CSCE 479/879 Lecture 5: Autoencoders

Stephen Scott

(Adapted from Eleanor Quint and Ian Goodfellow)

sscott@cse.unl.edu

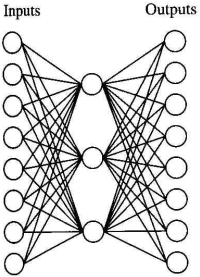
Introduction

- **Autoencoding** is training a network to replicate its input to its output
- Applications:
  - Unlabeled pre-training for semi-supervised learning
  - Learning **embeddings** to support information retrieval
  - Generation of new instances similar to those in the training set
  - Data compression

Outline

- Basic idea
- Stacking
- Types of autoencoders
  - Denoising
  - Sparse
  - Contractive
  - Variational
  - Generative adversarial networks

Basic Idea (Mitchell, 1997)

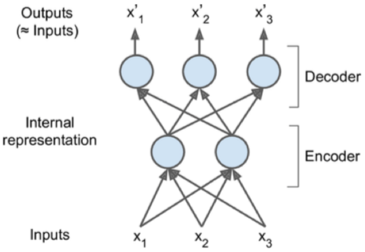


Input		Hidden Values				Output
10000000	→	.89	.04	.08	→	10000000
01000000	→	.15	.99	.99	→	01000000
00100000	→	.01	.97	.27	→	00100000
00010000	→	.99	.97	.71	→	00010000
00001000	→	.03	.05	.02	→	00001000
00000100	→	.01	.11	.88	→	00000100
00000010	→	.80	.01	.98	→	00000010
00000001	→	.60	.94	.01	→	00000001

- Sigmoid activation functions, 5000 training epochs, square loss, no regularization
- What's special about the hidden layer outputs?

Basic Idea

- An **autoencoder** is a network trained to learn the **identity function:** output = input



- Subnetwork called **encoder** $f(\cdot)$ maps input to an **embedded representation**
- Subnetwork called **decoder** $g(\cdot)$ maps back to input space

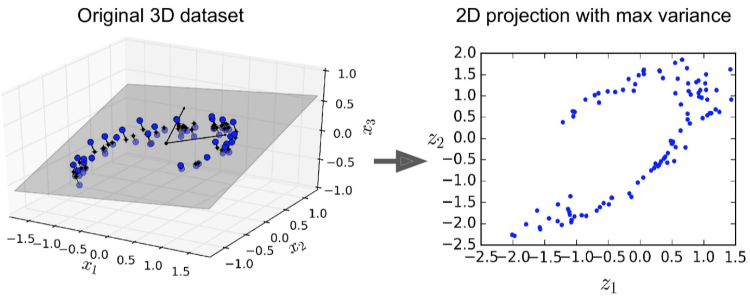
- Can be thought of as **lossy compression** of input
- Need to identify the important attributes of inputs to reproduce faithfully

Basic Idea

- General types of autoencoders based on size of hidden layer
  - **Undercomplete** autoencoders have hidden layer size smaller than input layer size
    - $\Rightarrow$ Dimension of embedded space lower than that of input space
    - $\Rightarrow$ Cannot simply memorize training instances
  - **Overcomplete** autoencoders have much larger hidden layer sizes
    - $\Rightarrow$ Regularize to avoid overfitting, e.g., enforce a **sparsity** constraint

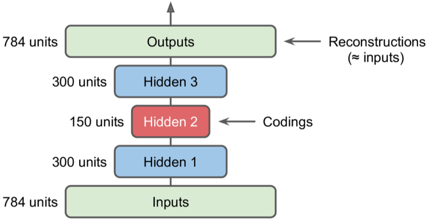
Basic Idea

Example: Principal Component Analysis



- A 3-2-3 autoencoder with linear units and square loss performs **principal component analysis**: Find linear transformation of data to maximize variance

Stacked Autoencoders

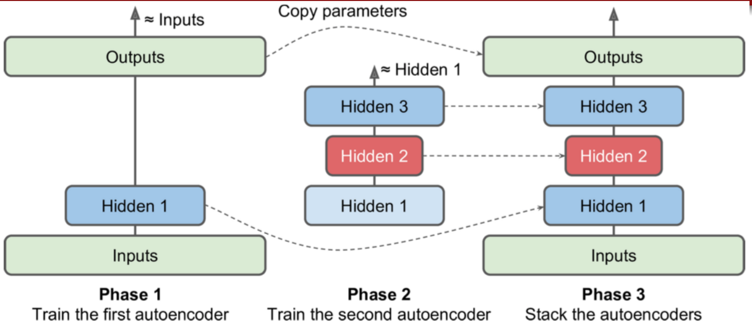


- A **stacked autoencoder** has multiple hidden layers

- Can share parameters to reduce their number by exploiting symmetry: $W_4 = W_1^\top$ and $W_3 = W_2^\top$

```
weights1 = tf.Variable(weights1_init, dtype=tf.float32, name="weights1")
weights2 = tf.Variable(weights2_init, dtype=tf.float32, name="weights2")
weights3 = tf.transpose(weights2, name="weights3")     # shared weights
weights4 = tf.transpose(weights1, name="weights4")     # shared weights
```

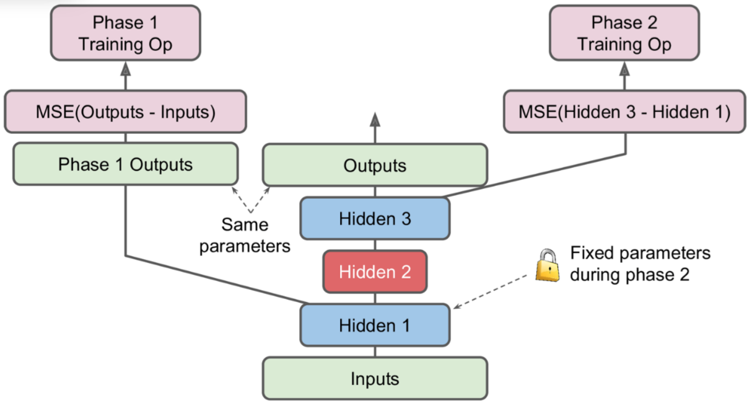
Stacked Autoencoders
Incremental Training



- Can simplify training by starting with single hidden layer H_1
- Then, train a second AE to mimic the output of H_1
- Insert this into first network
- Can build by using H_1's output as training set for Phase 2

Stacked Autoencoders

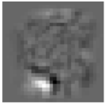
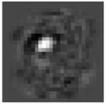
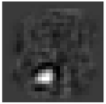
Incremental Training (Single TF Graph)



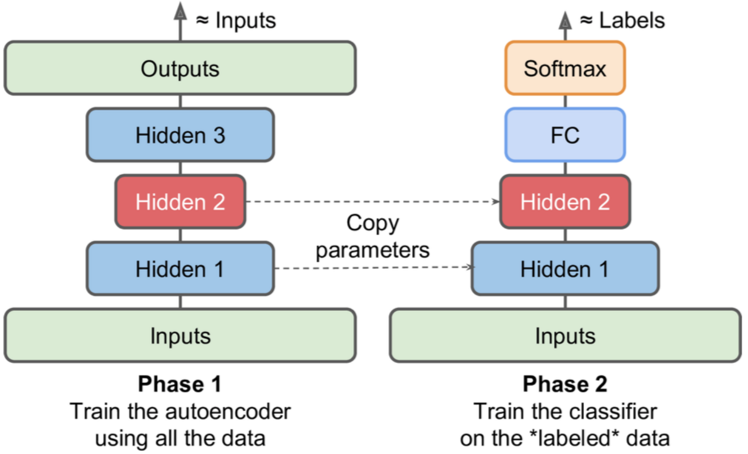
- Previous approach requires multiple TensorFlow graphs
- Can instead train both phases in a single graph: First left side, then right

Input MNIST Digit	Network Output
	
	

Weights (features selected) for five nodes from H_1:

Stacked Autoencoders
Semi-Supervised Learning

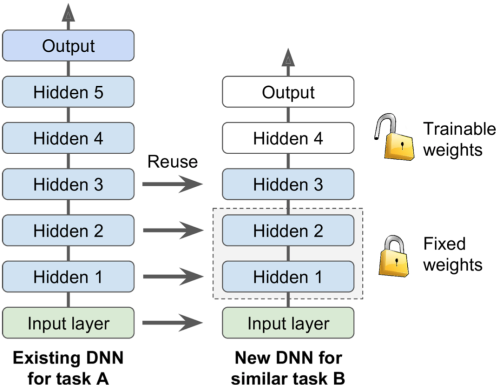


- Can **pre-train** network with unlabeled data

⇒ learn useful features and then train “logic” of dense layer with labeled data

Transfer Learning from Trained Classifier

- Can also transfer from a classifier trained on different task, e.g., transfer a GoogleNet architecture to ultrasound classification



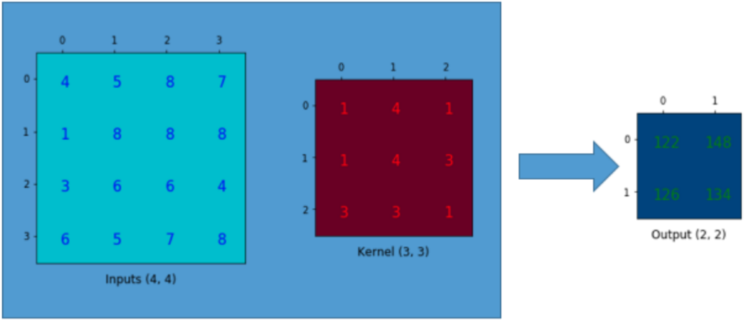
- Often choose existing one from a **model zoo**

Transposed Convolutions

- What if some encoder layers are convolutional? How to upsample to original resolution?
- Can use, e.g., **linear interpolation**, **bilinear interpolation**, etc.
- Or, **transposed convolution**, e.g., `tf.layers.conv2d_transpose`

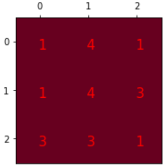
Transposed Convolutions (2)

Consider this example convolution

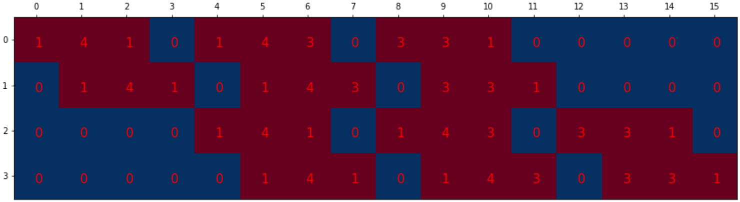


Transposed Convolutions (3)

An alternative way of representing the kernel



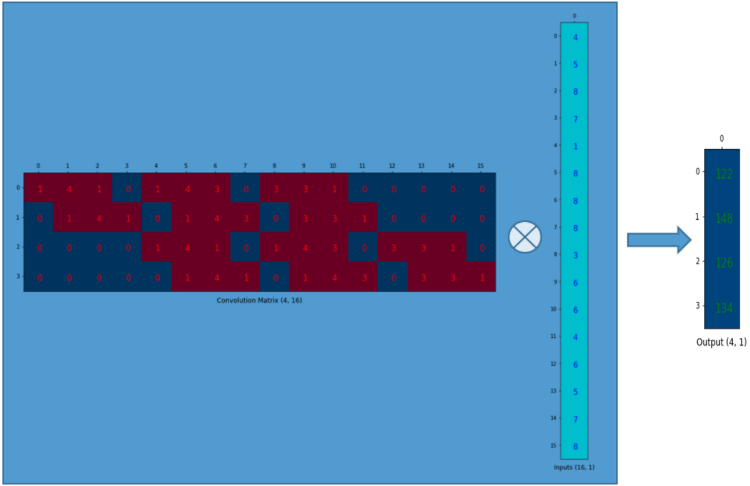
Kernel (3, 3)



Convolution Matrix (4, 16)

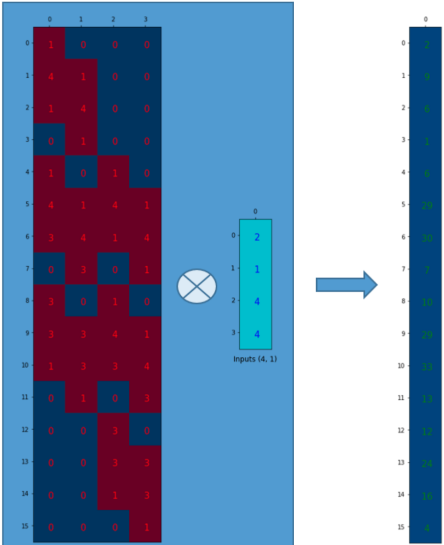
Transposed Convolutions (4)

This representation works with matrix multiplication on flattened input:



Transposed Convolutions (5)

Transpose kernel, multiply by flat 2×2 to get flat 4×4

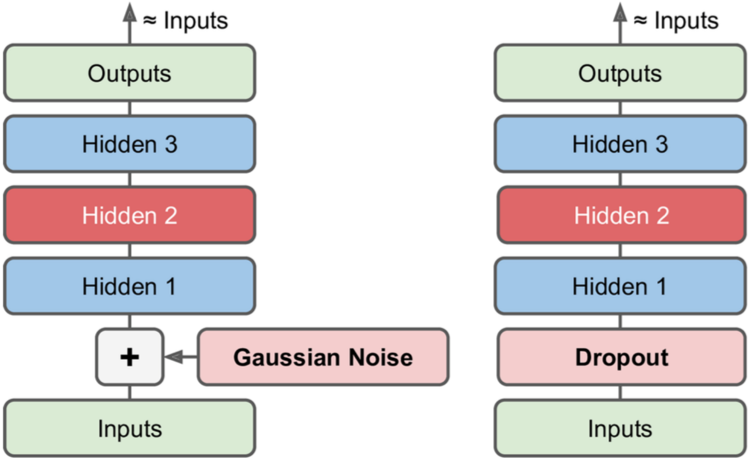


Denoising Autoencoders

Vincent et al. (2010)

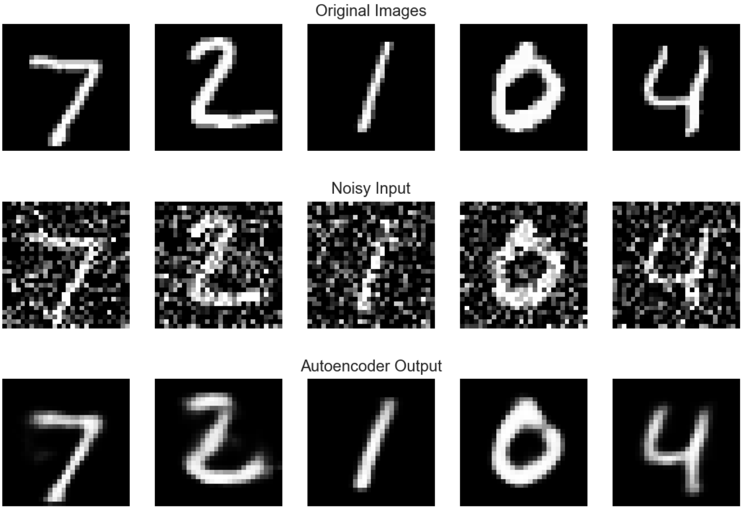
- Can train an autoencoder to learn to **denoise** input by giving input **corrupted** instance $\tilde{\boldsymbol{x}}$ and targeting **uncorrupted** instance $\boldsymbol{x}$
- Example noise models:
  - **Gaussian noise:** $\tilde{\boldsymbol{x}} = \boldsymbol{x} + z$, where $z \sim \mathcal{N}(\mathbf{0}, \sigma^2 I)$
  - **Masking noise:** zero out some fraction ν of components of $\boldsymbol{x}$
  - **Salt-and-pepper noise:** choose some fraction ν of components of $\boldsymbol{x}$ and set each to its min or max value (equally likely)

Denoising Autoencoders



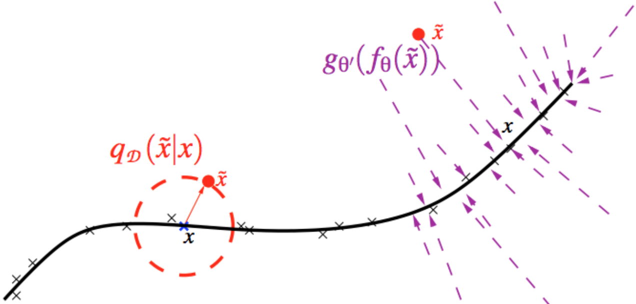
Denoising Autoencoders

Example



Denoising Autoencoders

- How does it work?
- Even though, e.g., MNIST data are in a 784-dimensional space, they lie on a low-dimensional **manifold** that captures their most important features
- Corruption process moves instance x off of manifold
- Encoder f_θ and decoder $g_{\theta'}$ are trained to project $\tilde{x}$ back onto manifold



Sparse Autoencoders

- An overcomplete architecture
- Regularize outputs of hidden layer to enforce **sparsity**:

$$\tilde{\mathcal{J}}(\boldsymbol{x}) = \mathcal{J}(\boldsymbol{x}, g(f(\boldsymbol{x}))) + \alpha\,\Omega(\boldsymbol{h}) \ ,$$

  where $\mathcal{J}$ is loss function, f is encoder, g is decoder, $\boldsymbol{h} = f(\boldsymbol{x})$, and Ω penalizes non-sparsity of $\boldsymbol{h}$
- E.g., can use $\Omega(\boldsymbol{h}) = \sum_i |h_i|$ and ReLU activation to force many zero outputs in hidden layer
- Can also measure average activation of h_i across mini-batch and compare it to user-specified **target sparsity** value p (e.g., 0.1) via square error or **Kullback-Leibler divergence**:

$$p \log \frac{p}{q} + (1 - p) \log \frac{1 - p}{1 - q} \ ,$$

  where q is average activation of h_i over mini-batch

Contractive Autoencoders

- Similar to sparse autoencoder, but use

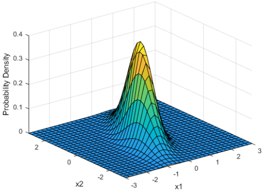
$$\Omega(\boldsymbol{h}) = \sum_{j=1}^{m} \sum_{i=1}^{n} \left(\frac{\partial h_i}{\partial x_j} \right)^2$$

- I.e., penalize large partial derivatives of encoder outputs wrt input values
- This **contracts** the output space by mapping input points in a neighborhood near $\boldsymbol{x}$ to a smaller output neighborhood near $f(\boldsymbol{x})$
  - $\Rightarrow$ Resists perturbations of input $\boldsymbol{x}$
- If $\boldsymbol{h}$ has sigmoid activation, encoding near binary and a CE pushes embeddings to corners of a hypercube

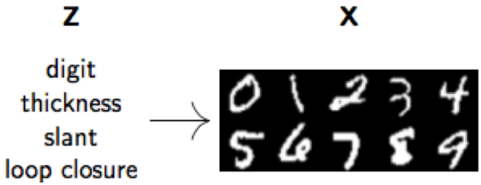
Variational Autoencoders

- VAE is an autoencoder that is also **generative model**
  - $\Rightarrow$ Can generate new instances according to a probability distribution
  - E.g., hidden Markov models, Bayesian networks
  - Contrast with **discriminative models**, which predict classifications

- Encoder f outputs $[\boldsymbol{\mu}, \boldsymbol{\sigma}]^\top$
  - Pair (μ_i, σ_i) parameterizes Gaussian distribution for dimension $i = 1, \ldots, n$
  - Draw $z_i \sim \mathcal{N}(\mu_i, \sigma_i)$
  - Decode this **latent variable** z to get $g(z)$

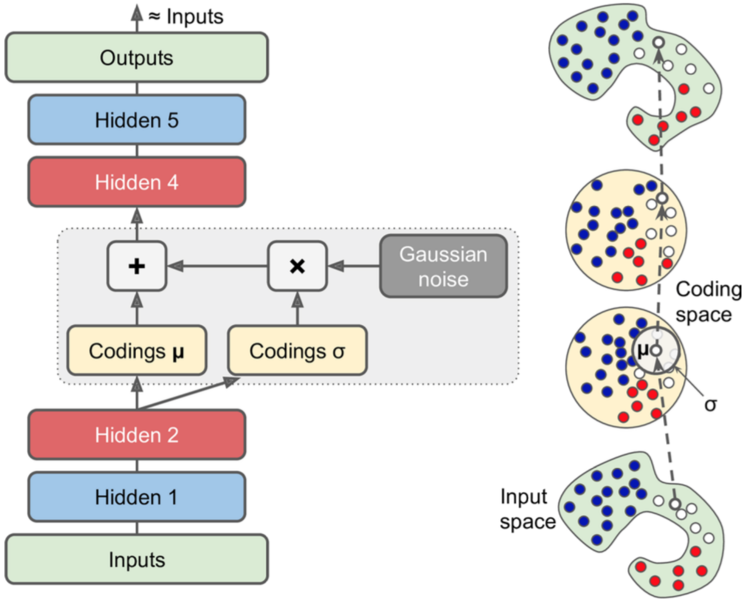


- Independence of z dimensions makes it easy to generate instances wrt complex distributions via decoder g
- Latent variables can be thought of as values of attributes describing inputs
  - E.g., for MNIST, latent variables might represent "thickness", "slant", "loop closure"



Variational Autoencoders

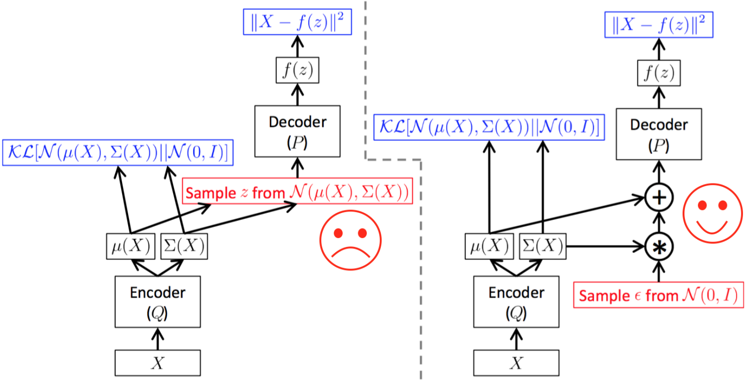
Architecture



- **Maximum likelihood** (ML) approach for training generative models: find a model ($\boldsymbol{\theta}$) with maximum probability of generating the training set $\mathcal{X}$
- Achieve this by minimizing the sum of:
  - End-to-end AE loss (e.g., square, cross-entropy)
  - Regularizer measuring distance (K-L divergence) from latent distribution $q(\boldsymbol{z} \mid \boldsymbol{x})$ and $\mathcal{N}(\mathbf{0}, I)$ (= standard multivariate Gaussian)
- $\mathcal{N}(\mathbf{0}, I)$ also considered the **prior distribution** over $\boldsymbol{z}$ (= distribution when no $\boldsymbol{x}$ is known)

```
eps = 1e-10
latent_loss = 0.5 * tf.reduce_sum(
        tf.square(hidden3_sigma) + tf.square(hidden3_mean)
        - 1 - tf.log(eps + tf.square(hidden3_sigma)))
```

- Cannot backprop error signal through random samples
- **Reparameterization trick** emulates $z \sim \mathcal{N}(\mu, \sigma)$ with $\epsilon \sim \mathcal{N}(0, 1)$, $z = \epsilon\sigma + \mu$

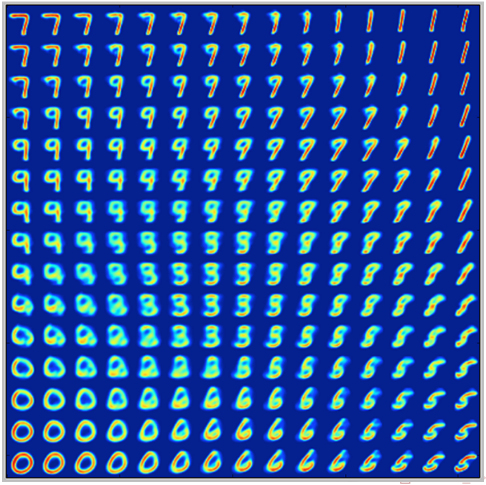


Variational Autoencoders

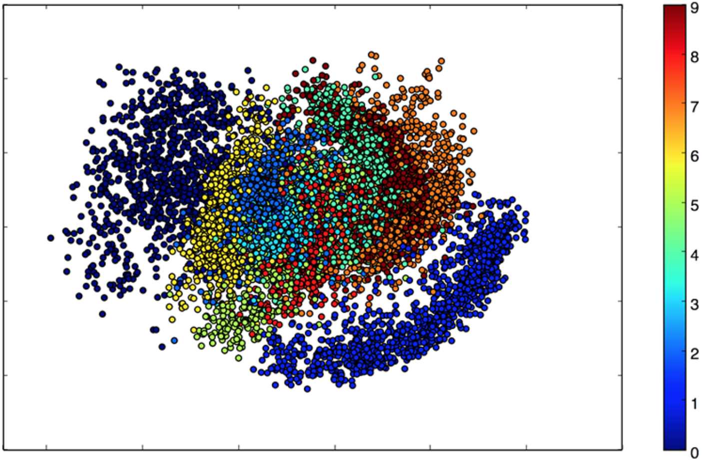
Example Generated Images: Random

- Draw $z \sim \mathcal{N}(\mathbf{0}, I)$ and display $g(z)$

- Uniformly sample points in (2-dimensional) z space and decode



- Cluster analysis by digit (2D latent space)



Aside: Visualizing with t-SNE

van der Maaten and Hinton (2008)

- Visualize high-dimensional data, e.g., embedded representations
- Want low-dimensional representation to have similar neighborhoods as high-dimensional one
- Map each high-dimensional $\boldsymbol{x}_1, \ldots, \boldsymbol{x}_N$ to low-dimensional $\boldsymbol{y}_1, \ldots, \boldsymbol{y}_N$ via matching **pairwise distributions** based on distance
  - $\Rightarrow$ Probability p_{ij} pair $(\boldsymbol{x}_i, \boldsymbol{x}_j)$ chosen similar to probability q_{ij} pair $(\boldsymbol{y}_i, \boldsymbol{y}_j)$ chosen
- Set $p_{ij} = (p_{j|i} + p_{i|j})/(2N)$ where

$$p_{j|i} = \frac{\exp\left(-\|\boldsymbol{x}_i - \boldsymbol{x}_j\|^2/(2\sigma_i^2)\right)}{\sum_{k \neq i} \exp\left(-\|\boldsymbol{x}_i - \boldsymbol{x}_k\|^2/(2\sigma_i^2)\right)}$$

  and σ_i chosen to control density of the distribution
- I.e., $p_{j|i}$ is probability of $\boldsymbol{x}_i$ choosing $\boldsymbol{x}_j$ as its neighbor if chosen in proportion of Gaussian density centered at $\boldsymbol{x}_i$

Aside: Visualizing with t-SNE (2)

van der Maaten and Hinton (2008)

- Also, define q via student's t distribution:

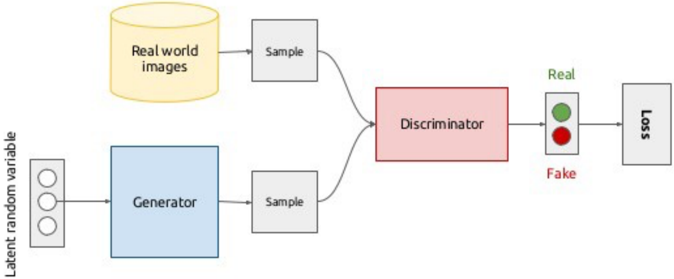
$$q_{ij} = \frac{\left(1 + \|\boldsymbol{y}_i - \boldsymbol{y}_j\|^2\right)^{-1}}{\sum_{k \neq \ell} \left(1 + \|\boldsymbol{y}_k - \boldsymbol{y}_\ell\|^2\right)^{-1}}$$

- Using student's t instead of Gaussian helps address **crowding problem** where distant clusters in $\boldsymbol{x}$ space squeeze together in $\boldsymbol{y}$ space
- Now choose $\boldsymbol{y}$ values to match distributions p and q via **Kullback-Leibler divergence**:

$$\sum_{i \neq j} p_{ij} \log \frac{p_{ij}}{q_{ij}}$$

Generative Adversarial Network

- GANs are also generative models, like VAEs
- Models a game between two players
  - **Generator** creates samples intended to come from training distribution
  - **Discriminator** attempts to discern the "real" (original training) samples from the "fake" (generated) ones
- Discriminator trains as a binary classifier, generator trains to fool the discriminator



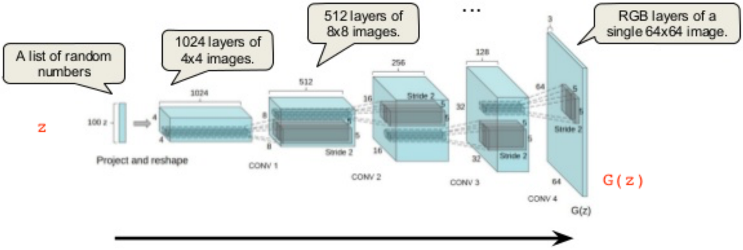
- Let $D(\boldsymbol{x})$ be discriminator parameterized by $\boldsymbol{\theta}^{(D)}$
  - Goal: Find $\boldsymbol{\theta}^{(D)}$ minimizing $J^{(D)}\left(\boldsymbol{\theta}^{(D)}, \boldsymbol{\theta}^{(G)}\right)$
- Let $G(\boldsymbol{z})$ be generator parameterized by $\boldsymbol{\theta}^{(G)}$
  - Goal: Find $\boldsymbol{\theta}^{(G)}$ minimizing $J^{(G)}\left(\boldsymbol{\theta}^{(D)}, \boldsymbol{\theta}^{(G)}\right)$
- A **Nash equilibrium** of this game is $\left(\boldsymbol{\theta}^{(D)}, \boldsymbol{\theta}^{(G)}\right)$ such that each $\boldsymbol{\theta}^{(i)}$, $i \in \{D, G\}$ yields a local minimum of its corresponding J

- Each training step:
  - Draw a minibatch of $\boldsymbol{x}$ values from dataset
  - Draw a minibatch of $\boldsymbol{z}$ values from prior (e.g., $\mathcal{N}(\mathbf{0}, I)$)
  - Simultaneously update $\boldsymbol{\theta}^{(G)}$ to reduce $J^{(G)}$ and $\boldsymbol{\theta}^{(D)}$ to reduce $J^{(D)}$, via, e.g., Adam
- For $J^{(D)}$, common to use cross-entropy where label is 1 for real and 0 for fake
- Since generator wants to trick discriminator, can use $J^{(G)} = -J^{(D)}$
  - Others exist that are generally better in practice, e.g., based on ML

Generative Adversarial Network

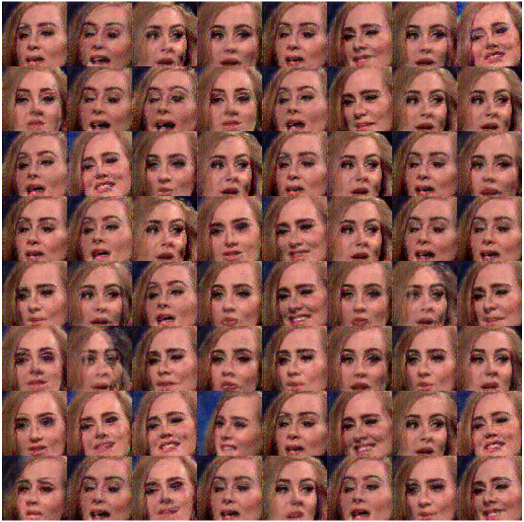
DCGAN: Radford et al. (2015)

- "Deep, convolution GAN"
- Generator uses **transposed convolutions** (e.g., `tf.layers.conv2d_transpose`) without pooling to upsample images for input to discriminator



Trained from LSUN dataset, sampled z space

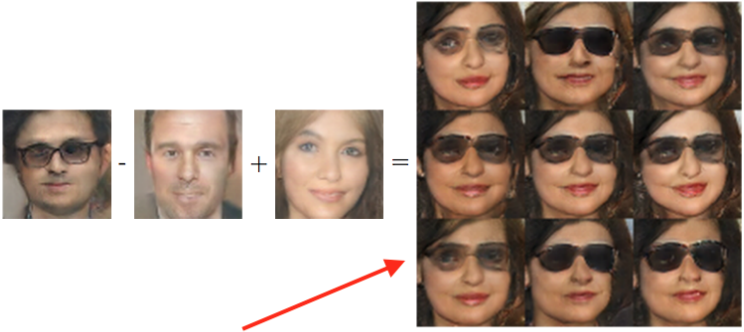
Trained from frame grabs of interview, sampled z space



Generative Adversarial Network

DCGAN Generated Images: Latent Space Arithmetic

Performed semantic arithmetic in z space!



(Non-center images have noise added in z space; center is noise-free)