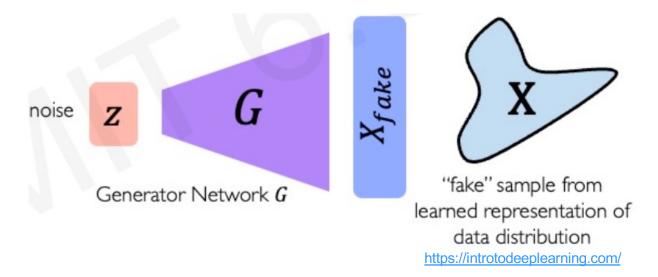
GANs: not modeling any explicit density function!

Slide credit: Fei-Fei Li

Generative Adversarial Networks (GANs)

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.



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

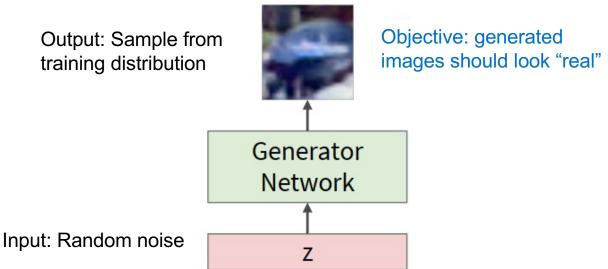
Slide credit: Fei-Fei Li

Generative Adversarial Networks (GANs)

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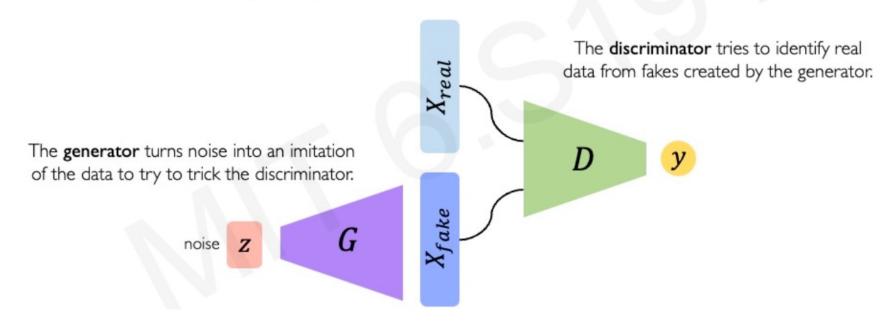
But we don't know which sample z maps to which training image -> can't learn by reconstructing training images



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

Generative Adversarial Networks (GANs)

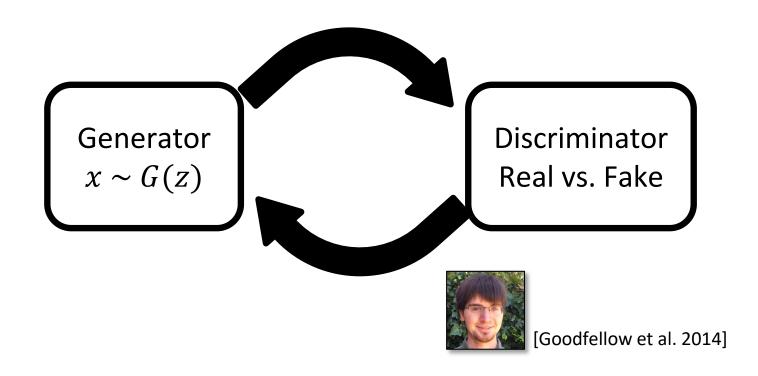
Generative Adversarial Networks (GANs) are a way to make a generative model by having two neural networks compete with each other.



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Adversarial Networks Framework

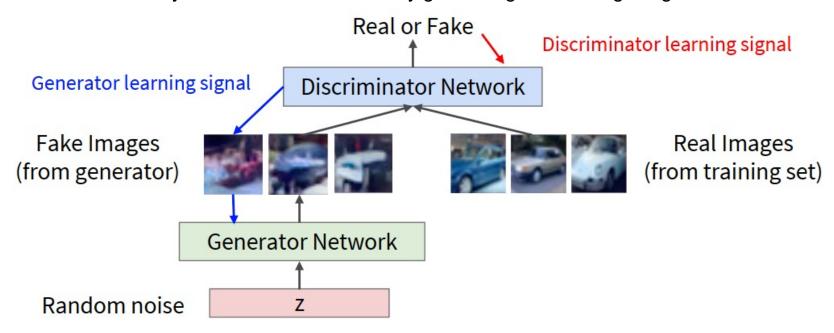


Jun-Yan Zhu

Training GANs: Two-player game

Discriminator network: try to distinguish between real and fake images

Generator network: try to fool the discriminator by generating real-looking images



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

Training GANs: Two-player game

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:

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

Training GANs: Two-player game

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

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

Minimax objective function:

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

$$\text{Discriminator output for generated fake data G(z)}$$

Training GANs: Two-player game

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

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

Minimax objective function:

$$\min_{\theta_g} \max_{\theta_d} \left[\mathbb{E}_{x \sim p_{data}} \log D_{\theta_d}(x) + \mathbb{E}_{z \sim p(z)} \log (1 - D_{\theta_d}(G_{\theta_g}(z))) \right] \\ \text{Discriminator output} \\ \text{for real data x} \\ \text{Discriminator output for generated fake data G(z)}$$

- 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)

Training GANs: Two-player game

Minimax objective function:

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

Alternate between:

1. Gradient ascent on discriminator

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

Gradient descent on generator

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

Training GANs: Two-player game

Minimax objective function:

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

Alternate between:

Gradient ascent on discriminator

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

axis).

Gradient descent on generator

$$\min_{ heta_g} \mathbb{E}_{z \sim p(z)} \log (1 - D_{ heta_d}(G_{ heta_g}(z)))$$
 it to improve generator

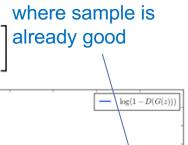
In practice, optimizing this generator objective does not work well!

But gradient in this region is relatively flat!

When sample is likely

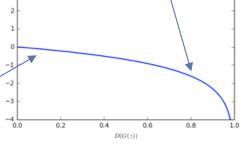
fake, want to learn from

(move to the right on X



dominated by region

Gradient signal



Slide credit: Fei-Fei Li

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

Training GANs: Two-player game

Minimax objective function:

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

Alternate between:

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. Instead: Gradient ascent on generator, different objective

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

Training GANs: Two-player game

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 $\{x^{(1)}, \dots, x^{(m)}\}$ from data generating distribution $p_{\text{data}}(x)$.
- Update the discriminator by ascending its stochastic gradient:

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

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!

end for

- Sample minibatch of m noise samples $\{z^{(1)}, \dots, z^{(m)}\}$ from noise prior $p_a(z)$.
- 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

Training GANs: Other Divergence

Least Squares GAN

$$\begin{split} & \min_{D} V_{\text{\tiny LSGAN}}(D) = & \frac{1}{2} \mathbb{E}_{\boldsymbol{x} \sim p_{\text{\tiny data}}(\boldsymbol{x})} \big[(D(\boldsymbol{x}) - 1)^2 \big] + \frac{1}{2} \mathbb{E}_{\boldsymbol{z} \sim p_{\boldsymbol{z}}(\boldsymbol{z})} \big[(D(G(\boldsymbol{z})))^2 \big] \\ & \min_{G} V_{\text{\tiny LSGAN}}(G) = & \frac{1}{2} \mathbb{E}_{\boldsymbol{z} \sim p_{\boldsymbol{z}}(\boldsymbol{z})} \big[(D(G(\boldsymbol{z})) - 1)^2 \big]. \end{split}$$

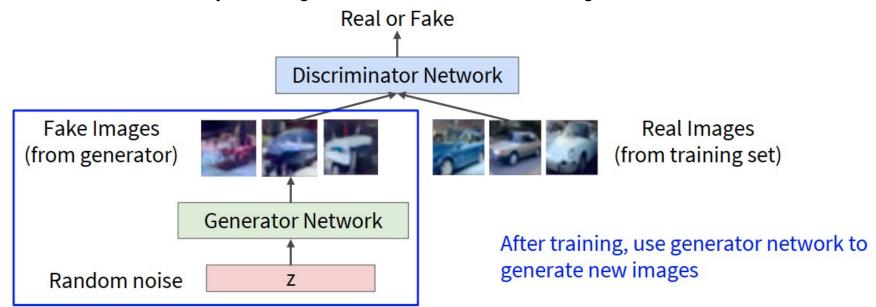
* Employed for our Assignment.

https://arxiv.org/pdf/1611.04076

https://sh-tsang.medium.com/review-lsgan-least-squares-generative-adversarial-networks-gan-bec12167e915

Training GANs: Two-player game

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



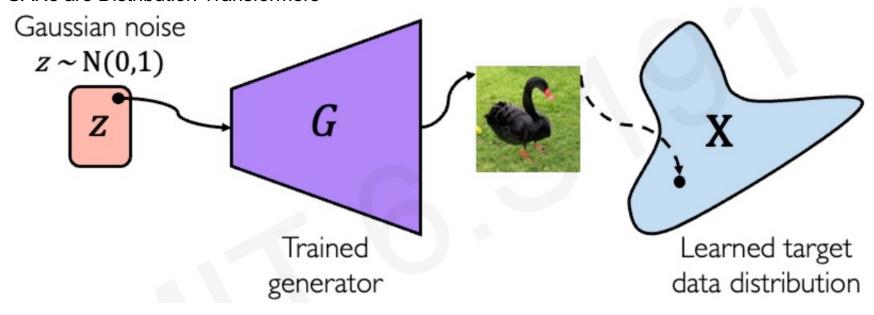
Fake and real images copyright Emily Denton et al. 2015

Slide credit: Fei-Fei Li

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

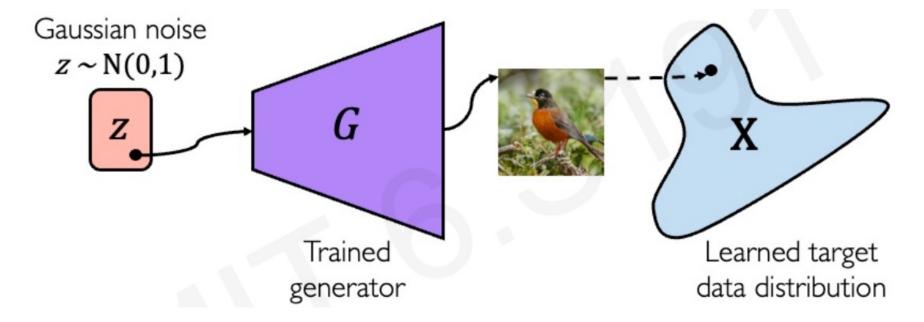
GANs: Generating New Data

GANs are Distribution Transformers



GANs: Generating New Data

GANs are Distribution Transformers



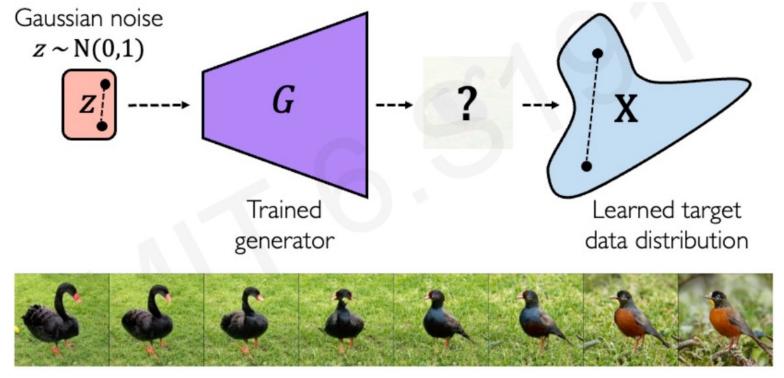
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GANs: Generating New Data

GANs are Distribution Transformers



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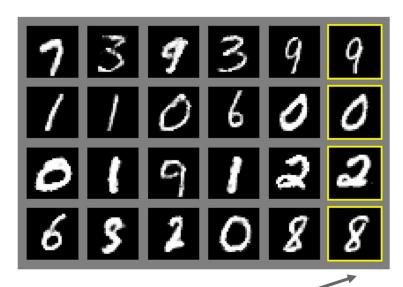
Lab 13a: Generative Adversarial Networks (GANs) for Digits

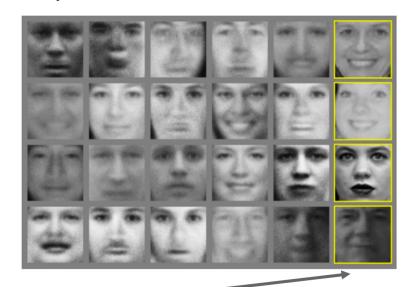
Duration: 10 min



Generative Adversarial Nets

Generated samples





Nearest neighbor from training set

Generative Adversarial Nets

Generated samples (CIFAR-10)





Nearest neighbor from training set

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.
- Use LeakyReLU activation in the discriminator for all layers.

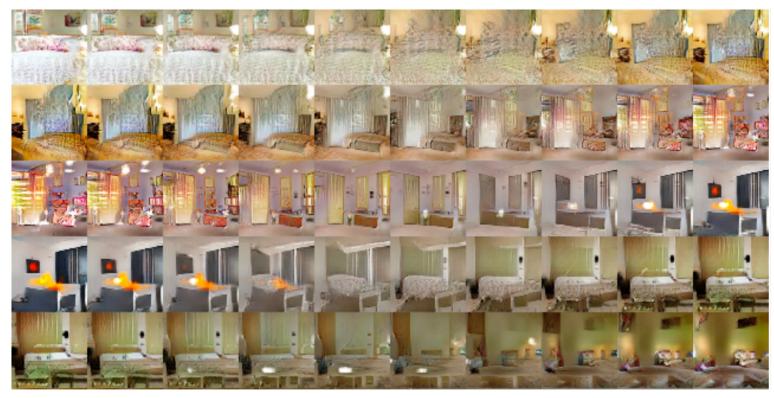
Generative Adversarial Nets: Convolutional Architectures

Samples from the model look much better!



Generative Adversarial Nets: Convolutional Architectures

Interpolating between random points in latent space



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

Slide credit: Fei-Fei Li

GANs: Interpretable Vector Math

Samples from the model



Smiling woman

Neutral woman



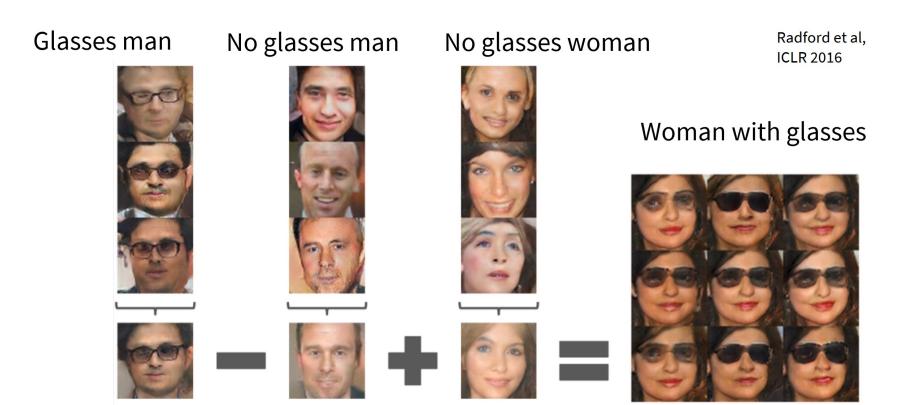
Neutral man



Radford et al, ICLR 2016

Adapted from Serena Young

GANs: Interpretable Vector Math



Adapted from Serena Young

2017: Explosion of 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

2017: Explosion of GANs

Better training and generation

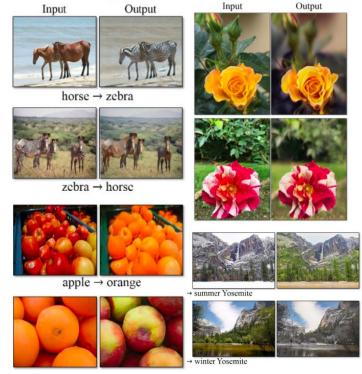


LSGAN. Mao et al. 2017.



BEGAN. Bertholet et al. 2017. Adapted from Serena Young

Source->Target domain transfer



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. crest, and white cheek patch.

this magnificent fellow is





Reed et al. 2017.

Many GAN applications



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

Summary: 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 samples!

Cons:

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

Active areas of research:

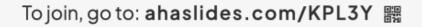
- Better loss functions, more stable training (Wasserstein GAN, LSGAN, many others)
- Conditional GANs, GANs for all kinds of applications

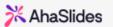
Adapted from Serena Young

Lab 13b: Generative Adversarial Networks (GANs)

Duration: 10 min







Please, from Lab 13: GAN [Section 1.2], submit your interpolation plot result.













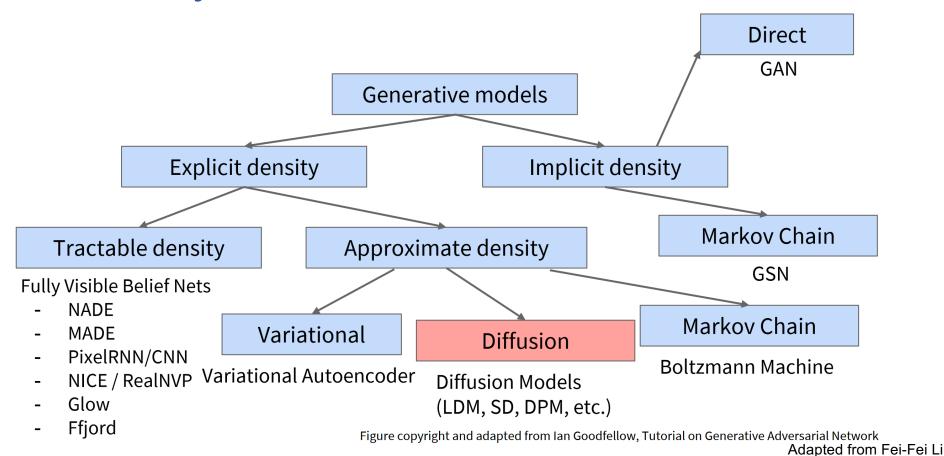








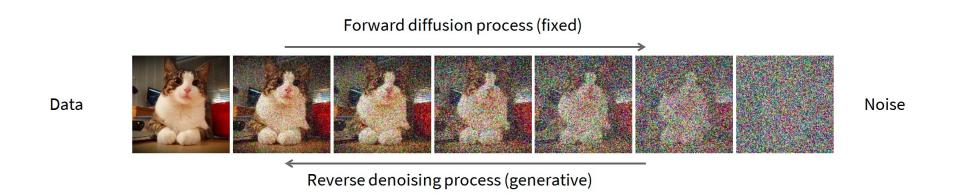
Taxonomy of Generative Models



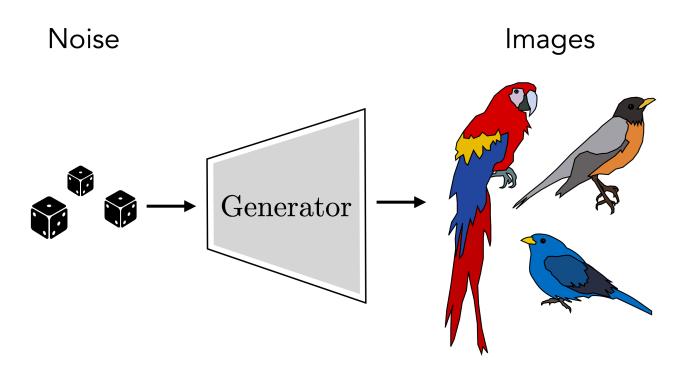
Denoising Diffusion Models

Learning to generate by denoising Denoising diffusion models consist of two processes:

- Forward diffusion process that gradually adds noise to input
- Reverse denoising process that learns to generate data by denoising

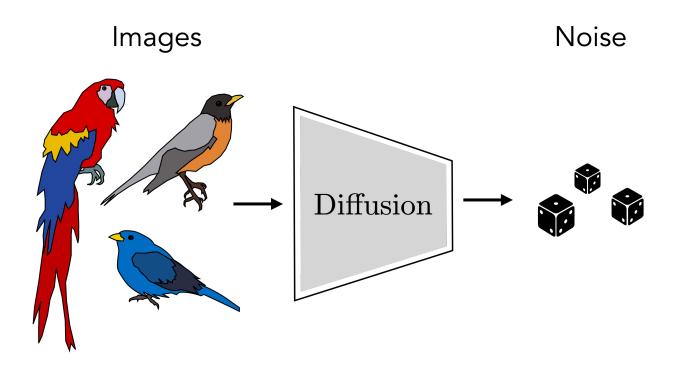


Sohl-Dickstein et al., Deep Unsupervised Learning using Nonequilibrium Thermodynamics, ICML 2015 Ho et al., Denoising Diffusion Probabilistic Models, NeurIPS 2020 Song et al., Score-Based Generative Modeling through Stochastic Differential Equations, ICLR 2021

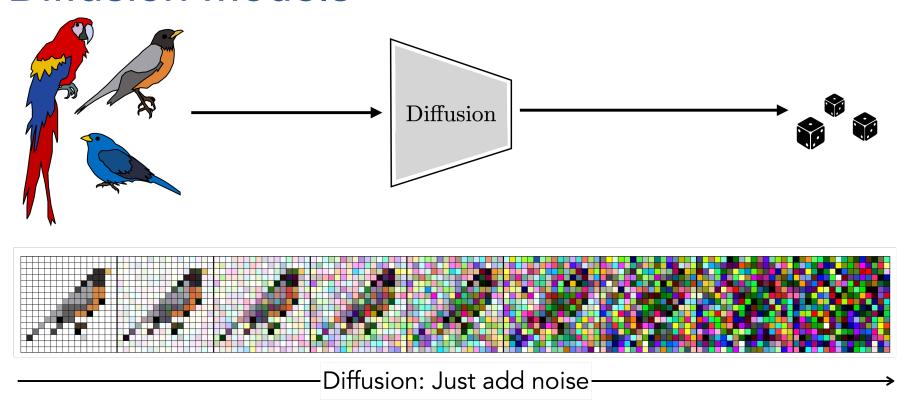


Foundations of Computer Vision

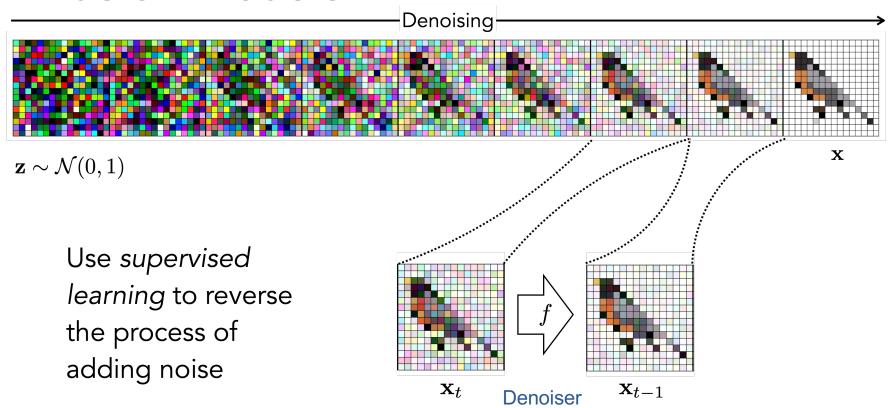
Torralba, Isola, Freeman



Foundations of Computer Vision Torralba, Isola, Freeman 2024



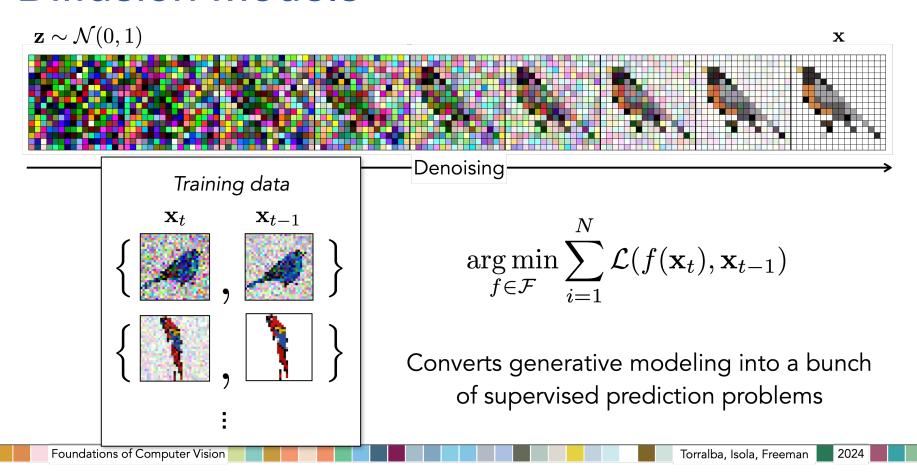
Foundations of Computer Vision Torralba, Isola, Freeman 2024



Foundations of Computer Vision

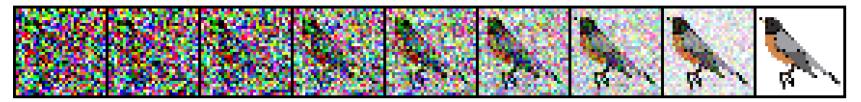
Torralba, Isola, Freeman

202/



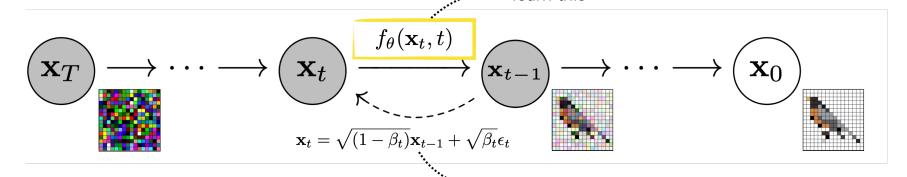
Different noise samples (dice rolls) result in different images





Foundations of Computer Vision Torralba, Isola, Freeman 2024

Gaussian Diffusion Models



~~which inverts this

Forward process:

$$\epsilon_t \sim \mathcal{N}(\mathbf{0}, \mathbf{I})$$
 $\mathbf{x}_t = \sqrt{(1 - \beta_t)} \mathbf{x}_{t-1} + \sqrt{\beta_t} \epsilon_t$

Reverse process:

$$\mathbf{x}_{t-1} = f_{\theta}(\mathbf{x}_t, t)$$

The variances, beta and sigma, are modeling choices. See Ho, Jain, and Abbeel for details.

Diffusion Models: Training

- Generate Training data by corrupting a bunch of images (forward process; noising)
- 2. Train a neural net to invert each step of corruption (reverse process; denoising)



Diffusion Models: Training

Algorithm 1.2: Training a diffusion model.

- 1 **Input:** training data $\{\mathbf{x}^{(i)}\}_{i=1}^{N}$
- 2 Output: trained model f_{θ}
- **3 Generate training sequences via diffusion:**

Forward Process.

4 for
$$i = 1, ..., N$$
 do
5 | for $t = 1, ..., T$ do
6 | $\epsilon_t \sim \mathcal{N}(\mathbf{0}, \mathbf{I})$
7 | $\mathbf{x}_t^{(i)} \leftarrow \sqrt{(1 - \beta_t)} \mathbf{x}_{t-1}^{(i)} + \sqrt{\beta_t} \epsilon_t$



Lab 13c

Reverse Process. Denoising

9 Train denoiser f_{θ} to reverse these sequences:

10
$$\theta^* = \arg\min_{\theta} \sum_{i=1}^{N} \sum_{t=1}^{T} \mathcal{L}(f_{\theta}(\mathbf{x}_{t}^{(i)}, t), \mathbf{x}_{t-1}^{(i)}))$$

11 **Return:** f_{θ^*}

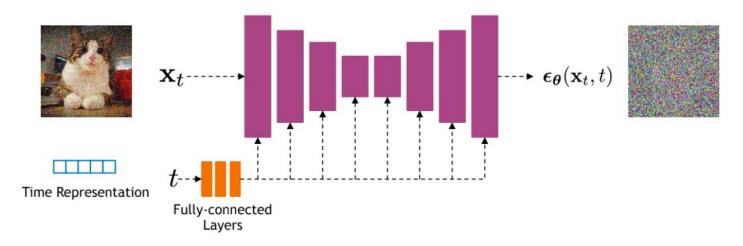
Lab 13c: Diffusion Models

Duration: 10 min



Diffusion Models: Training – Unet model transition

Diffusion models often use U-Net architectures with ResNet blocks and self-attention layers to represent $\epsilon_{\theta}(\mathbf{x}_t,t)$

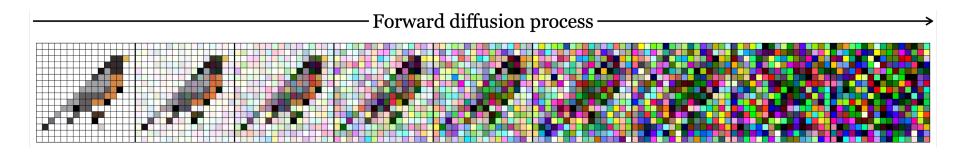


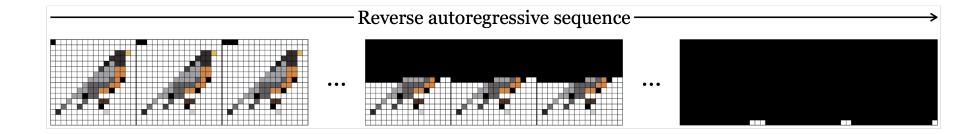
Time representation: sinusoidal positional embeddings or random Fourier features.

Time features are fed to the residual blocks using either simple spatial addition or using adaptive group normalization layers. (see <u>Dhariywal and Nichol NeurIPS 2021</u>)

https://cvpr2022-tutorial-diffusion-models.github.io/

Autoregressive Modes vs Diffusion Models

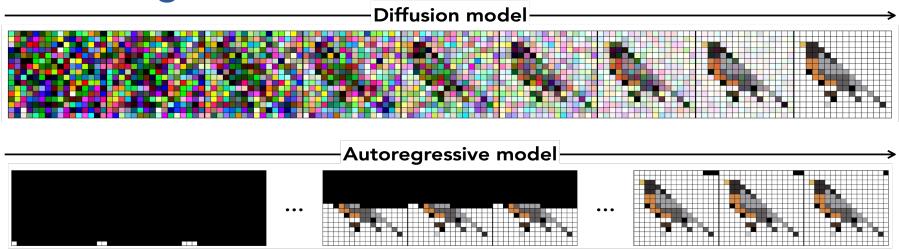




Foundations of Computer Vision

Torralba, Isola, Freeman

Autoregressive Modes vs Diffusion Models



A common strategy is to turn generative modeling into a sequence of supervised learning problems

Foundations of Computer Vision Torralba, Isola, Freeman 2024

2022 / 2023 : The year of diffusion and generative modeling?











slide from https://cvpr2022-tutorial-diffusion-models.github.io/ Courtesy of Ruiqi Gao

Useful Resources on Generative Models

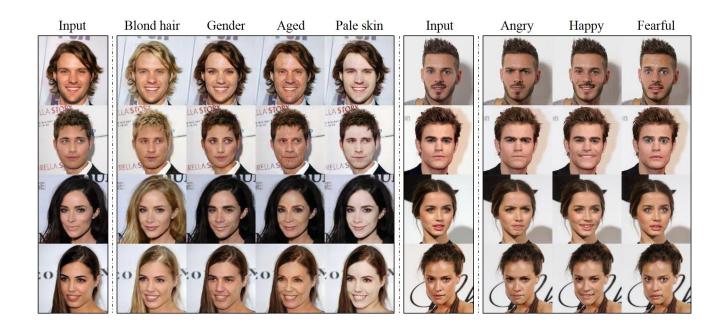
CS 236: <u>Deep Generative Models</u> (Stanford)

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

Applications: Celebrities Who Never Existed



Applications: StarGAN

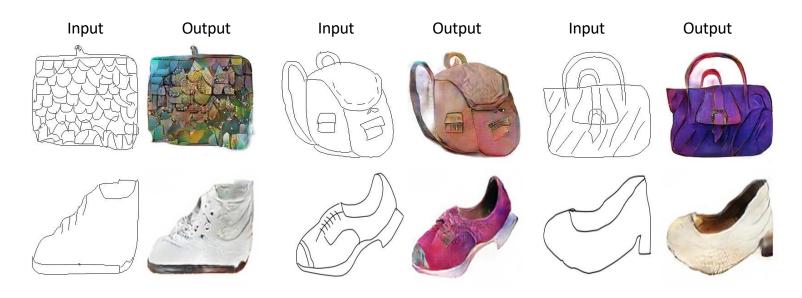


Applications: Edges to Images



Edges from [Xie & Tu, 2015]

Applications: Sketches to Images

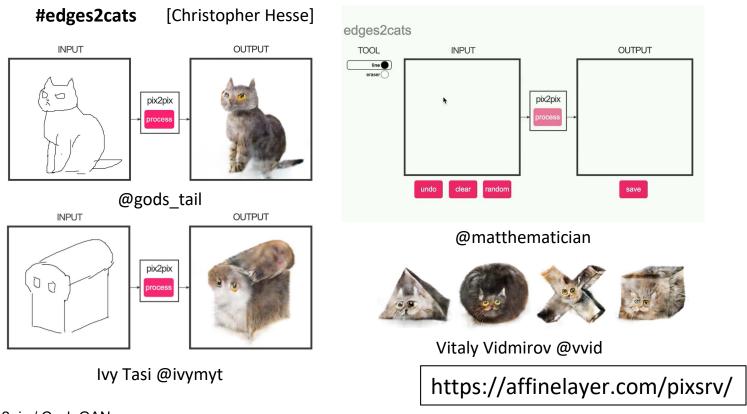


Trained on Edges → Images

Data from [Eitz, Hays, Alexa, 2012]

Pix2pix / CycleGAN

Applications: Edges to Images



Pix2pix / CycleGAN

Applications: Changing Artistic Style



Pix2pix / CycleGAN

Applications: Changing Seasons



Pix2pix / CycleGAN

Extra

Taxonomy of Generative Models

Ffjord

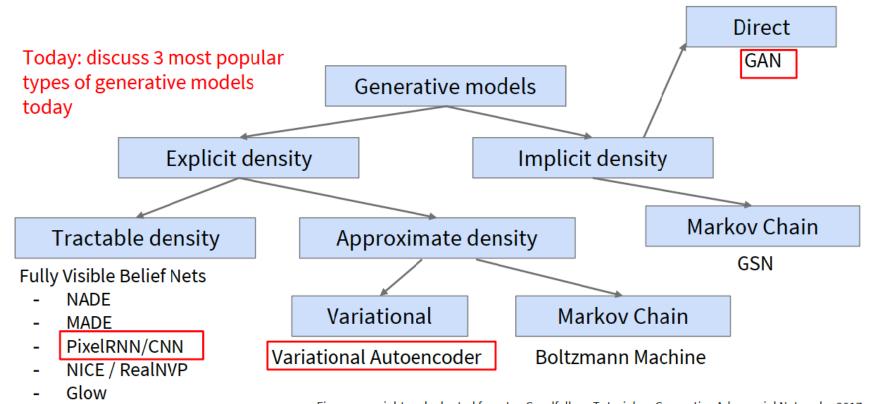


Figure copyright and adapted from Ian Goodfellow, Tutorial on Generative Adversarial Networks, 2017.

PixelCNN [van der Oord et al. 2016]

Still generate image pixels starting from corner

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

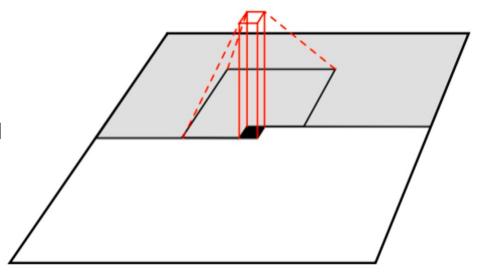


Figure copyright van der Oord et al., 2016

Pixe CNN [van der Oord et al. 2016]

Still generate image pixels starting from corner

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

Training is faster than PixelRNN (can parallelize convolutions since context Region values known from training images)

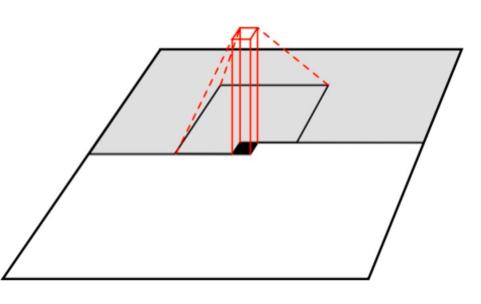
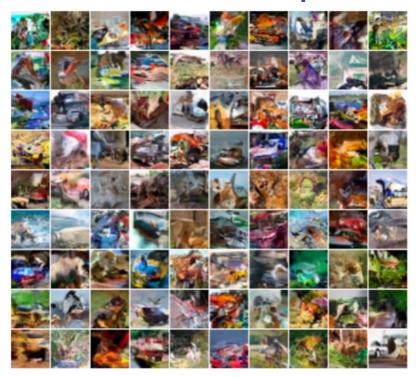


Figure copyright van der Oord et al., 2016

Generation is still slow:

For a 32x32 image, we need to do forward passes of the network 1024 times for a single image

Generation Samples





32x32 CIFAR-10

32x32 ImageNet

Figures copyright Aaron van der Oord et al., 2016

PixelRNN and PixelCNN

Pros:

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

Cons:

- 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++)

How to improve PixelCNN?

What are the limitations of PixelCNN/RNN?

- Slow sampling time.
- May accumulate errors over multiple steps. (might not be a big issue for image completion)



How can we further improve results?

VQ-VAE-2: VAE+PixelCNN

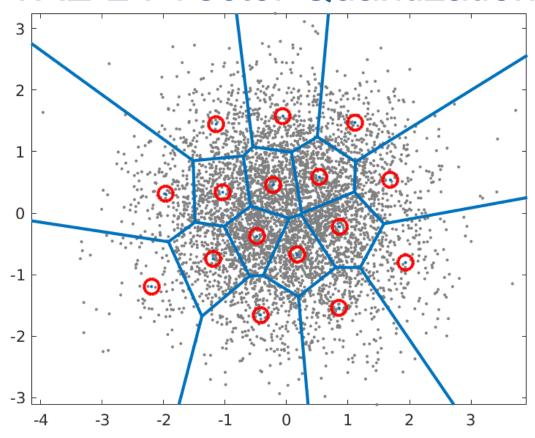


VQ (Vector quantization) maps continuous vectors into discrete codes

Common methods: clustering (e.g., k-means)

Generating Diverse High-Fidelity Images with VQ 45 -VAE-2 [Razavi et al., 2019]

VQ-VAE-2: Vector Quantization

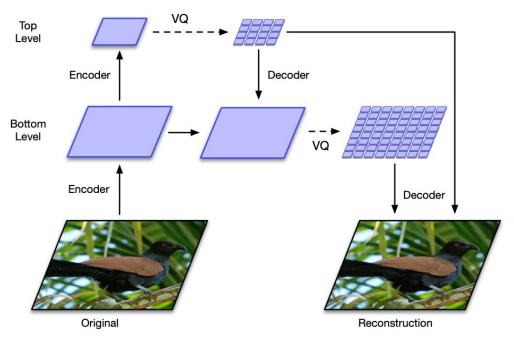


K-means, EM (GMM), end-to-end learning

https://wiki.aalto.fi/pages/viewpage.action?pageId=149883153

VQ-VAE-2: VAE+PixelCNN

VQ-VAE Encoder and Decoder Training

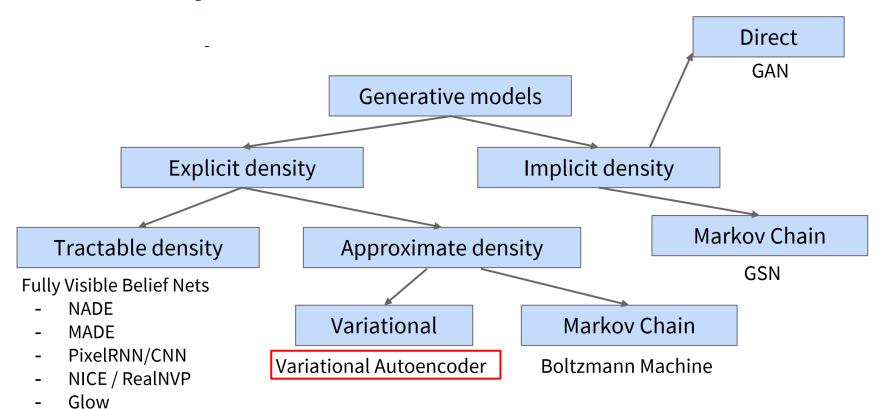


VAE+VQ: learn a more compact codebook for PixelCNN (instead of pixels) PixelCNN: use a more expressive bottleneck for VAE (instead of Gaussian

Generating Diverse High-Fidelity Images with VQ 45 -VAE-2 [Razavi et al., 2019]

Taxonomy of Generative Models

Ffjord



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

The Myth of the Cave



https://www.youtube.com/watch?v=1RWOpQXTItA&ab_channel=TED-Ed

What is a Latent Variable?



https://en.wikipedia.org/wiki/Myth of the Cave

The Myth of the Cave



https://en.wikipedia.org/wiki/Myth_of_the_Cave

Can we learn the true explanatory factors (e.g. latent variables) from only observed data?

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MIT Introduction to Deep Learning

<u>IntroToDeepLearning.com</u>

Variational AutoEncoders (VAE)

PixelRNN/CNNs define tractable density function, optimize likelihood of training data:

$$p_{\theta}(x) = \prod_{i=1}^{n} p_{\theta}(x_i|x_1, ..., x_{i-1})$$

Variational Autoencoders (VAEs) define intractable density function with latent z:

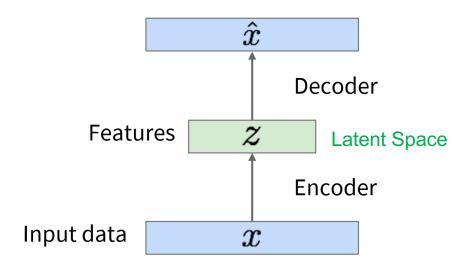
$$p_{ heta}(x) = \int p_{ heta}(z) p_{ heta}(x|z) dz$$

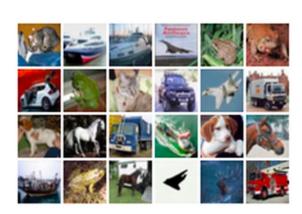
No dependencies among pixels, can generate all pixels at the same time!

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

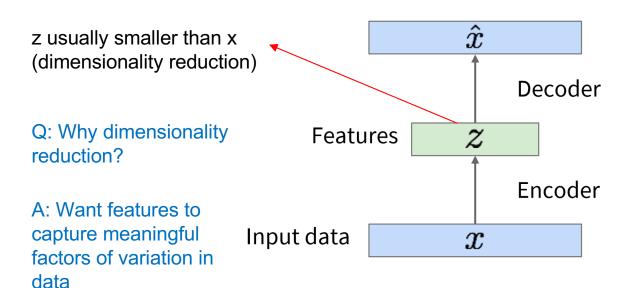
Why latent z?

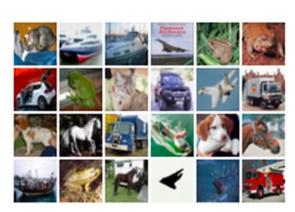
Unsupervised approach for learning a lower-dimensional feature representation from unlabeled training data





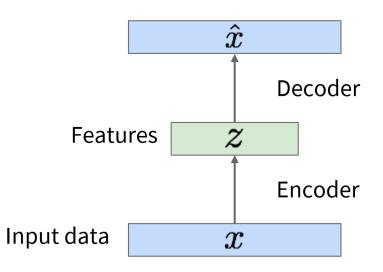
Unsupervised approach for learning a lower-dimensional feature representation from unlabeled training data

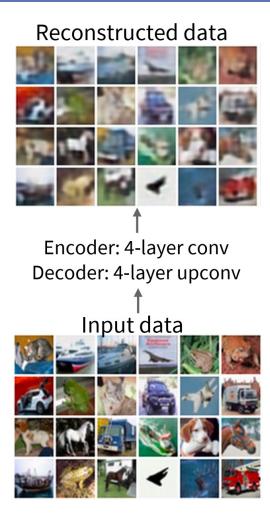




How to learn this feature representation?

Train such that features can be used to reconstruct original data "Autoencoding" - encoding input itself



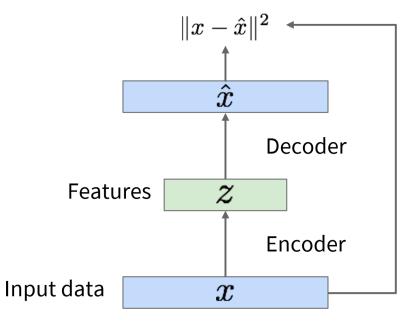


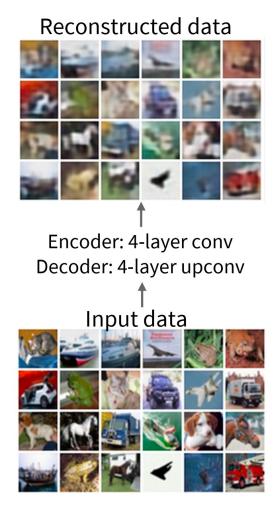
Slide credit: Fei-Fei Li

Train such that features can be used to reconstruct original data

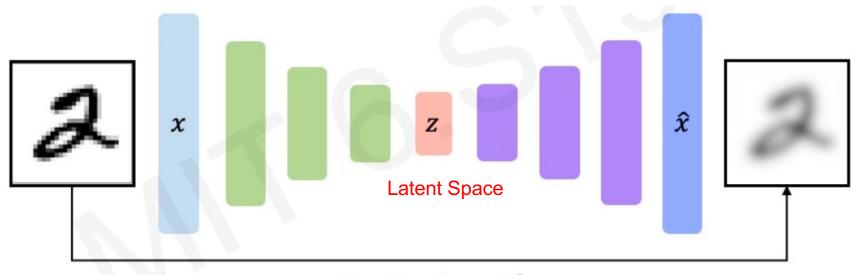
Doesn't use labels!

L2 Loss function:





How can we learn this latent space? Train the model to use these features to **reconstruct the original data**.



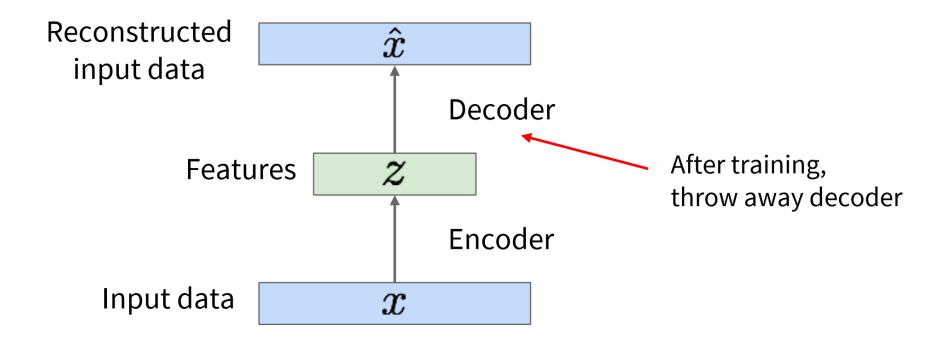
$$\mathcal{L}(x,\hat{x}) = \|x - \hat{x}\|^2$$

Loss function doesn't use any labels!!

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MIT Introduction to Deep Learning

IntroToDeepLearning.com



Background: AutoEncoders – Reconstruction Quality

Autoencoding is a form of compression!

Smaller latent space will force a larger training bottleneck

2D latent space



5D latent space



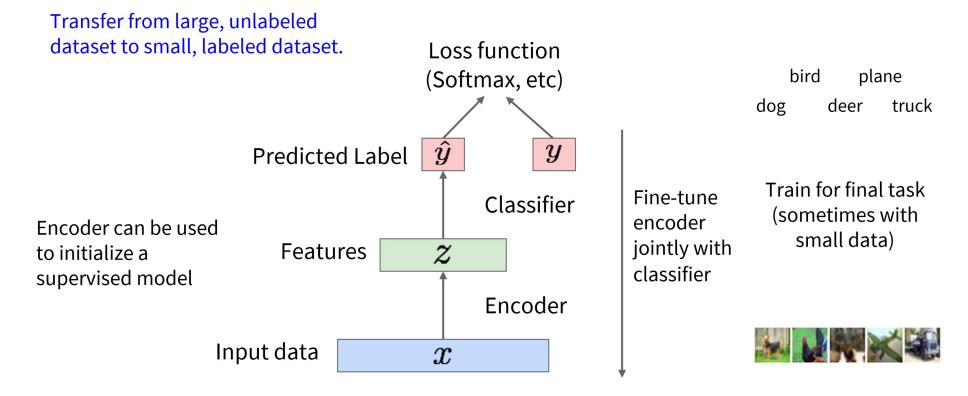
Ground Truth



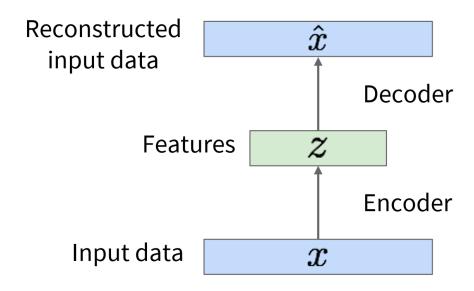
https://introtodeeplearning.com/

Slide credit: Ava Amini

Background: AutoEncoders



Background: AutoEncoders



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?

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

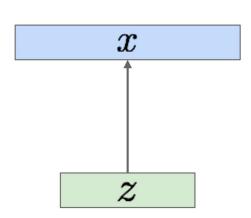
 $\{x^{(i)}\}_{i=1}^N$ is generated from the distribution of unobserved (latent) Assume training data representation z

Sample from true conditional

 $p_{\theta^*}(x \mid z^{(i)})$

Sample from true prior

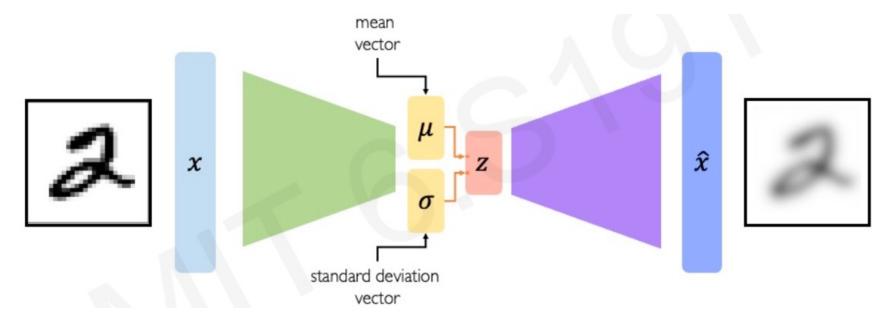
 $z^{(i)} \sim p_{ heta^*}(z)$



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

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

Variational AutoEncoders: Key Difference with AutoEncoders



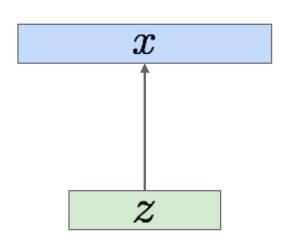
Variational autoencoders are a probabilistic twist on autoencoders! Sample from the mean and standard deviation to compute latent sample

Sample from true conditional

$$p_{\theta^*}(x \mid z^{(i)})$$

Sample from true prior

$$z^{(i)} \sim p_{ heta^*}(z)$$



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.

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

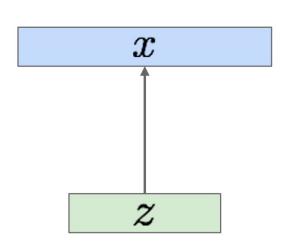
Kingma and Welling, "Auto-Encoding Variational Bayes", ICLR 2014

Sample from true conditional

$$p_{\theta^*}(x \mid z^{(i)})$$

Sample from true prior

$$z^{(i)} \sim p_{ heta^*}(z)$$



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

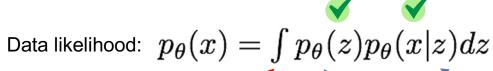
$$p_{\theta}(x) = \int p_{\theta}(z) p_{\theta}(x|z) dz$$

Q: What is the problem with this?

A: Intractable!

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

Variational AutoEncoders: Intractability



Simple Gaussian prior

Decoder neural network

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

Slide credit: Serena Young

Variational AutoEncoders: Intractability

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

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

Intractable data likelihood

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

Variational AutoEncoders: Intractability

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

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

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

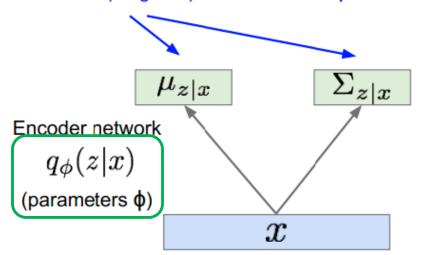
Will see that the approximate posterior allows us to derive a lower bound on the data likelihood that is tractable, which we can optimize.

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

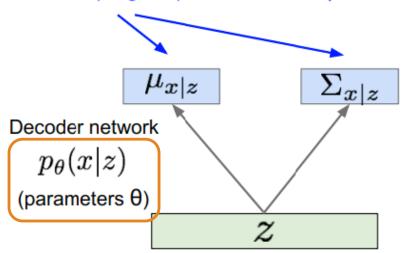
Kingma and Welling, "Auto-Encoding Variational Bayes", ICLR 2014

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

Mean and (diagonal) covariance of **z | x**

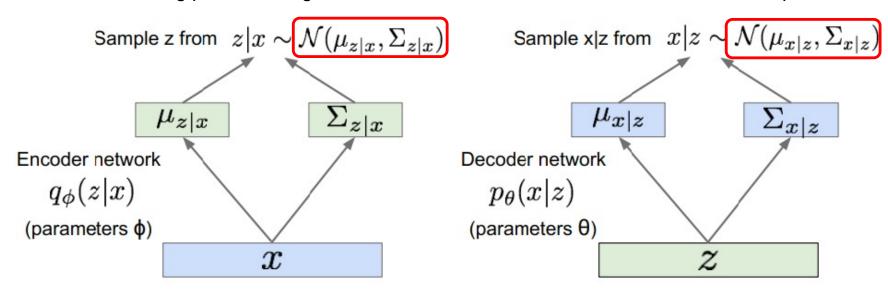


Mean and (diagonal) covariance of x | z



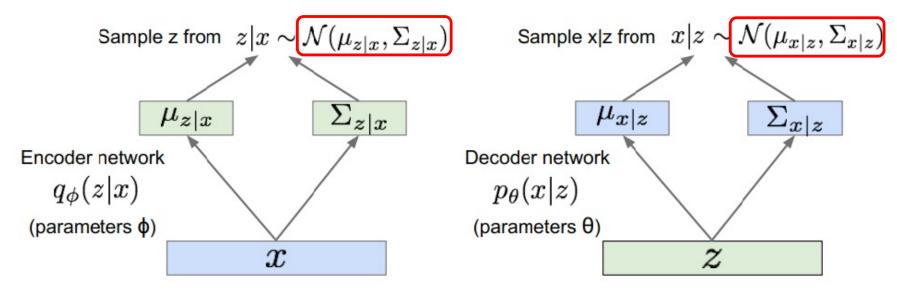
Kingma and Welling, "Auto-Encoding Variational Bayes", ICLR 2014

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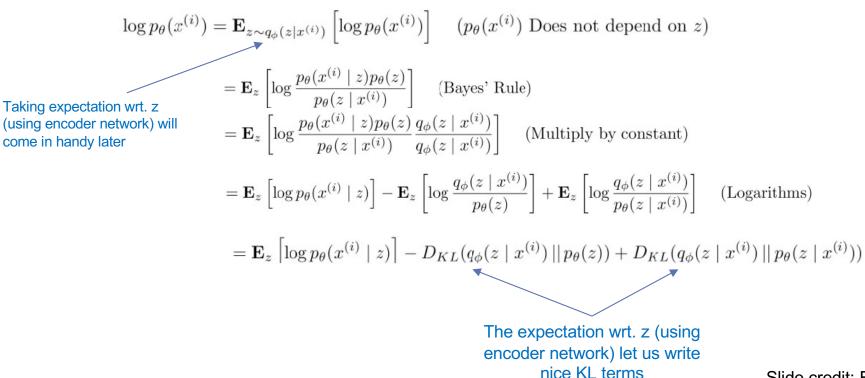
Since we're modeling probabilistic generation of data, encoder and decoder networks are probabilistic



Encoder and decoder networks also called "recognition"/"inference" and "generation" networks

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

Now equipped with our encoder and decoder networks, let's work out the (log) data likelihood:



Now equipped with our encoder and decoder networks, let's work out the (log) data likelihood:

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

$$= \mathbf{E}_{z} \left[\log \frac{p_{\theta}(x^{(i)}|z)p_{\theta}(z)}{p_{\theta}(z|x^{(i)})} \right] \qquad (\text{Bayes' Rule})$$

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

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

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

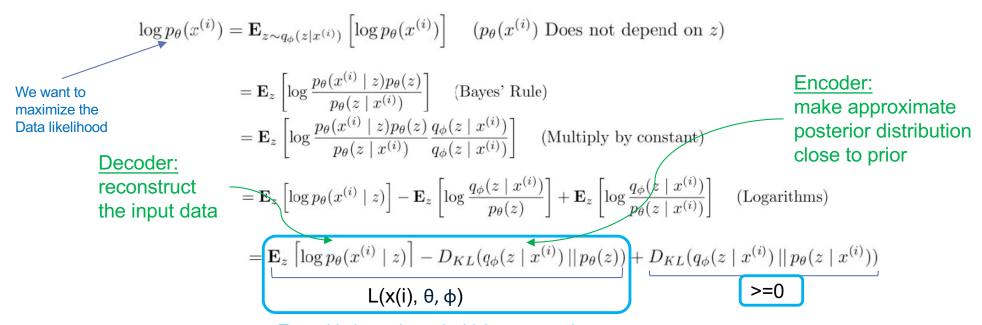
Decoder network gives $p\theta(x|z)$, can compute estimate of this term through sampling (need some trick to differentiate through sampling).

This KL term (between
Gaussians for encoder and z
prior) has nice closed-form
solution!

¹ https://statproofbook.github.io/P/kl-nonneg.html

pθ(z|x) intractable (saw earlier), can't compute this KL term :(But we know KL divergence always >= 0¹

Now equipped with our encoder and decoder networks, let's work out the (log) data likelihood:

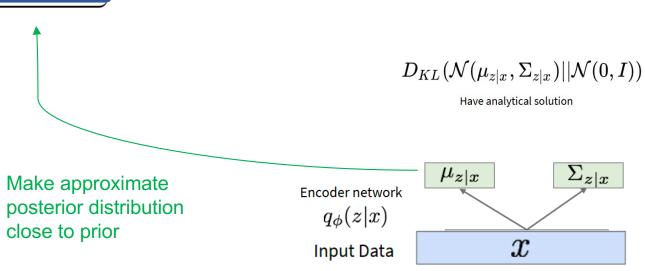


Tractable lower bound which we can take gradient of and optimize! ($p_{\theta}(x|z)$ differentiable, KL term differentiable)

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



Variational AutoEncoders: KL Divergence

$$D_{KL}(\mathcal{N}(\mu_{z|x},\Sigma_{z|x})||\mathcal{N}(0,I))$$

Inferred Latent
Distribution

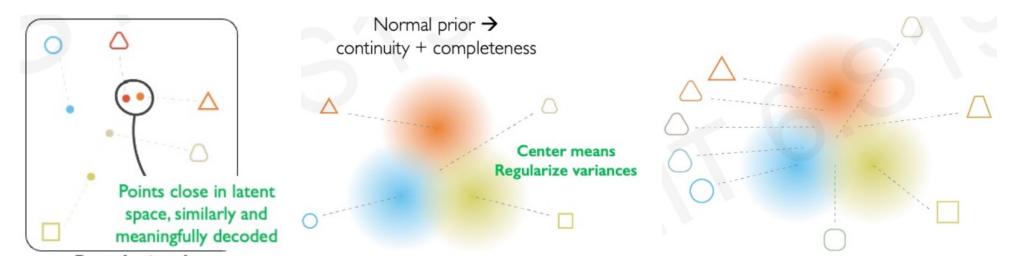
Fixed Prior on Latent Distribution

- Encourage encodings to distribute them evenly around the center of the latent space
- Penalize the network when it tries to "cheat" by clustering points in specific regions (i.e. memorizing data)

Variational AutoEncoders: KL Divergence

What properties do we want to achieve from KL Divergence?

- 1. Continuity: Points that are close in latent space → similar content after decoding
- 2. Completeness: sampling from latent space → "meaningful" content after decoding

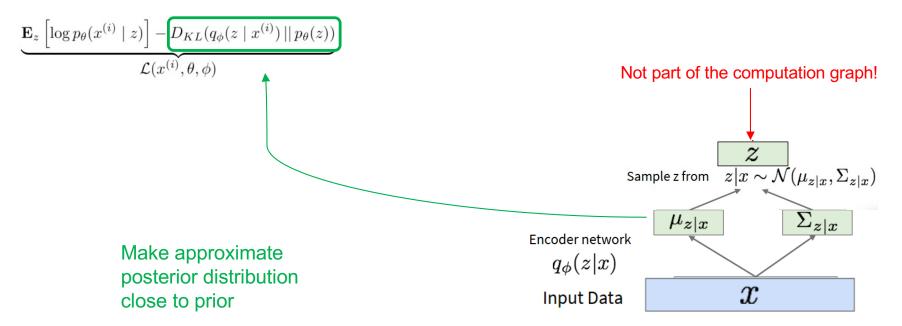


© Alexander Amini and Ava Amini

MIT Introduction to Deep Learning

<u>IntroToDeepLearning.com</u>

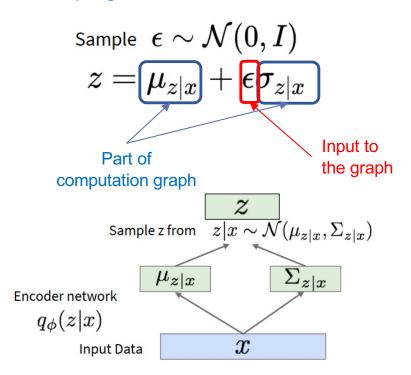
Putting it all together: maximizing the likelihood lower bound



Putting it all together: maximizing the likelihood lower bound

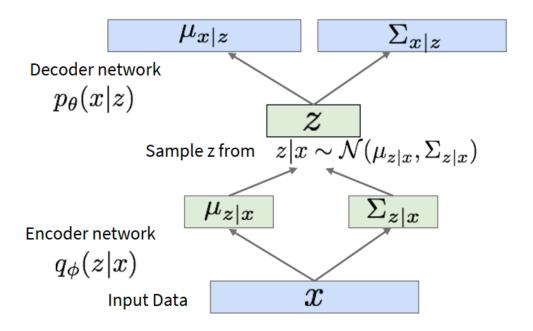
$$\underbrace{\mathbf{E}_{z} \left[\log p_{\theta}(x^{(i)} \mid z) \right] - D_{KL}(q_{\phi}(z \mid x^{(i)}) \mid\mid p_{\theta}(z))}_{\mathcal{L}(x^{(i)}, \theta, \phi)}$$

Reparameterization trick to make sampling differentiable:

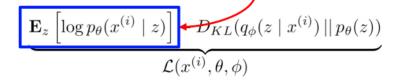


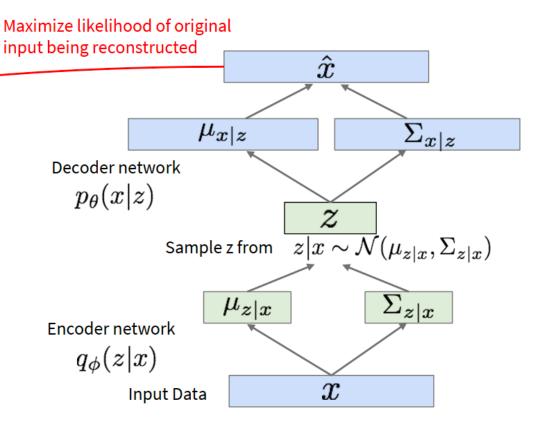
Putting it all together: maximizing the likelihood lower bound

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Putting it all together: maximizing the likelihood lower bound

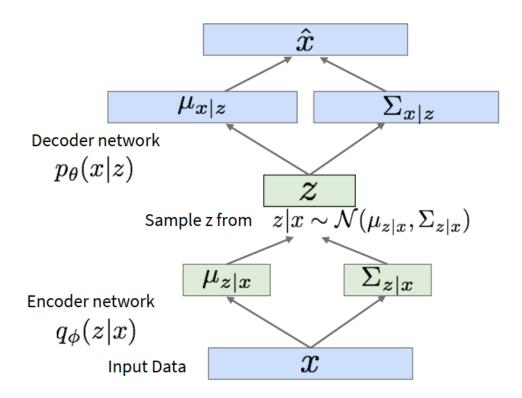




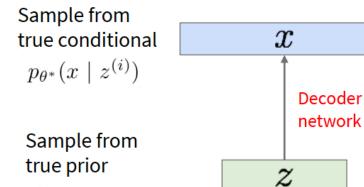
Putting it all together: maximizing the likelihood lower bound

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

For every minibatch of input data: compute this forward pass, and then backprop!

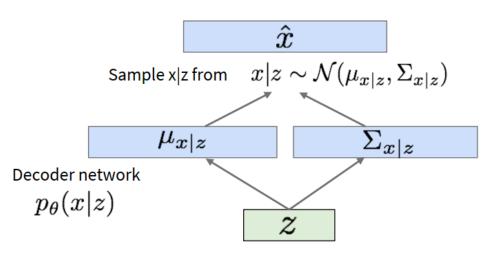


Our assumption about data generation process



 $z^{(i)} \sim p_{ heta^*}(z)$

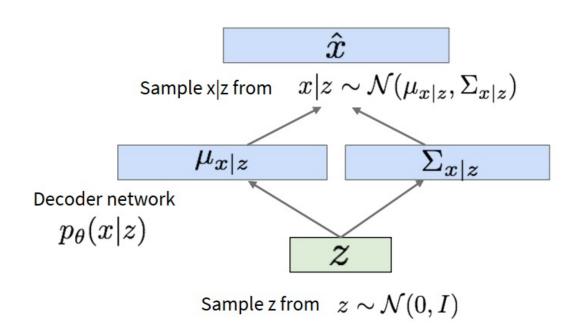
Now given a trained VAE: use decoder network & sample z from prior!



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

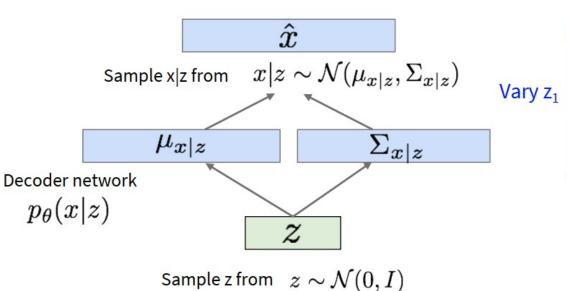
Kingma and Welling, "Auto-Encoding Variational Bayes", ICLR 2014

Use decoder network. Now sample z from prior!



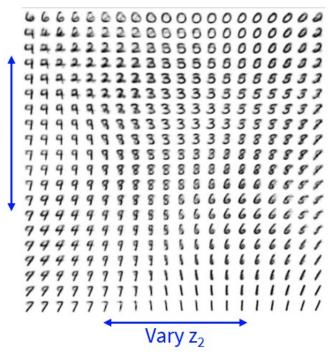
Kingma and Welling, "Auto-Encoding Variational Bayes", ICLR 2014

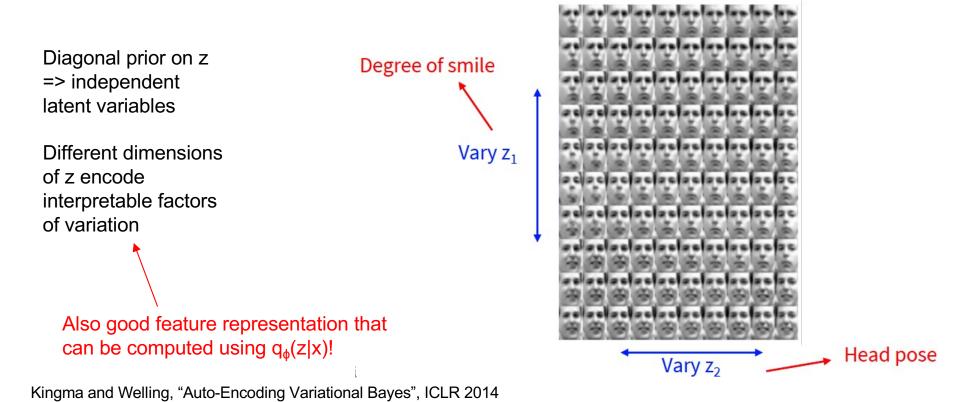
Use decoder network. Now sample z from prior!



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

Data manifold for 2-d z









Labeled Faces in the Wild

32x32 CIFAR-10

Figures copyright (L) Dirk Kingma et al. 2016; (R) Anders Larsen et al. 2017.

Music VAE

https://magenta.tensorflow.org/music-vae

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:

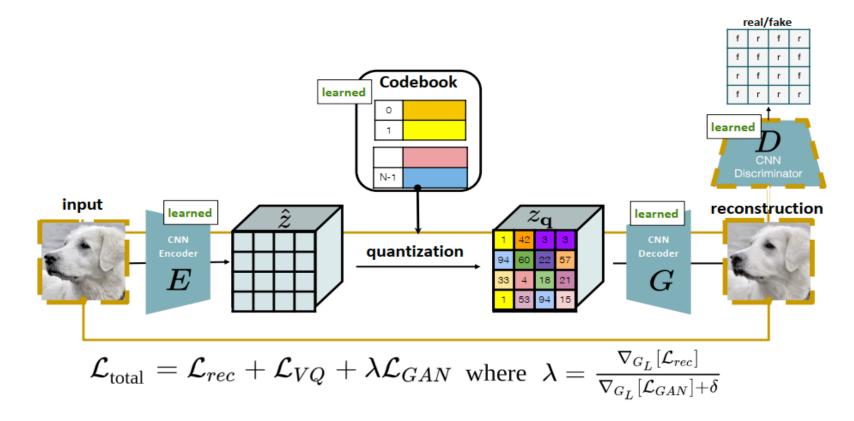
- More flexible approximations, e.g. richer approximate posterior instead of diagonal Gaussian, e.g., Gaussian Mixture Models (GMMs), Categorical Distributions.
- Learning disentangled representations.

GAN Example for Digits on Numpy

https://nbviewer.org/url/www.cs.toronto.edu/~rgrosse/courses/csc321 2018/tutorials/tut9 GAN.ipynb#



From VQ-VAE to VQGAN



Slide credit: Robin Rombach

From VQ-VAE to VQGAN



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