Unsupervised Learning: PCA, Clustering, AutoEncoder, and Generative Adversarial Networks

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Supervised Learning

- **Data**: (x, y)
  x is input, y is output/response (label)
- **Goal**: Learn a *function* to map x -> y
- **Examples**:
  - Classification,
  - regression,
  - object detection,
  - semantic segmentation,
  - image captioning, etc.

Cat

Today: Unsupervised Learning

- **Data**: x
  Just input data, no output labels!
- **Goal**: Learn some underlying hidden *structure* of the data
- **Examples**:
  - Clustering,
  - dimensionality reduction (manifold learning),
  - Density (probability) estimation,
  - Generative models:
    - Autoencoder
    - GANs, etc.

Generative Models

Given training data, generate new samples from same distribution

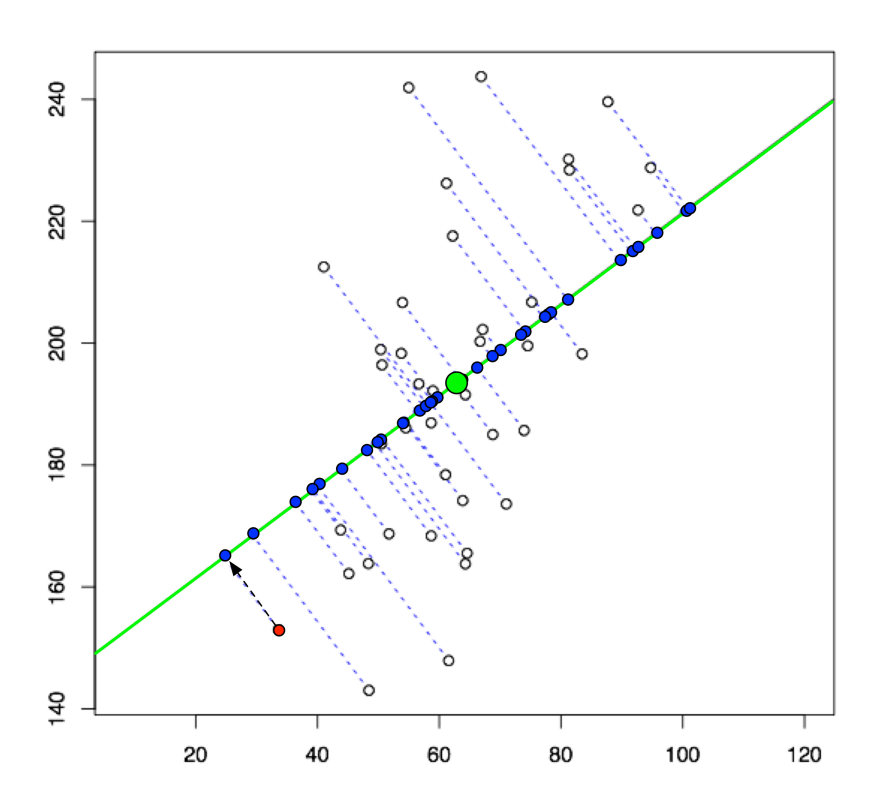
Training data ~ $p_{data}(x)$

Generated samples ~ $p_{model}(x)$

Want to learn $p_{model}(x)$ similar to $p_{data}(x)$

PCA: Principal Component Analysis

Can you find a low dimensional affine representation?



- Data: $\mathbf{x}_i = (x_{i1}, ..., x_{ip})$, $i = 1, ..., n$.
- Compute sample covariance matrix, e.g. $\mathbf{S} = \frac{1}{n}\sum_{i=1}^{n}(\mathbf{x}_i - \hat{\mu})^T(\mathbf{x}_i - \hat{\mu})$.
- Decompose into eigenvalue-eigenvector pairs:

$$\mathbf{S} = \hat{\mathbf{e}}\hat{\Lambda}\hat{\mathbf{e}}^T = (\hat{\mathbf{e}}_1 \vdots ... \vdots \hat{\mathbf{e}}_p)\hat{\Lambda}\begin{pmatrix}\hat{\mathbf{e}}_1 \\ \vdots \\ \hat{\mathbf{e}}_p\end{pmatrix}$$

  where $\hat{\Lambda} = diag(\hat{\lambda}_1, ..., \hat{\lambda}_p)$.
- $(\hat{\lambda}_k, \hat{\mathbf{e}}_k)$ are eigen-value-eigenvector pairs, $\hat{\lambda}_1 \geq ... \geq \hat{\lambda}_p$.

PCA

- The k-th sample PC.s:

$$Z_k = \begin{pmatrix} z_{1k} \\ \vdots \\ z_{nk} \end{pmatrix} = (\mathbf{X} - \mathbf{1}\hat{\mu}^T)\hat{\mathbf{e}}_k$$

  - $\hat{\mathbf{e}}_k$ is called the k-th *loading vector*
  - Component-wise, $z_{ik} = (\mathbf{x}_i - \hat{\mu})^T\hat{\mathbf{e}}_k$ are the k-th *principle component scores* of the i-th observation.
- $\hat{\lambda}_k$ measures the importance of the k-th PC.
- $\hat{\lambda}_k/(\hat{\lambda}_1 + ... + \hat{\lambda}_p) = \hat{\lambda}_k/trace(\mathbf{S})$ is interpreted as percentage of the total variation explained by Y_k.
- Usually retain the first few PCs.
- PCs are uncorrelated with each other.

Example: USArrests Data

For each of the 50 states in the United States, the data set contains the number of arrests per 100, 000 residents for each of three crimes: Assault, Murder, and Rape.
We also record UrbanPop (the percent of the population in each state living in urban areas).
The principal component score vectors Z_k have length $n = 50$, and the principal component loading vectors ($\hat{\mathbf{e}}_k$) have length $p = 4$.
PCA was performed after standardizing each variable to have mean zero and standard deviation one.

	PC1	PC2
Murder	0.5358995	0.4181809
Assault	0.5831836	0.1879856
UrbanPop	0.2781909	0.8728062
Rape	0.5434321	0.1673186

Table 10.1. The principal component loading vectors, $\hat{\mathbf{e}}_1$ and $\hat{\mathbf{e}}_2$, for the USArrests data. These are also displayed in Figure 10.1.

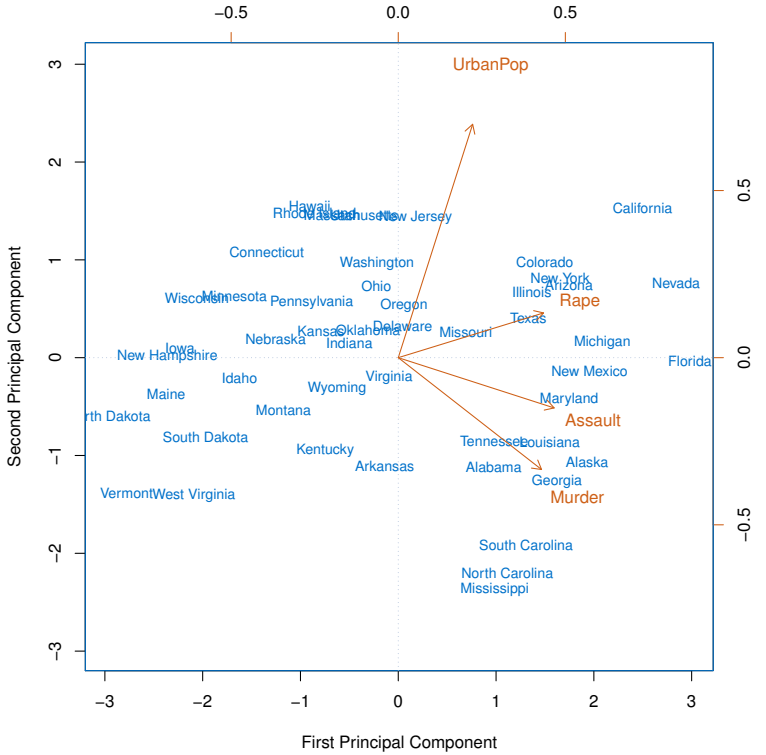


Figure: 10.1. Next page

Manifold Learning: Nonlinear Dimensionality Reduction

- MDS
- ISOMAP
- LLE: Locally linear Embedding
- Laplacian Eigenmap
- Hessian Eigenmap
- Diffusion Map
- LTSA: Local Tangent Space Alignment
- *MDS-SDP (Sensor-Network-Localization)
- t-SNE
- https://scikit-learn.org/stable/modules/manifold.html
- https://yao-lab.github.io/2020.csic5011/

K-Means Clustering

Algorithm 10.1 K-Means Clustering

- 1. Randomly assign a number, from 1 to K, to each of the observations. These serve as initial cluster assignments for the observations.
- 2. Iterate until the cluster assignments stop changing:
  1. For each of the K clusters, compute the cluster centroid. The kth cluster centroid is the vector of the p feature means for the observations in the kth cluster.
  2. Assign each observation to the cluster whose centroid is closest (where closest is defined using Euclidean distance).

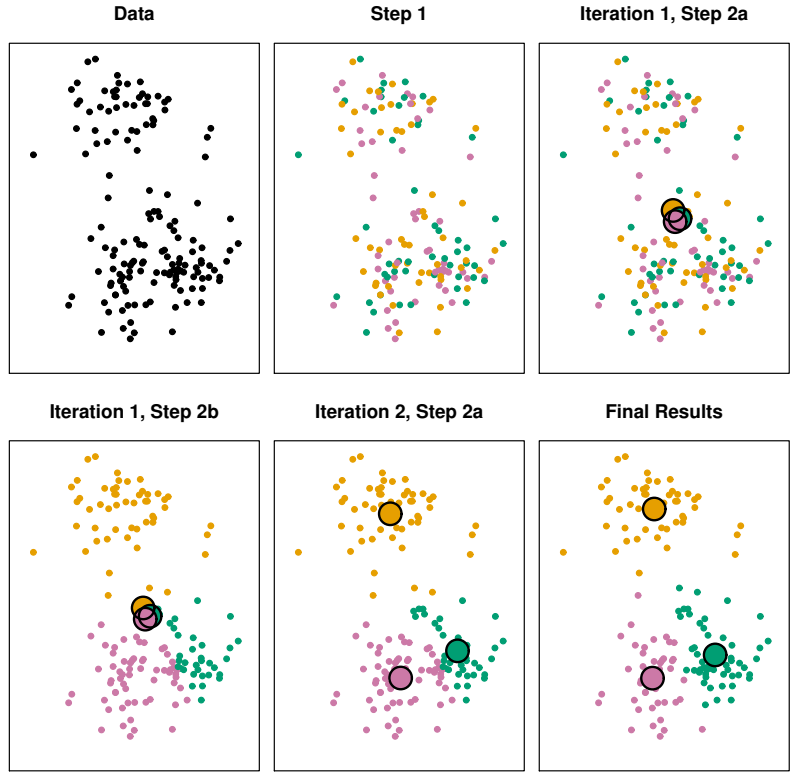


FIGURE 10.6. The progress of the K-means algorithm on the example of Figure 10.5 with $K = 3$. Top left: the observations are shown. Top center: in Step 1 of the algorithm, each observation is randomly assigned to a cluster. Top right: in Step 2(a), the cluster centroids are computed. These are shown as large colored disks. Initially the centroids are almost completely overlapping because the initial cluster assignments were chosen at random. Bottom left: in Step 2(b), each observation is assigned to the nearest centroid. Bottom center: Step 2(a) is once again performed, leading to new cluster centroids. Bottom right: the results obtained after ten iterations.

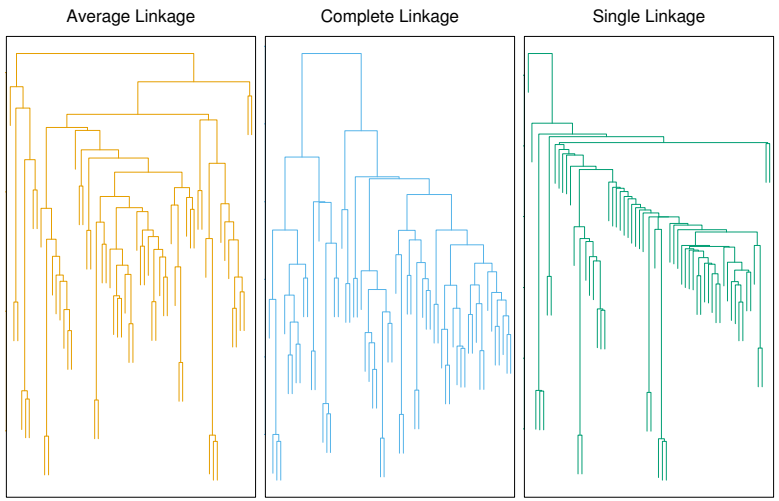
Figure: 10.6

Hierarchical Clustering Algorithms (Agglomerative)

- 1. Begin with n observations and a measure (such as Euclidean distance) of all the $\binom{n}{2} = n(n-1)/2$ pairwise dissimilarities. Treat each observation as its own cluster.
- 2. For $i = n, n-1, ...2$:
  1. Examine all pairwise inter-cluster dissimilarities among the i clusters and identify the pair of clusters that are least dissimilar (that is, most similar). Fuse these two clusters. The dissimilarity between these two clusters indicates the height in the dendrogram at which the fusion should be placed.
  2. Compute the new pairwise inter-cluster dissimilarities among the $i-1$ remaining clusters.

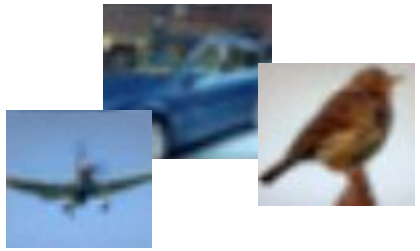
Linkage	Description
Complete	Maximal intercluster dissimilarity. Compute all pairwise dissimilarities between the observations in cluster A and the observations in cluster B, and record the largest of these dissimilarities.
Single	Minimal intercluster dissimilarity. Compute all pairwise dissimilarities between the observations in cluster A and the observations in cluster B, and record the smallest of these dissimilarities. Single linkage can result in extended, trailing clusters in which single observations are fused one-at-a-time.
Average	Mean intercluster dissimilarity. Compute all pairwise dissimilarities between the observations in cluster A and the observations in cluster B, and record the average of these dissimilarities.
Centroid	Dissimilarity between the centroid for cluster A (a mean vector of length p) and the centroid for cluster B. Centroid linkage can result in undesirable inversions.

TABLE 10.2. A summary of the four most commonly-used types of linkage



Generative Models

Given training data, generate new samples from same distribution



Training data ~ $p_{data}(x)$

Generated samples ~ $p_{model}(x)$

Want to learn $p_{model}(x)$ similar to $p_{data}(x)$

Generative Models

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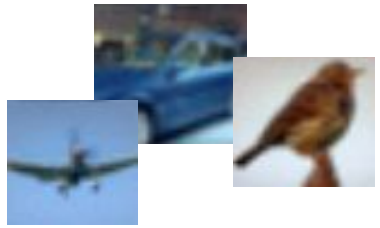


Training data ~ $p_{data}(x)$

Generated samples ~ $p_{model}(x)$

Want to learn $p_{model}(x)$ similar to $p_{data}(x)$

Addresses density estimation, a core problem in unsupervised learning

Several flavors:

- Explicit density estimation: explicitly define and solve for $p_{model}(x)$
- Implicit density estimation: learn model that can sample from $p_{model}(x)$ w/o explicitly defining it

Taxonomy of Generative Models

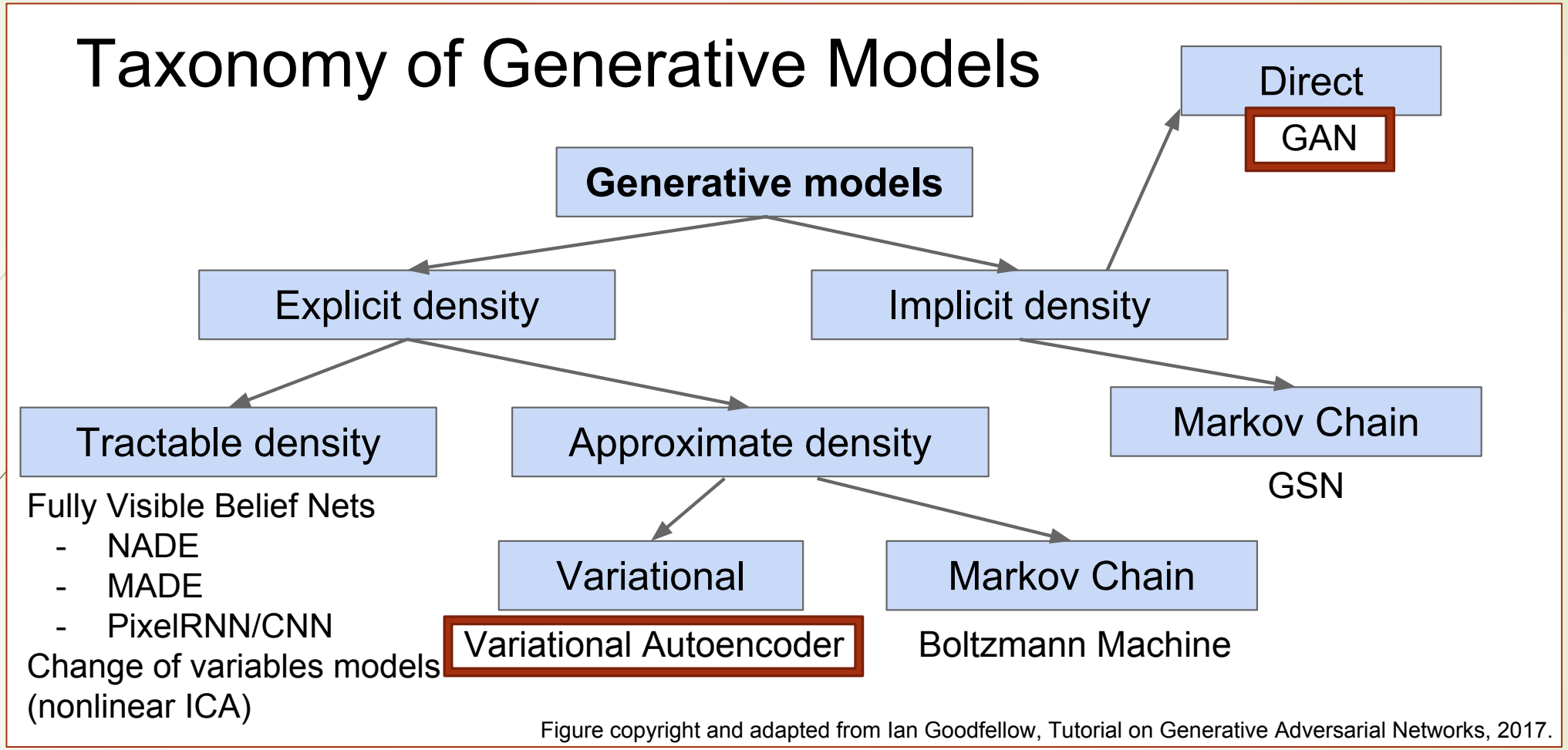


Figure copyright and adapted from Ian Goodfellow, Tutorial on Generative Adversarial Networks, 2017.

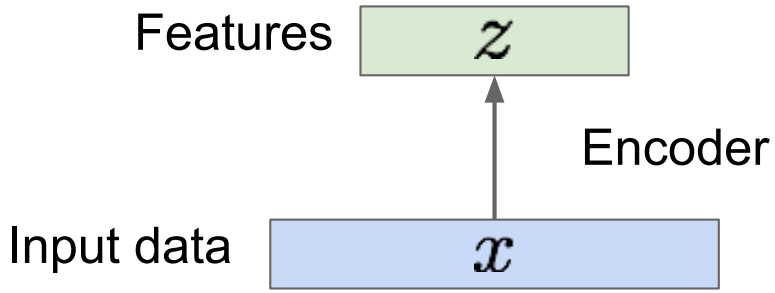
- We are going to focus on:
  - Variational AutoEncoder (VAE)
  - Generative Adversarial Network (GAN)

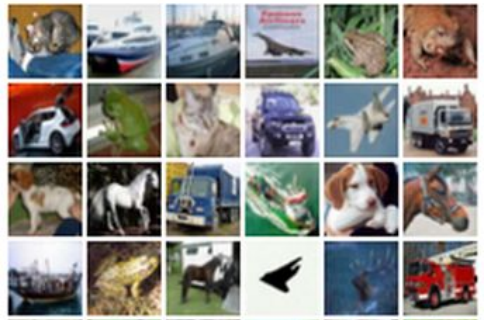
Variational Autoencoders (VAE)

Some background first: Autoencoders

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

e.g. PCA, Manifold Learning, Dictionary Learning

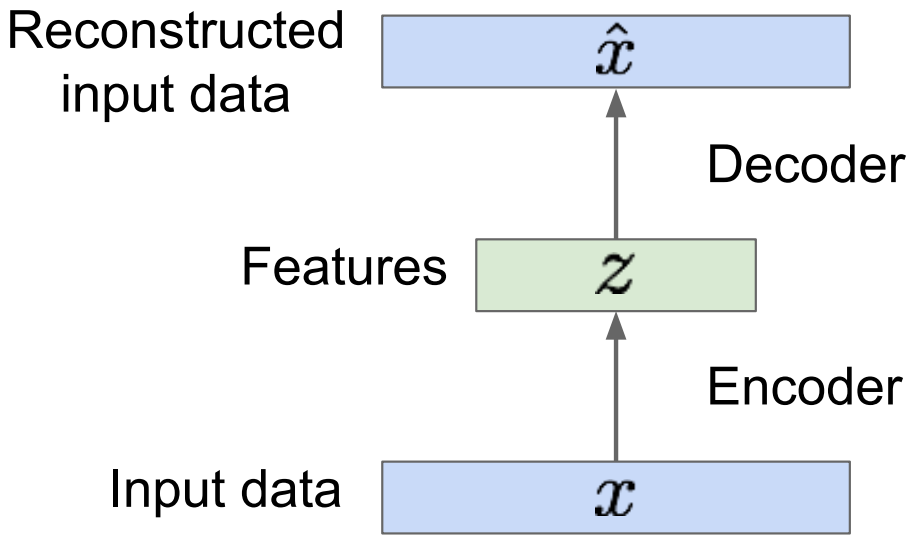




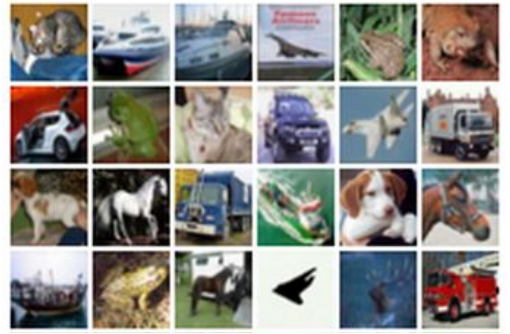
How to learn this feature representation?

Train such that features can be used to reconstruct original data

"Autoencoding" - encoding itself



e.g. PCA, Manifold Learning, Dictionary Learning, Matrix Factorization: D = E'



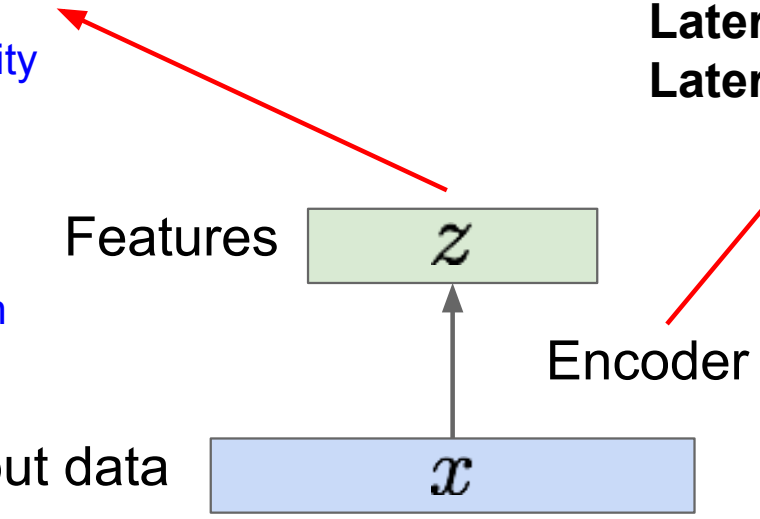
Deep Autoencoder

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

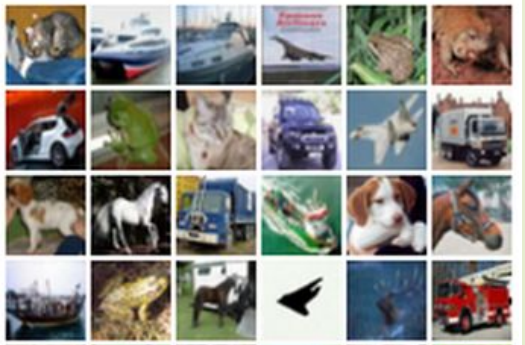
z usually smaller than **x** (dimensionality reduction)

Q: Why dimensionality reduction?

A: Want features to capture meaningful factors of variation in data



Originally: Linear + nonlinearity (sigmoid)
Later: Deep, fully-connected
Later: ReLU CNN

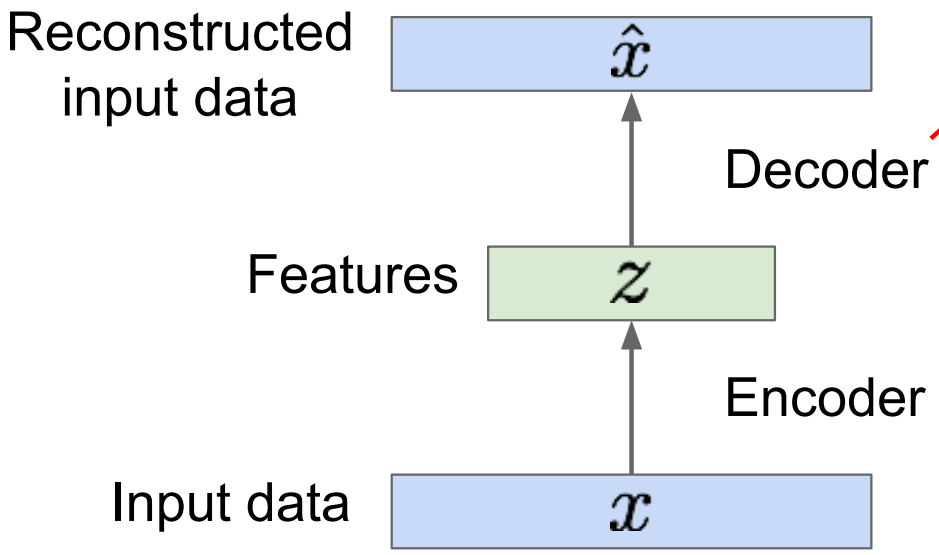


Deep Learning for decoders

How to learn this feature representation?

Train such that features can be used to reconstruct original data

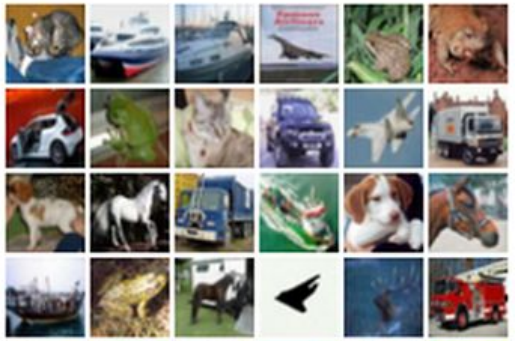
“Autoencoding” - encoding itself



Originally: Linear + nonlinearity (sigmoid)

Later: Deep, fully-connected

Later: ReLU CNN (upconv)

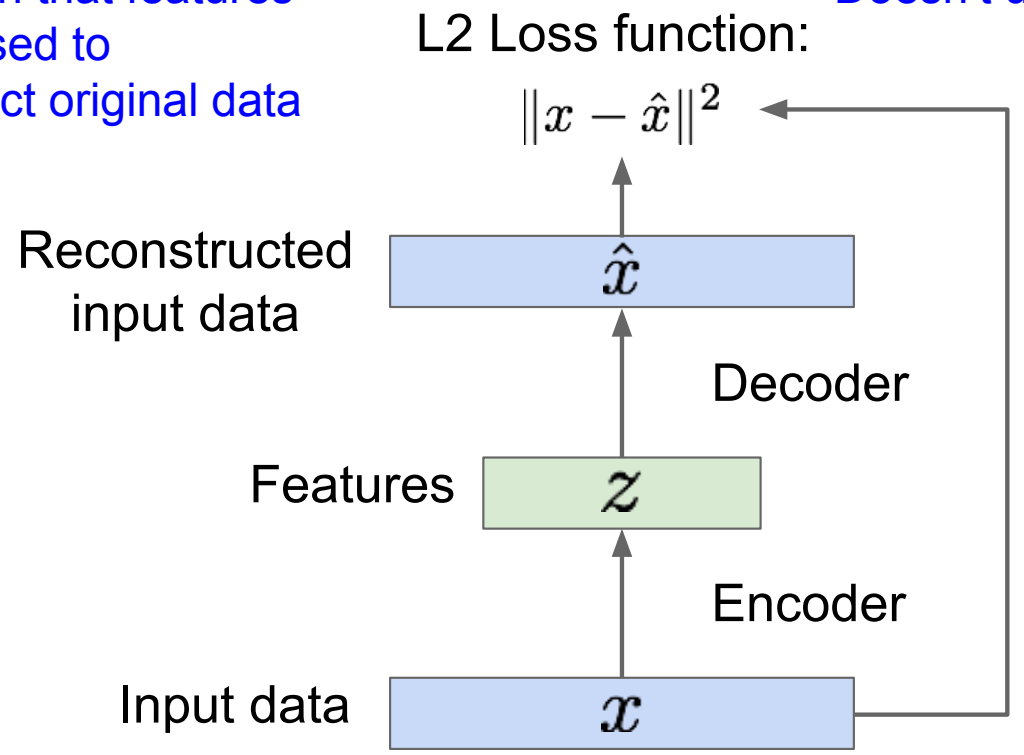


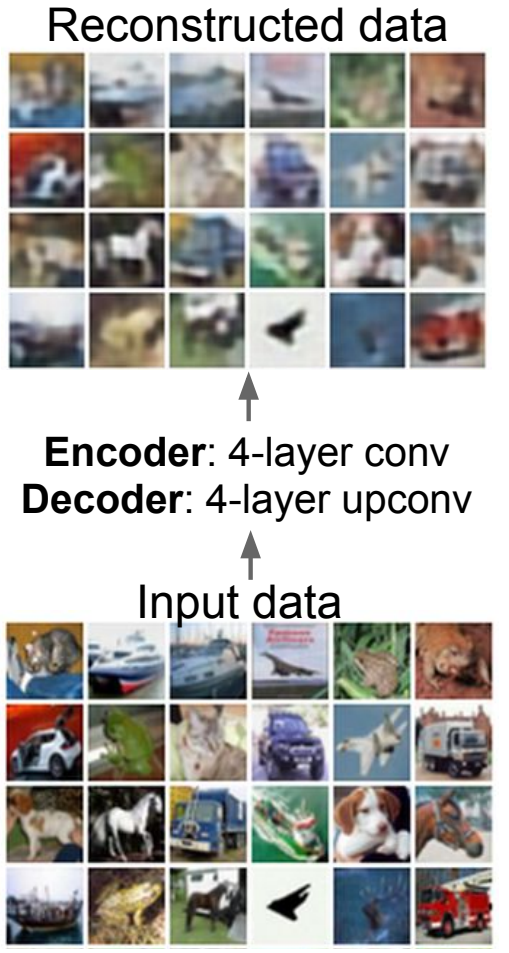
L2 Loss functions

Some background first: Autoencoders

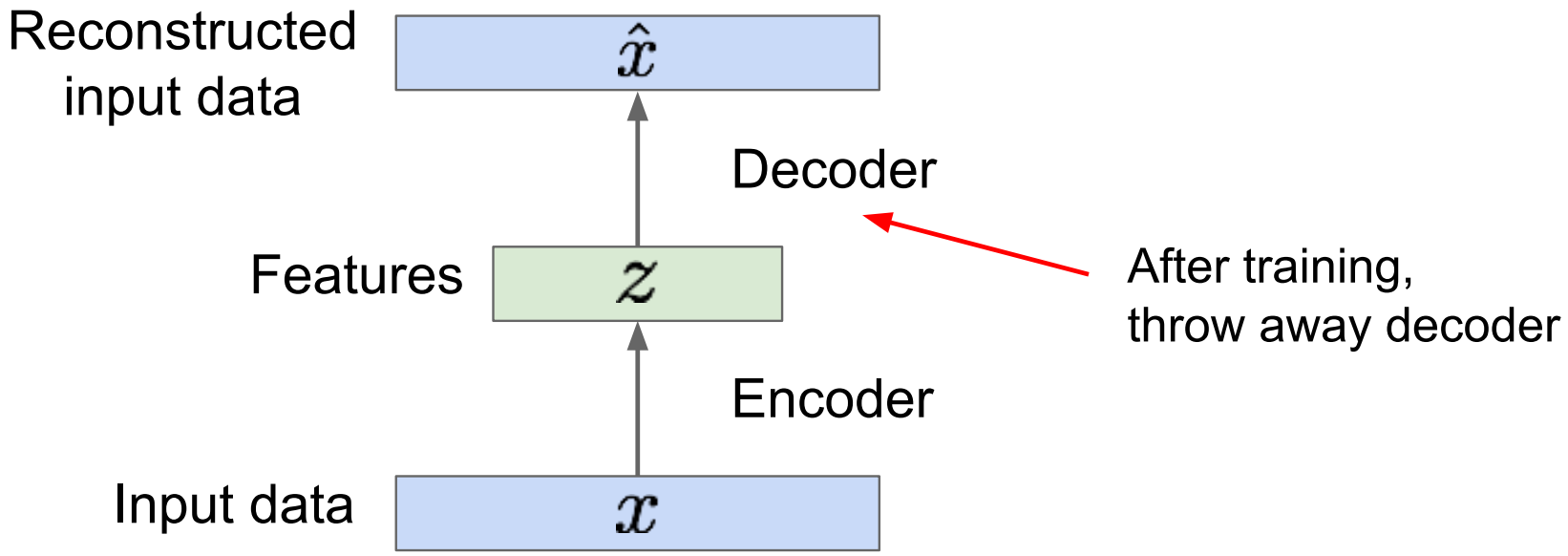
Train such that features can be used to reconstruct original data

Doesn't use labels!

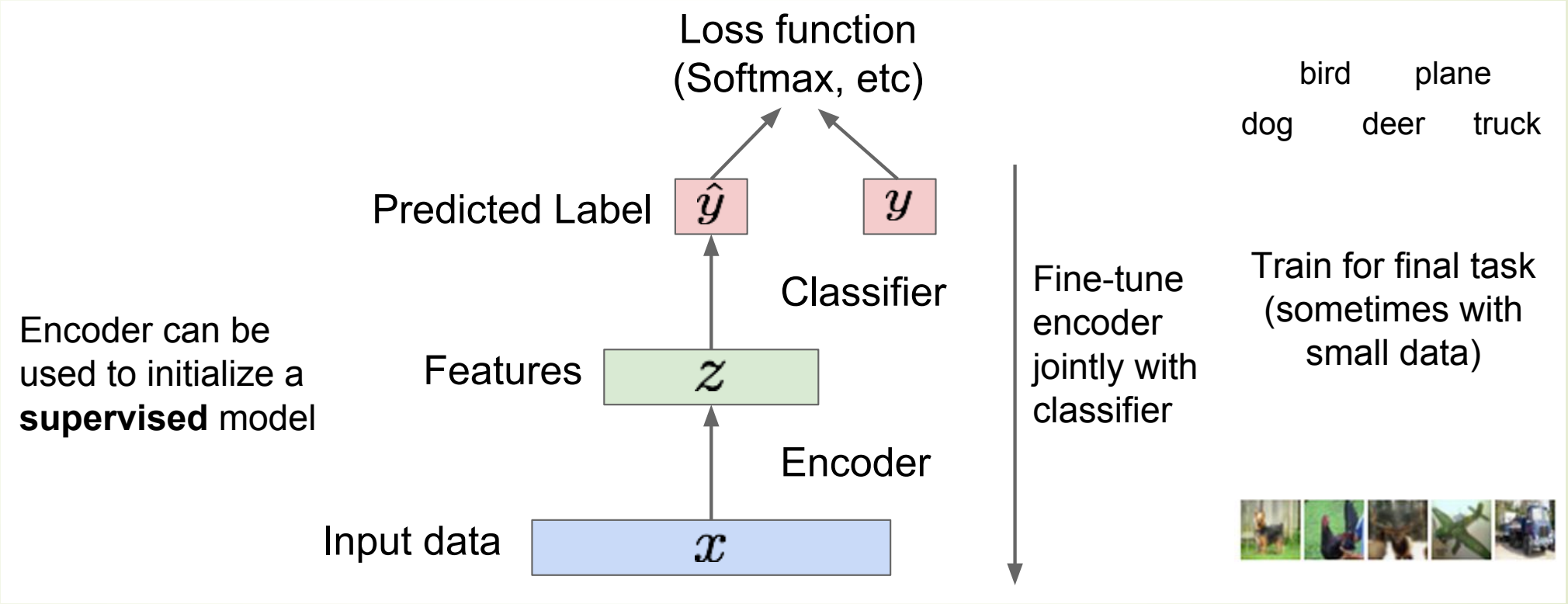


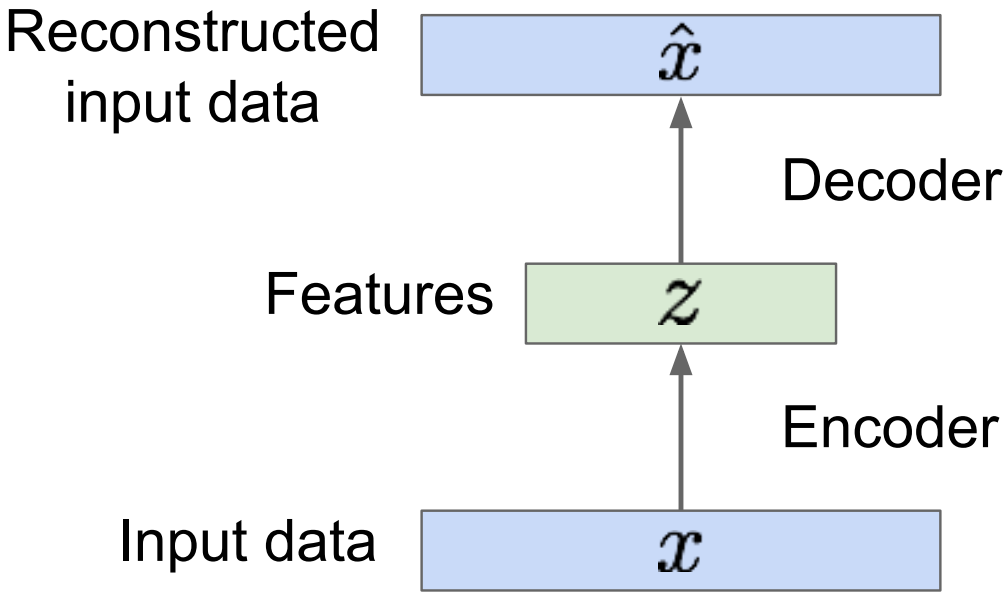


Some background first: Autoencoders



Autoencoders for Transfer Learning





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

Features capture factors of variation in training data. Can we generate new images from an autoencoder?

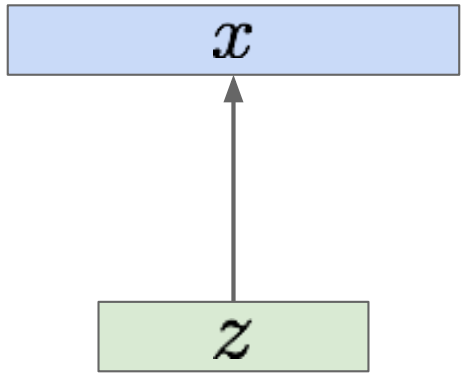
Variational Autoencoders

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 underlying unobserved (latent) representation **z**

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

Sample from true prior $p_{\theta^*}(z)$



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

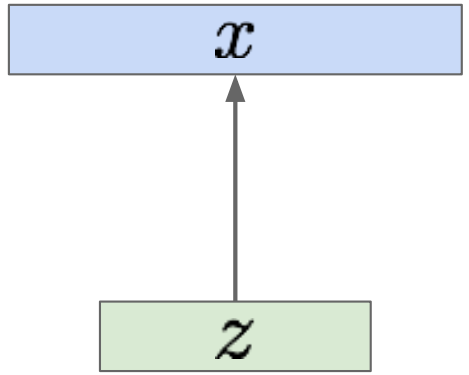
Variational Autoencoders

Sample from true conditional

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

Sample from true prior

$p_{\theta^*}(z)$



We want to estimate the true parameters θ^* of this generative model.

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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Sample from true conditional

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

Sample from true prior

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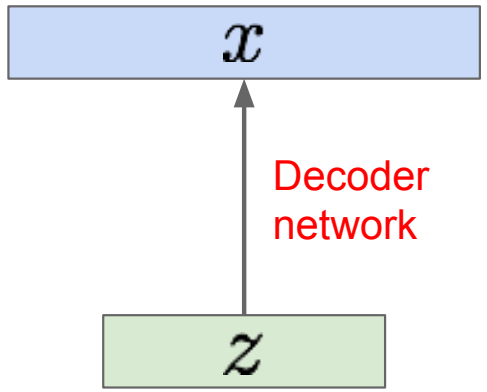


We want to estimate the true parameters θ^* of this generative model.

How should we represent this model?

Choose prior p(z) to be simple, e.g. Gaussian.

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

Kingma and Welling, “Auto-Encoding Variational Bayes”, ICLR 2014

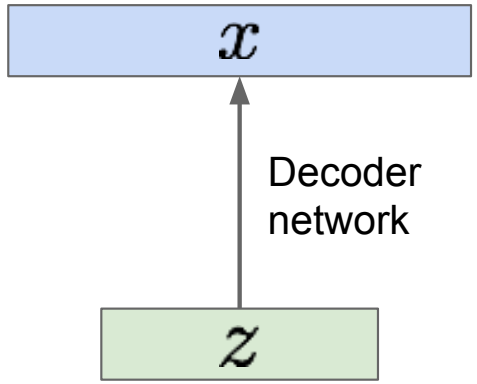
Variational Autoencoders

Sample from true conditional

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

Sample from true prior

$p_{\theta^*}(z)$



We want to estimate the true parameters θ^* of this generative model.

How to train the model?

Remember strategy for training generative models from FVBNs. Learn model parameters to maximize likelihood of training data

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

Now with latent z

Kingma and Welling, “Auto-Encoding Variational Bayes”, ICLR 2014

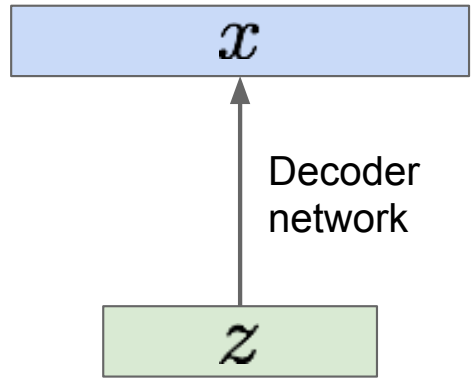
Variational Autoencoders

Sample from true conditional

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

Sample from true prior

$p_{\theta^*}(z)$



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Remember strategy for training generative models from FVBNs. 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

Variational Autoencoders: Intractability

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

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

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

Intractable data likelihood

Variational Lower Bounds

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

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

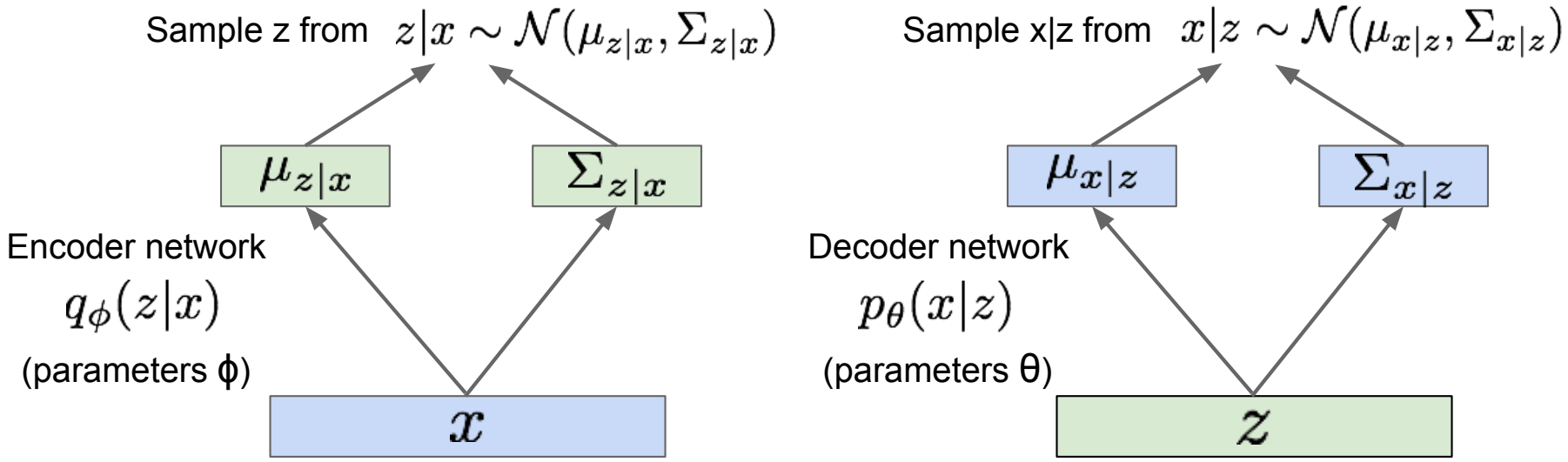
Solution: In addition to decoder network modeling $p_\theta(x|z)$, define additional encoder network $q_\phi(z|x)$ that approximates $p_\theta(z|x)$

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

Kingma and Welling, “Auto-Encoding Variational Bayes”, ICLR 2014

Variational Autoencoders

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

Assume that $\Sigma_{x|z}$ and $\Sigma_{z|x}$ are both diagonal, *i.e.* conditional independence.

Variational Autoencoders

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

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

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

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

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

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

Decoder network gives $p_\theta(x|z)$, can compute estimate of this term through sampling. (Sampling differentiable through reparam. trick, see paper.)

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

$p_\theta(z|x)$ intractable (saw earlier), can't compute this KL term :(But we know KL divergence always >= 0.

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

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

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

Variational Autoencoders

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

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

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

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

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

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

Reconstruct the input data

Make approximate posterior distribution close to prior

$$\log p_\theta(x^{(i)}) \geq \mathcal{L}(x^{(i)}, \theta, \phi)$$

Variational lower bound ("ELBO")

$$\theta^*, \phi^* = \arg\max_{\theta,\phi} \sum_{i=1}^{N} \mathcal{L}(x^{(i)}, \theta, \phi)$$

Training: Maximize lower bound

Stage I: Encoder

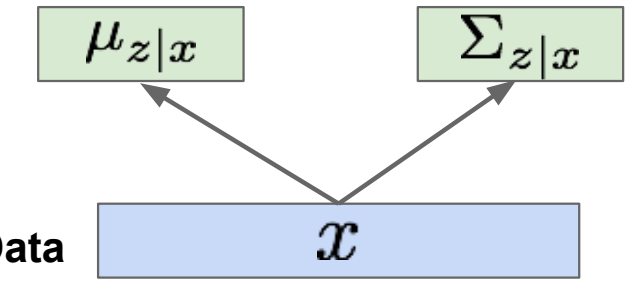
Putting it all together: maximizing the likelihood lower bound

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

Make approximate posterior distribution close to prior

Encoder network

$q_\phi(z|x)$



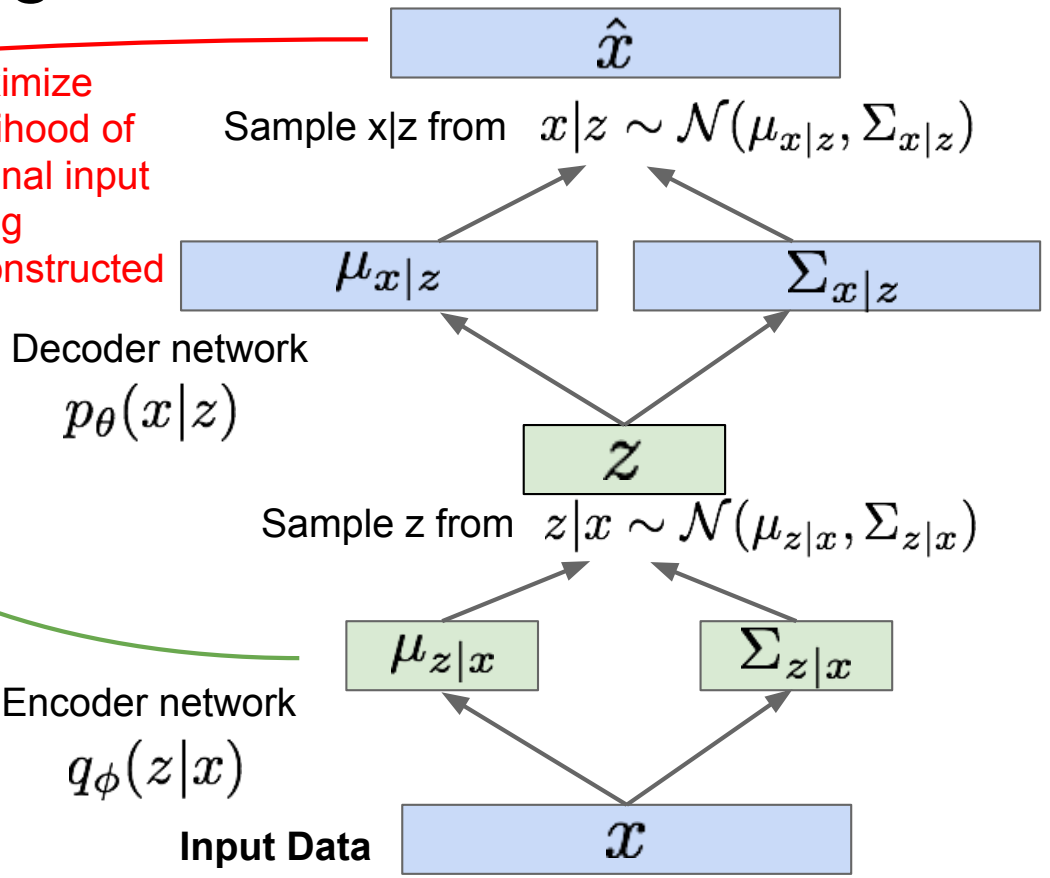
Stage II: Decoder.

Variational Autoencoders

Putting it all together: maximizing the likelihood lower bound

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

Maximize likelihood of original input being reconstructed

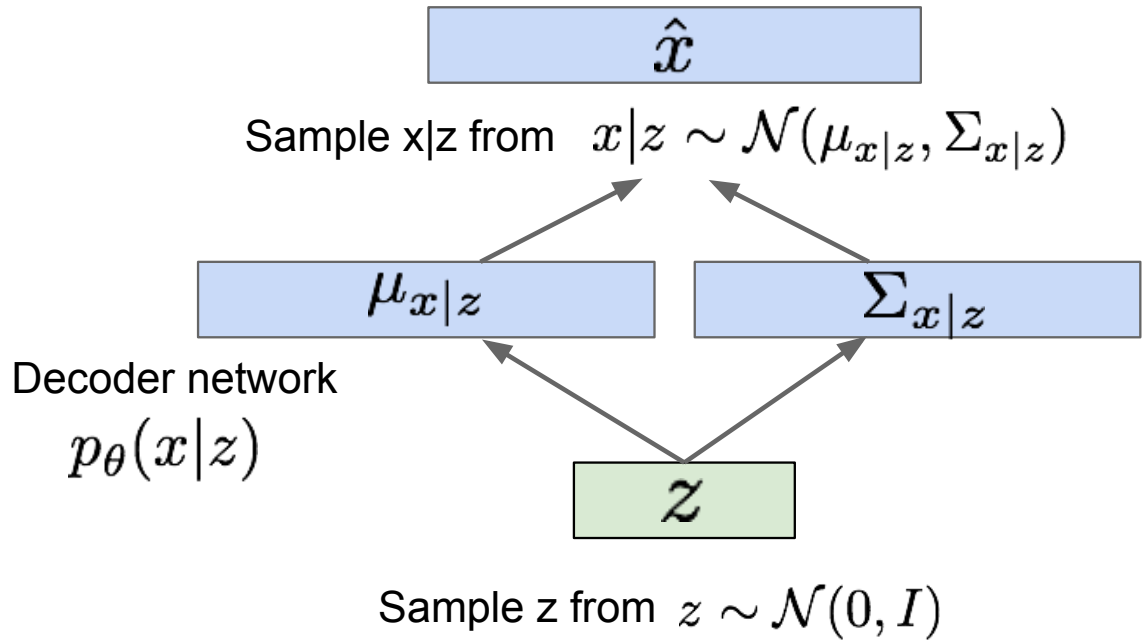


Make approximate posterior distribution close to prior

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

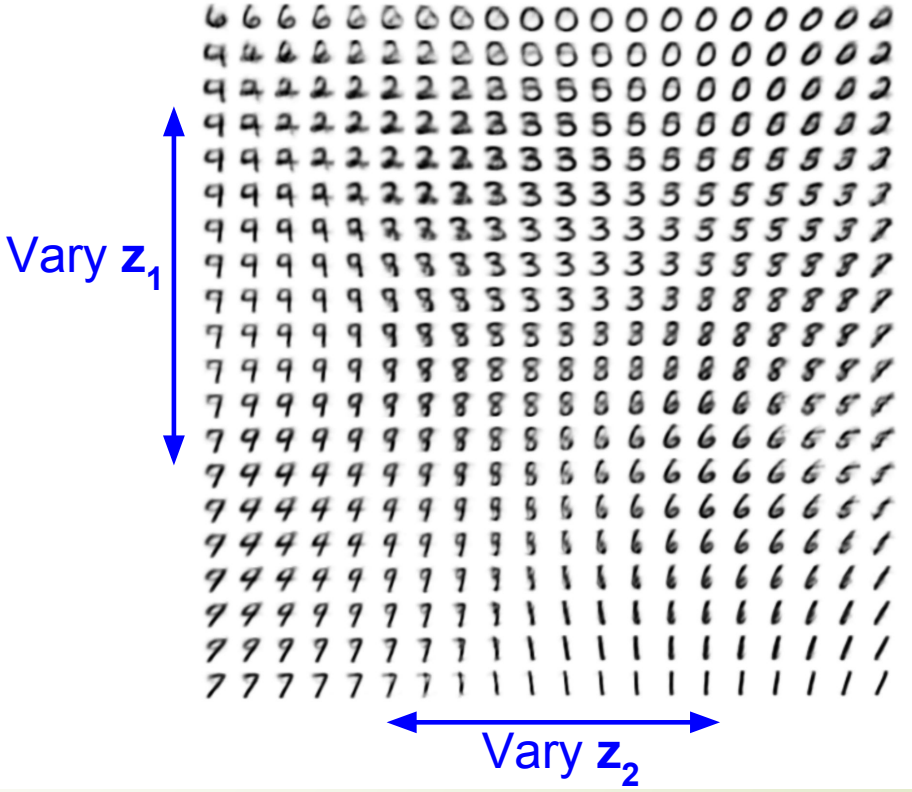
VAE: generating data

Use decoder network. Now sample z from prior!



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

Data manifold for 2-d **z**



VAE: generating data

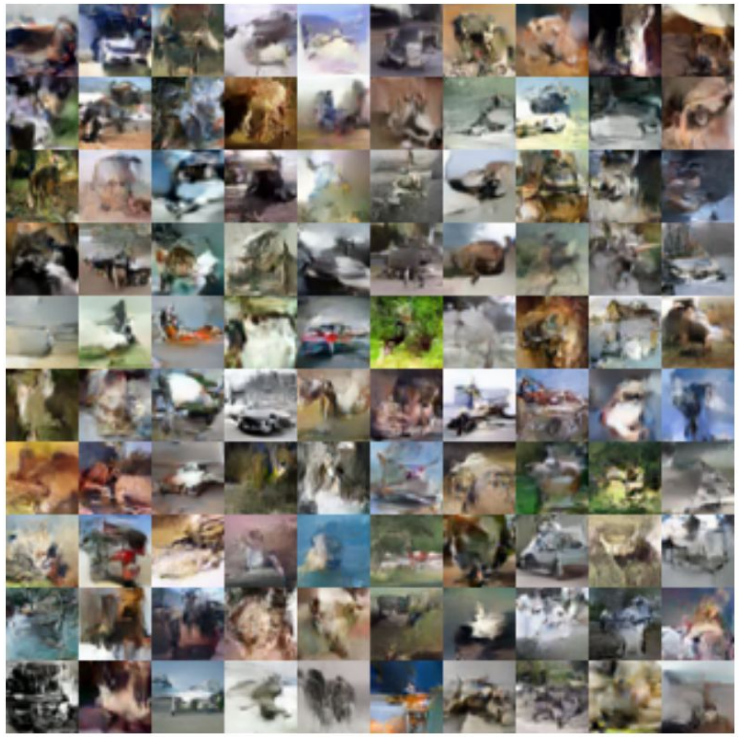
Diagonal prior on **z**
=> independent
latent variables

Different
dimensions of **z**
encode
interpretable factors
of variation

Also good feature representation that can be computed using $q_\phi(z|x)$!

Kingma and Welling, “Auto-Encoding Variational Bayes”, ICLR 2014

VAE: Generating Data



32x32 CIFAR-10

Labeled Faces in the Wild

Variational Autoencoders

- 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
  - Allows inference of q(z|x), can be useful feature representation for other tasks
- Cons:
  - Maximizes lower bound of likelihood
  - 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
  - Incorporating structure in latent variables

Generative Adversarial Networks (GAN)

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**:

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

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: don't work with any explicit density function!
Instead, take game-theoretic approach: learn to generate from training distribution through 2-player game

Generative Adversarial Networks

Ian Goodfellow et al., “Generative Adversarial Nets”, NIPS 2014

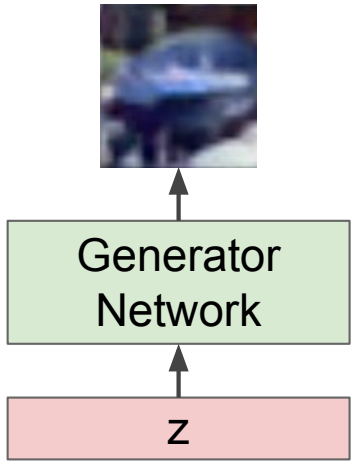
Problem: Want to sample from complex, high-dimensional training distribution. No direct way to do this!

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

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

A: A neural network!

Output: Sample from training distribution

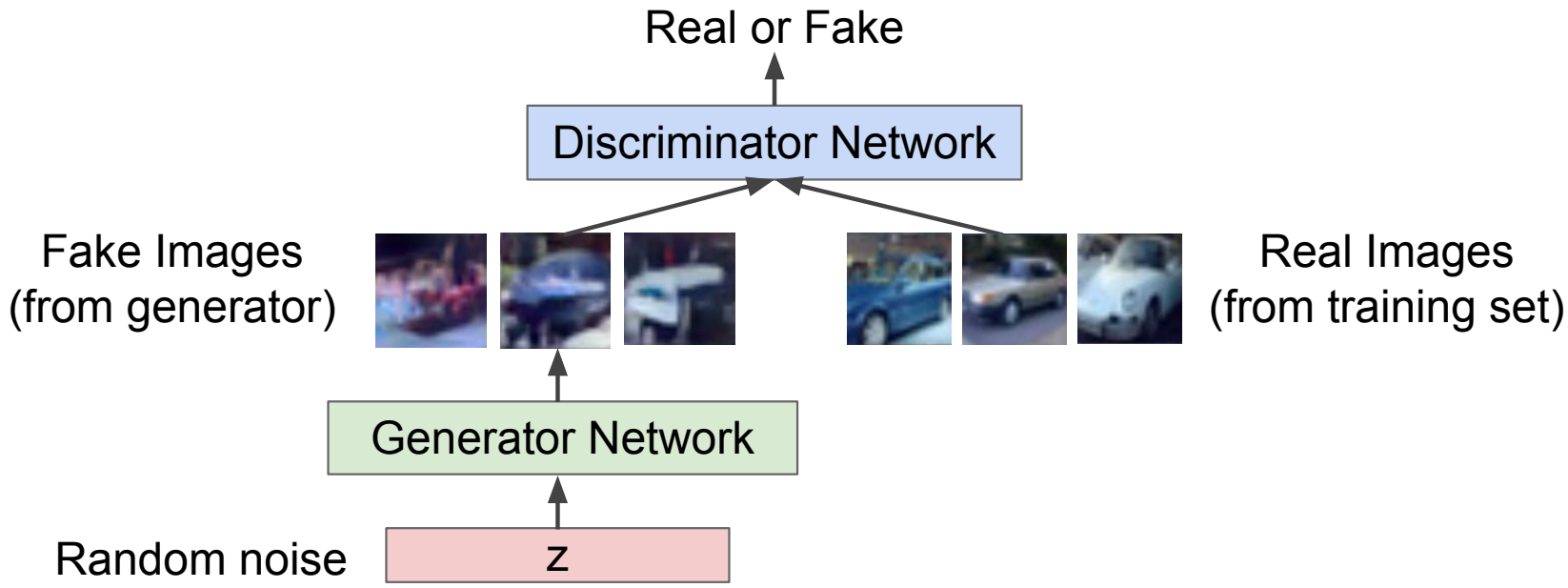


Input: Random noise

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



Training GANs: Minimax Game

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

Train jointly in **minimax game**

Minimax objective function:

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

Training GANs: Minimax Game

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

Train jointly in **minimax game**

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

Minimax objective function:

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

Discriminator output for real data x

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

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

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

The Issue in Training GANs

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

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

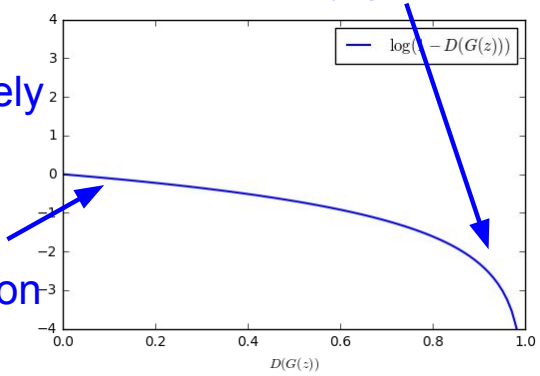
2. **Gradient descent** on generator

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

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

When sample is likely fake, want to learn from it to improve generator. But gradient in this region is relatively flat!

Gradient signal dominated by region where sample is already good



The Log D trick

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:

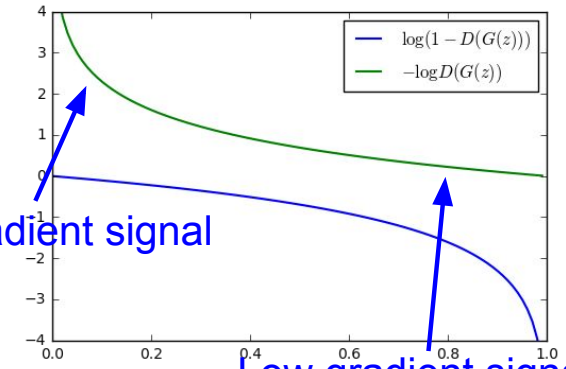
1. **Gradient ascent** on discriminator

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

2. **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.



Putting it together: GAN training algorithm

for number of training iterations **do**

  for k steps **do**

- Sample minibatch of m noise samples $\{\boldsymbol{z}^{(1)}, \ldots, \boldsymbol{z}^{(m)}\}$ from noise prior $p_g(\boldsymbol{z})$.
- Sample minibatch of m examples $\{\boldsymbol{x}^{(1)}, \ldots, \boldsymbol{x}^{(m)}\}$ from data generating distribution $p_{\text{data}}(\boldsymbol{x})$.
- 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

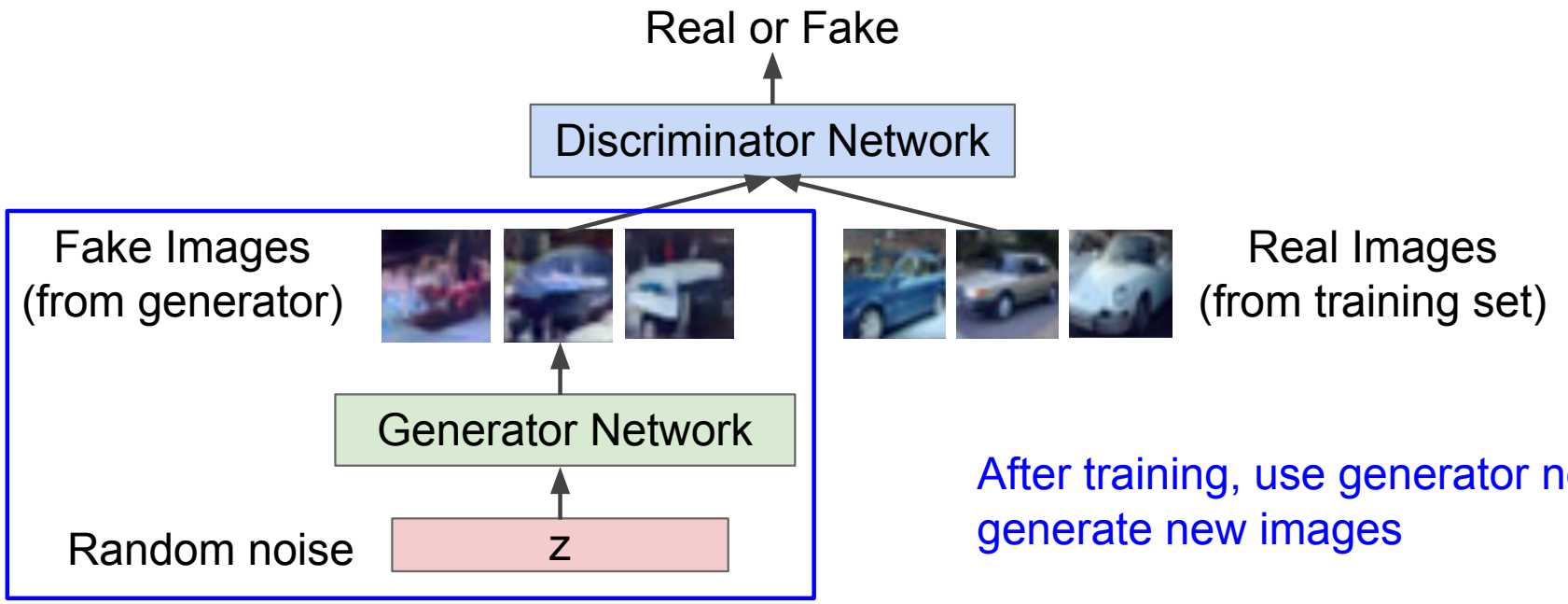
- Sample minibatch of m noise samples $\{\boldsymbol{z}^{(1)}, \ldots, \boldsymbol{z}^{(m)}\}$ from noise prior $p_g(\boldsymbol{z})$.
- Update the generator by ascending its stochastic gradient (improved objective):

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

end for

Other Losses (Wasserstein Distance, KL-divergence) are better in stability!

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

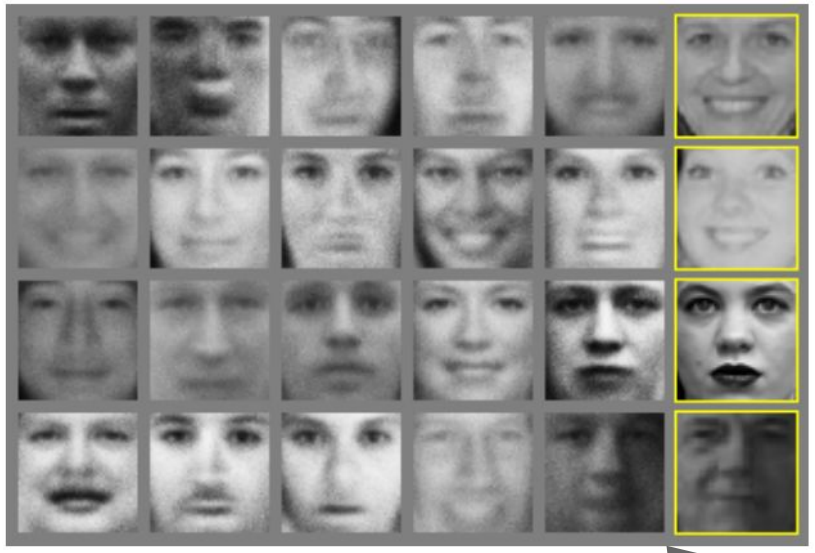


After training, use generator network to generate new images

Ian Goodfellow et al., “Generative Adversarial Nets”, NIPS 2014

Generative Adversarial Nets

Generated samples

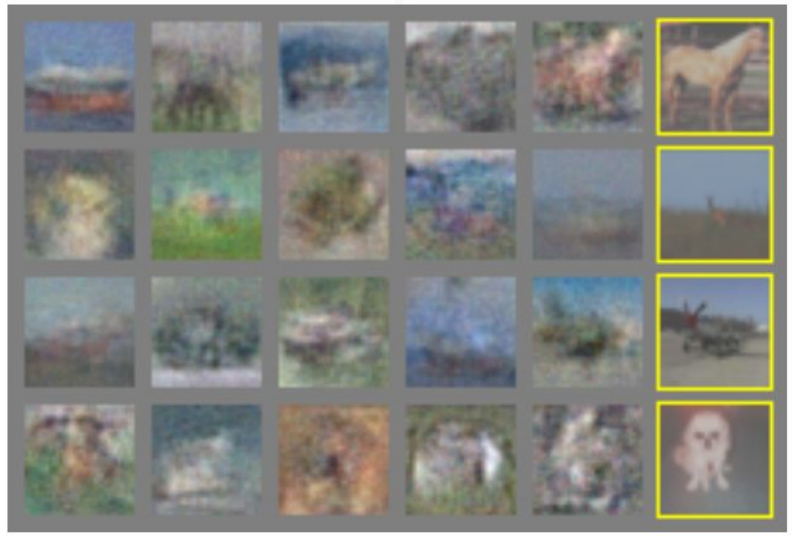


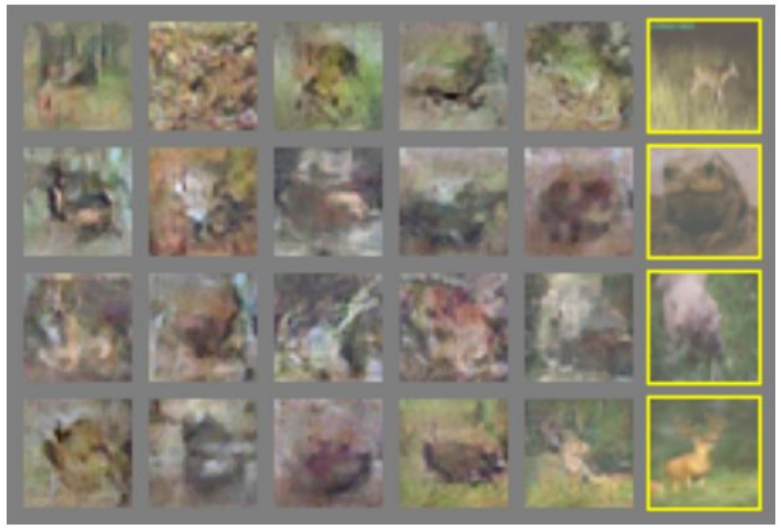
Nearest neighbor from training set

Ian Goodfellow et al., “Generative Adversarial Nets”, NIPS 2014

Generative Adversarial Nets

Generated samples (CIFAR-10)





Nearest neighbor from training set

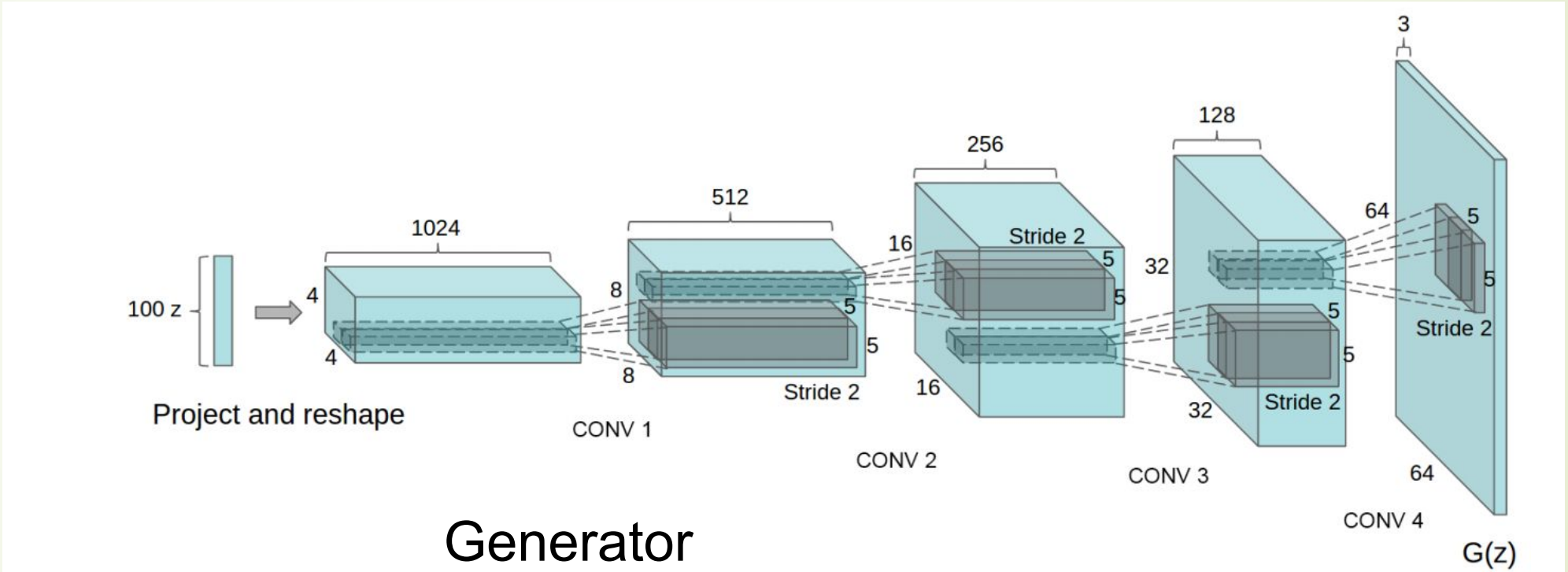
Generative Adversarial Nets: Convolutional Architectures

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.

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

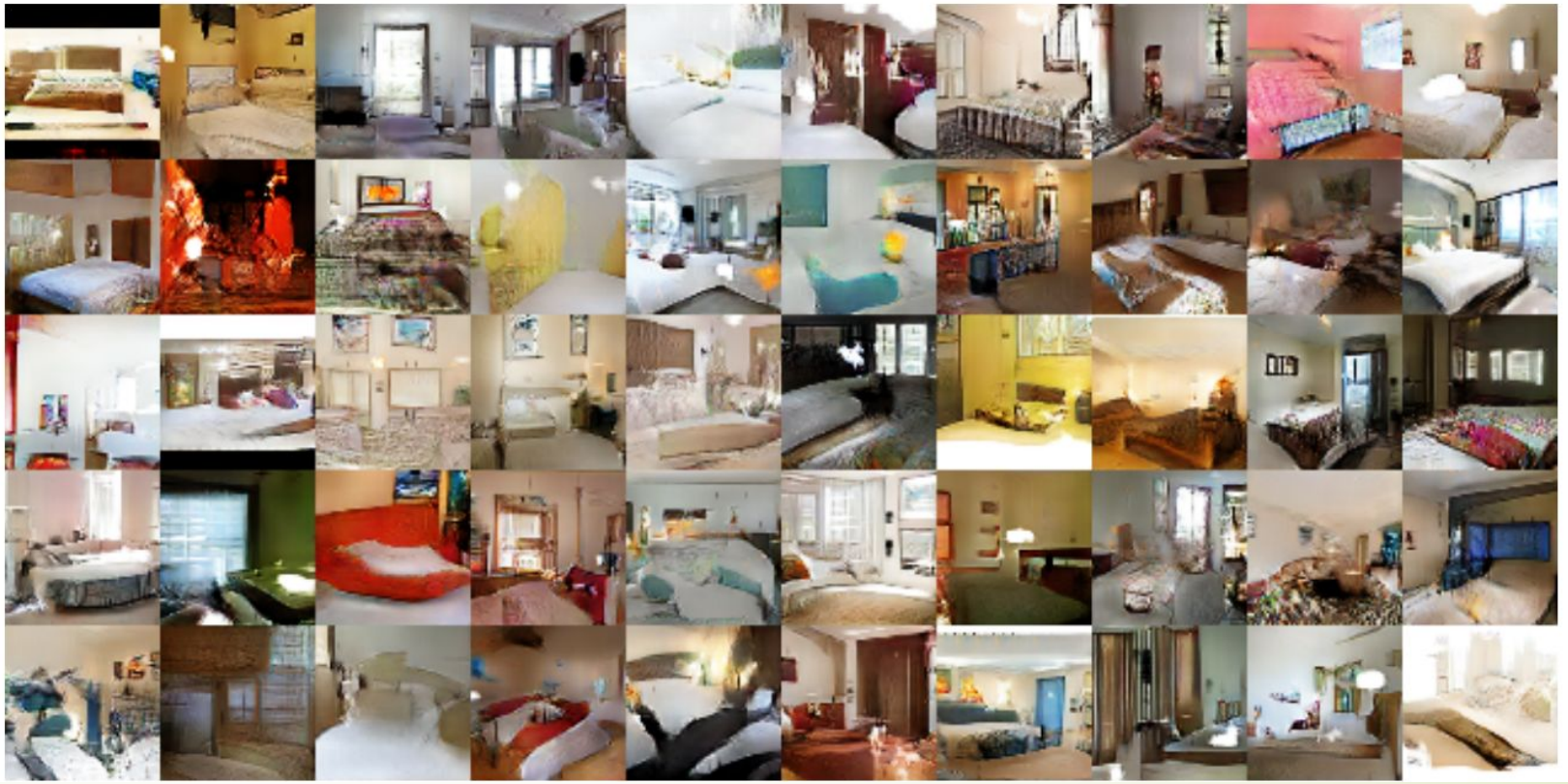


Generator

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

Generative Adversarial Nets: Convolutional Architectures

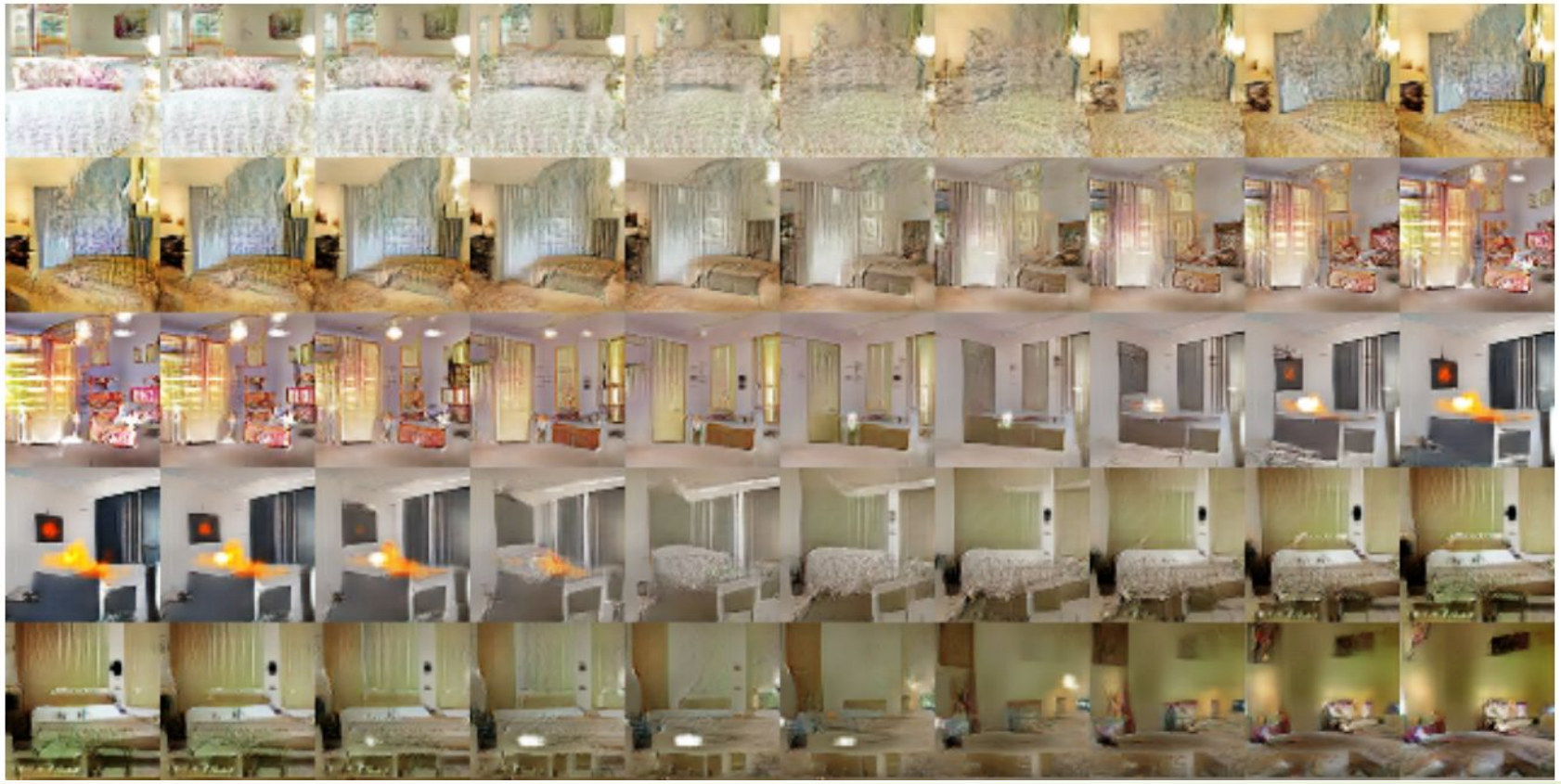
Samples from the model look amazing!



Radford et al, ICLR 2016

Generative Adversarial Nets: Convolutional Architectures

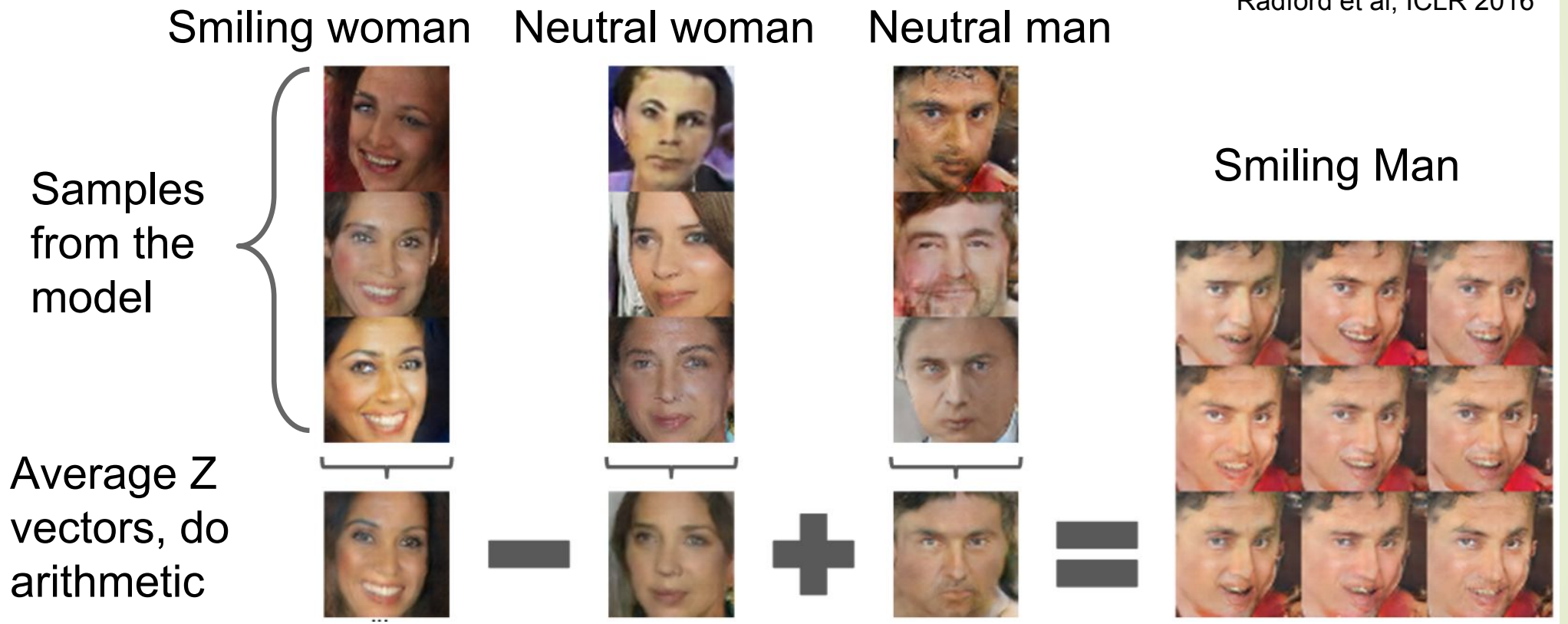
Interpolating between random points in laten space



Radford et al, ICLR 2016

Generative Adversarial Nets: Interpretable Vector Math

Radford et al, ICLR 2016



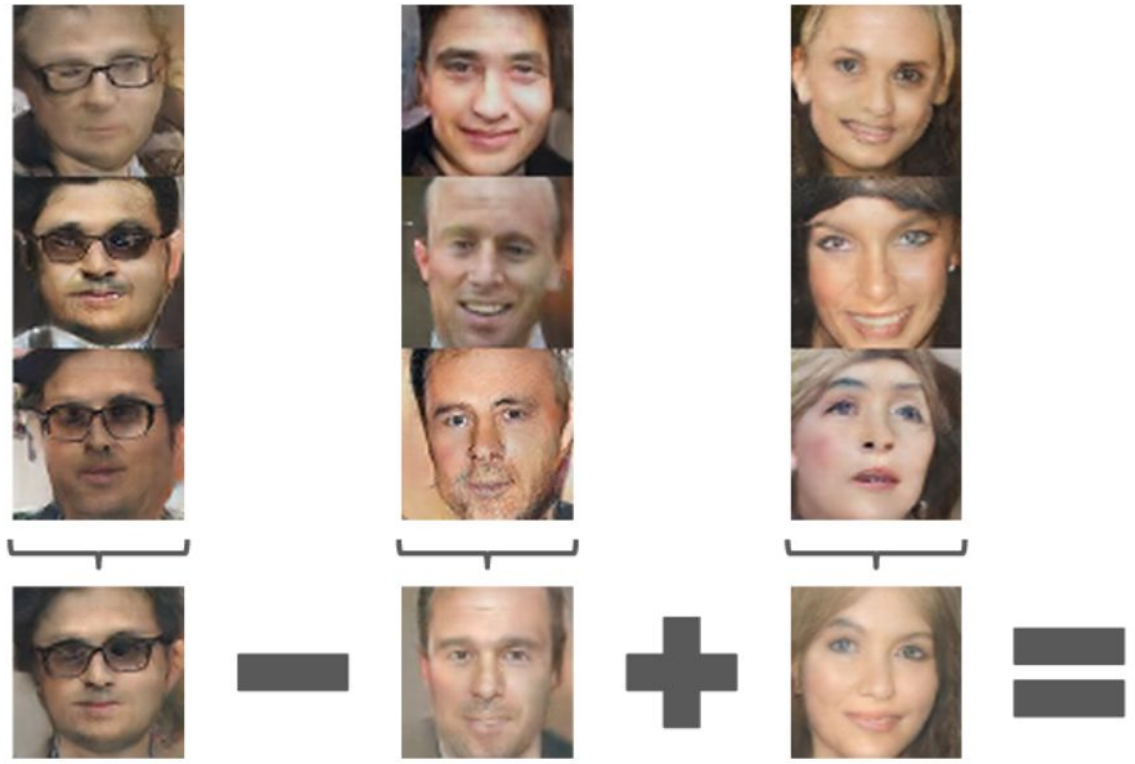
Generative Adversarial Nets: Interpretable Vector Math

Glasses man

No glasses man

No glasses woman

Radford et al, ICLR 2016



Woman with glasses

2017: Explosion of GANs

Better training and generation

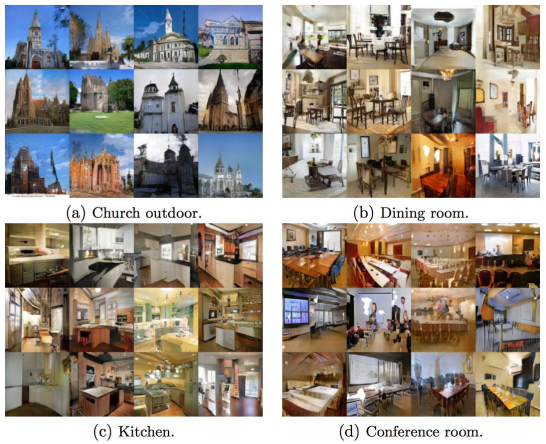
LSGAN, Zhu 2017.

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

Progressive GAN, Karras 2018.

2017: Year of the GAN

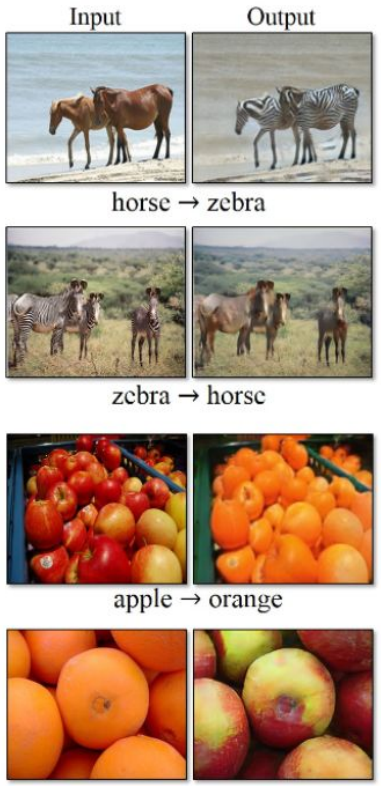
Better training and generation

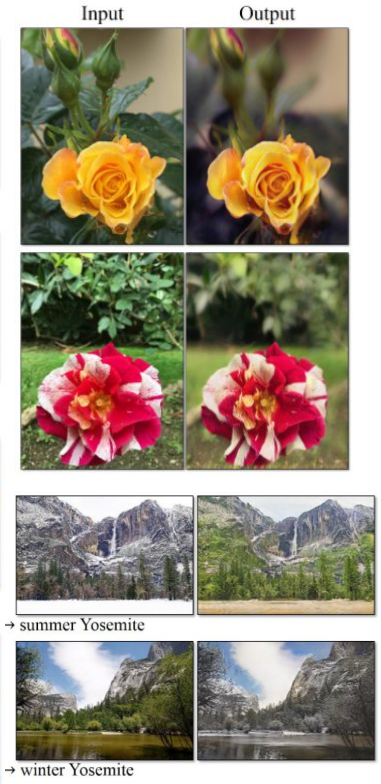


LSGAN. Mao et al. 2017.

BEGAN. Bertholet et al. 2017.

Source->Target domain transfer





CycleGAN. Zhu et al. 2017.

Text -> Image Synthesis

Reed et al. 2017.

Many GAN applications

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

2019: BigGAN

Brock et al., 2019

Reference of GANs

- The GAN zoo: https://github.com/hindupuravinash/the-gan-zoo
- See also: https://github.com/soumith/ganhacks for tips and tricks for trainings GANs

GANs

- Don't work with an explicit density function
  Take game-theoretic approach: learn to generate from training distribution through 2-player minimax zero-sum 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, etc.)
  - Conditional GANs, GANs for all kinds of applications

Thank you!