CS 3750 Machine Learning

PCA and Autoencoders

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PCA: Introduction

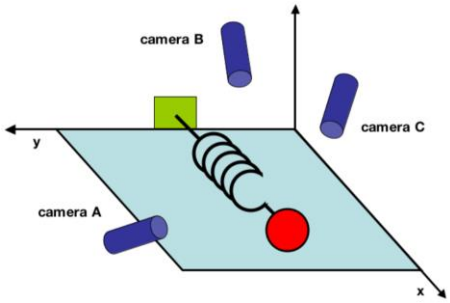
- **PCA: Principal Component Analysis**
- Provides a roadmap for dimension reduction
- Used for:
  - Visualization
  - Preprocessing
  - Compression

PCA: Example

- A ball is attached to a massless frictionless spring
- The ball is released a small distance away from equilibrium
- It oscillates along the x-axis at a set frequency
- We want to find the dynamics of the ball
- We place three cameras to observe the ball's movement
- Each camera records the ball's position in a 2-D plane
- Due to our ignorance, we choose three camera axes at some arbitrary angles

PCA: Example

- Goal: Based on the camera records, determine that the dynamics are along the x-axis



PCA: A Naïve Basis

- Each data point is expressed along the x, y axis of the 3 camera planes (6 dimension in total)

$$\vec{X} = \begin{bmatrix} x_A \\ y_A \\ x_B \\ y_B \\ x_C \\ y_C \end{bmatrix}$$

- If we choose a naïve basis with orthonormal basis vectors $\mathbf{b}_i$

$$\mathbf{B} = \begin{bmatrix} \mathbf{b_1} \\ \mathbf{b_2} \\ \vdots \\ \mathbf{b_m} \end{bmatrix} = \begin{bmatrix} 1 & 0 & \cdots & 0 \\ 0 & 1 & \cdots & 0 \\ \vdots & \vdots & \ddots & \vdots \\ 0 & 0 & \cdots & 1 \end{bmatrix} = \mathbf{I}$$

- All data can be trivially expressed as a linear combination of $\{\mathbf{b}_i\}$

$$\boldsymbol{X = BX}$$

PCA: Change of Basis

- PCA is trying to re-express the data as a **linear combination** of its naïve basis vectors:

$$\boldsymbol{Y = PBX = PX} \quad (1)$$

with the following quantity definition:

- $\boldsymbol{p_i}$ are the rows of $\boldsymbol{P}$
- $\boldsymbol{x_i}$ are the columns of $\boldsymbol{X}$
- $\boldsymbol{y_i}$ are the columns of $\boldsymbol{Y}$

PCA: Change of Basis

- Equation 1 represents a **change of basis** and can have many interpretations:
  - $\boldsymbol{P}$ is a matrix that transforms $\boldsymbol{X}$ to $\boldsymbol{Y}$
  - Geometrically, $\boldsymbol{P}$ is a rotation and a stretch which again transforms $\boldsymbol{X}$ to $\boldsymbol{Y}$
  - The rows of $\boldsymbol{P}$, namely $\{\boldsymbol{p}_1, \ldots, \boldsymbol{p}_m\}$, are a set of new basis vectors for expressing the columns of $\boldsymbol{X}$, namely each $\boldsymbol{x_i}$ of $\boldsymbol{X}$

PCA: Change of Basis

- The last interpretation can be seen clearly by writing out the explicit dot products of ***PX***:

$$\mathbf{PX} = \begin{bmatrix} \mathbf{p_1} \\ \vdots \\ \mathbf{p_m} \end{bmatrix} \begin{bmatrix} \mathbf{x_1} & \cdots & \mathbf{x_n} \end{bmatrix}$$

$$\mathbf{Y} = \begin{bmatrix} \mathbf{p_1} \cdot \mathbf{x_1} & \cdots & \mathbf{p_1} \cdot \mathbf{x_n} \\ \vdots & \ddots & \vdots \\ \mathbf{p_m} \cdot \mathbf{x_1} & \cdots & \mathbf{p_m} \cdot \mathbf{x_n} \end{bmatrix}$$

- Each column of ***Y*** is:

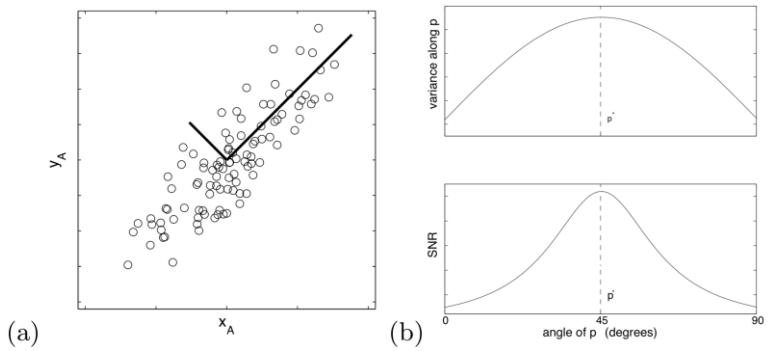
$$\mathbf{y}_i = \begin{bmatrix} \mathbf{p_1} \cdot \mathbf{x_i} \\ \vdots \\ \mathbf{p_m} \cdot \mathbf{x_i} \end{bmatrix}$$

PCA: Goal

- Goal:
  - Find the best way to "re-express" ***X***
  - Find a good choice of basis ***P***
- What does "best express" the data mean?
- Three potential confounds that "garbles" the data:
  - Noise
  - Rotation
  - Redundancy

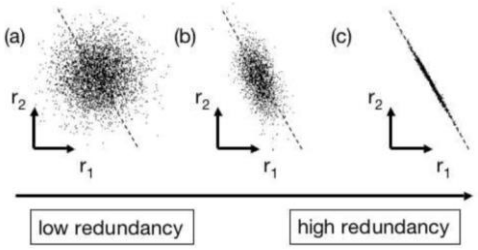
PCA: Noise and Rotation

- Signal-to-noise ratio: $SNR = \sigma^2_{signal}/\sigma^2_{noise}$
- Dynamics of interest is along direction with high SNR
- Rotate the naïve basis to lie parallel to p^*



PCA: Redundancy

- More meaningful to record one variable in panel (c)
- Because one can calculate r_1 from r_2 using best-fit line
- Removing redundancy is the very idea behind dimension reduction



PCA: Covariance Matrix

- Consider a data set in **mean deviation form**

$$\mathbf{X} = \begin{bmatrix} \mathbf{x}_1 \\ \vdots \\ \mathbf{x}_m \end{bmatrix}$$

- The covariance matrix is $\boldsymbol{C_X} = \frac{1}{n-1}\boldsymbol{X}\boldsymbol{X}^T$
  - $\boldsymbol{C_X}$ is a square symmetric matrix
  - The diagonal terms are variance of measurement
    - Large values correspond to **interesting dynamics**
  - The off-diagonal terms are covariance between measurement
    - Large values correspond to **high redundancy**

PCA: Diagonalize Covariance Matrix

- We want to transform $\boldsymbol{X}$ to $\boldsymbol{Y}$ using a new basis $\boldsymbol{P}$ such that the covariance matrix becomes $\boldsymbol{C_Y}$
- $\boldsymbol{C_Y}$ must be diagonal
- $\{\boldsymbol{p}_1, \ldots, \boldsymbol{p}_m\}$ in $\boldsymbol{P}$ are the principal components
- To find $\boldsymbol{P}$
  - Find $\boldsymbol{p}_1$ corresponds to the vector parallel to the direction with largest variance in $\boldsymbol{X}$
  - Find $\boldsymbol{p}_2$ with the second largest variance in the remaining directions orthogonal to previously selected directions
  - Repeat until m vectors are selected

PCA: Assumptions and Limits

- Linearity
  - Linearity frames the problem as a change of basis
  - Kernel PCA: PCA with nonlinear kernels
- Mean and variance are sufficient statistics
  - Mean and variance fully describe the distribution
  - Gaussian, Exponential distribution, etc.
- Large variances have important dynamics
- The principal components are orthogonal
  - Soluble with linear algebra decomposition techniques

PCA: Eigenvectors of Covariance

- Find some orthonormal matrix $\boldsymbol{P}$ where $\boldsymbol{Y} = \boldsymbol{PX}$ such that $\boldsymbol{C_Y} = \frac{1}{n-1}\boldsymbol{YY}^T$ is diagonalized.
- The rows of $\boldsymbol{P}$ are the principal components of $\boldsymbol{X}$.

PCA: Eigenvectors of Covariance

- Rewrite $\boldsymbol{C_Y}$ in terms of our variable of choice $\boldsymbol{P}$

$$\begin{aligned}
\mathbf{C_Y} &= \frac{1}{n-1}\mathbf{Y}\mathbf{Y}^T \\
&= \frac{1}{n-1}(\mathbf{P}\mathbf{X})(\mathbf{P}\mathbf{X})^T \\
&= \frac{1}{n-1}\mathbf{P}\mathbf{X}\mathbf{X}^T\mathbf{P}^T \\
&= \frac{1}{n-1}\mathbf{P}(\mathbf{X}\mathbf{X}^T)\mathbf{P}^T \\
\mathbf{C_Y} &= \frac{1}{n-1}\mathbf{P}\mathbf{A}\mathbf{P}^T
\end{aligned}$$

PCA: Eigenvectors of Covariance

- With $\boldsymbol{A} = \boldsymbol{E}\boldsymbol{D}\boldsymbol{E}^T$ ($\boldsymbol{E}$ is a matrix of eigenvectors of $\boldsymbol{A}$) and $\boldsymbol{P} \equiv \boldsymbol{E}^T$ and $\boldsymbol{P}^{-1} = \boldsymbol{P}^T$, we have:

$$\begin{aligned}
\mathbf{C_Y} &= \frac{1}{n-1}\mathbf{P}\mathbf{A}\mathbf{P}^T \\
&= \frac{1}{n-1}\mathbf{P}(\mathbf{P}^T\mathbf{D}\mathbf{P})\mathbf{P}^T \\
&= \frac{1}{n-1}(\mathbf{P}\mathbf{P}^T)\mathbf{D}(\mathbf{P}\mathbf{P}^T) \\
&= \frac{1}{n-1}(\mathbf{P}\mathbf{P}^{-1})\mathbf{D}(\mathbf{P}\mathbf{P}^{-1}) \\
\mathbf{C_Y} &= \frac{1}{n-1}\mathbf{D}
\end{aligned}$$

PCA: Eigenvectors of Covariance

- Results of PCA in the matrices $\boldsymbol{P}$ and $\boldsymbol{C_Y}$
  - The principal components of $\boldsymbol{X}$ are the eigenvectors of $\boldsymbol{XX^T}$; or the rows of $\boldsymbol{P}$.
  - The i^{th} diagonal value of $\boldsymbol{C_Y}$ is the variance of $\boldsymbol{X}$ along $\boldsymbol{p}_i$.

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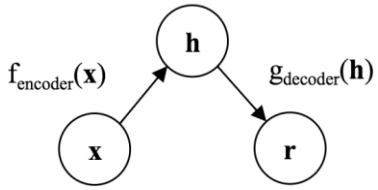
Introduction to Autoencoders

- An autoencoder is a type of **artificial neural network** used to learn **efficient data codings** in an **unsupervised** manner.
- The aim of an autoencoder is to learn a representation (encoding) for a set of data, typically for the purpose of **dimensionality reduction**.
- Recently, the autoencoder concept has become more widely used for learning **generative models** of data.

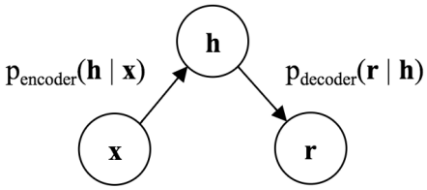
Introduction to Autoencoders

- The network may be viewed as consisting of two parts:
  - An **encoder** function **h** = f(**x**) and
  - A **decoder** that produces a reconstruction **r** = g(**h**)



Introduction to Autoencoders

- Modern autoencoders have generalized the idea of an encoder and a decoder beyond **deterministic functions** to **stochastic mappings** $p_{encoder}(\mathbf{h} \mid \mathbf{x})$ and $p_{decoder}(\mathbf{x} \mid \mathbf{h})$.

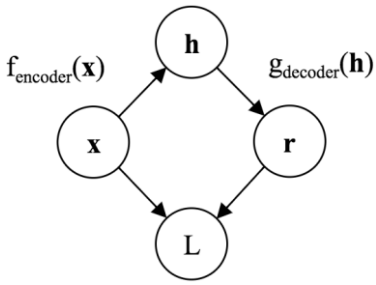


Introduction to Autoencoders

- The learning process is minimizing a loss function

$$L\left(\boldsymbol{x}, g\left(f\left(\boldsymbol{x}\right)\right)\right)$$

where L is a loss function penalizing g(f(**x**)) for being dissimilar from **x**, such as the mean squared error.



Undercomplete Autoencoders

- If the code dimension is larger than the input dimension, an autoencoder tends to learn $g \circ f$ as a **identity function**.
- An autoencoder whose code dimension is smaller than the input dimension is called **undercomplete**.
- When the encoder and decoder are linear and L is the mean squared error, an undercomplete autoencoder learns to span the same subspace as PCA.

Undercomplete Autoencoders

- Define $\boldsymbol{h} = f(\boldsymbol{W}\boldsymbol{x});\ \boldsymbol{r} = g(\boldsymbol{V}\boldsymbol{h})$
- Goal $\min_{\boldsymbol{W},\boldsymbol{V}} \frac{1}{2N} \sum_{n=1}^{N} \left\| \boldsymbol{x}^{(n)} - \boldsymbol{r}^{(n)} \right\|^2$
- If f and g are linear $\min_{\boldsymbol{W},\boldsymbol{V}} \frac{1}{2N} \sum_{n=1}^{N} \left\| \boldsymbol{x}^{(n)} - \boldsymbol{V}\boldsymbol{W}\boldsymbol{x}^{(n)} \right\|^2$
- In other words, the optimal solution is PCA

Regularized Autoencoders

- Undercomplete autoencoders can also fail to learn anything useful if the encoder and decoder are given too much capacity e.g. **nonlinearity**.
- Regularized autoencoders use a loss function that encourages the model to have other properties besides the ability to copy its input to its output:
  - **Sparsity** of the representation
  - **Robustness** to noise or to missing inputs
  - **Smallness** of the derivative of the representation

Sparse Autoencoders

- A sparse autoencoder involves a **sparsity penalty** $\Omega(\mathbf{h})$ on the code layer **h**, in addition to the reconstruction error:

$$L\left(\boldsymbol{x}, g\left(f\left(\boldsymbol{x}\right)\right)\right) + \Omega(\boldsymbol{h})$$

  where g(**h**) is the decoder output and typically we have **h** = f(**x**), the encoder output.
- Regularized maximum likelihood corresponds to maximizing p(θ | x), which is equivalent to maximizing log p(x | θ) + log p(θ). The log p(x | θ) term is the usual data log-likelihood term and the log p(θ) term, the log-prior over parameters, incorporates the preference over particular values of θ.

Sparse Autoencoders

- Regularized autoencoders defy such an interpretation because the regularizer depends on the data
- But, we still can think of the entire sparse autoencoder framework as approximating maximum likelihood training of a generative model that has **latent variables**.
- Suppose we have a model with visible variables x and latent variables h, with an explicit joint distribution:

$$p_{model}(x,h) = p_{model}(h)\, p_{model}(x \mid h)$$

Sparse Autoencoders

- We refer to $p_{model}(h)$ as the model's **prior distribution** over the latent variables, representing the model's beliefs prior to seeing x.
- Then the likelihood can be decomposed as:

$$\log p_{model}(x) = \log \sum_{h} p_{model}(h, x)$$

- We can think of the autoencoder as approximating this sum with a point estimate for just **one highly likely** value for h.

Sparse Autoencoders

- From this point of view, with this chosen h, we maximize

$$\log p_{model}(h, x) = \log p_{model}(h) + \log p_{model}(x|h)$$

- The log p_{model} (h) term can be **sparsity-inducing**. For example, the Laplace prior,

$$p_{model}(h_i) = \frac{\lambda}{2} e^{-\lambda|h_i|}$$

corresponds to an absolute value sparsity penalty. Expressing the log-prior as an absolute value penalty, we obtain

$$\Omega(\mathbf{h}) = \lambda \sum_i |h_i|$$

Sparse Autoencoders

- This view provides a different motivation for training an autoencoder: it is a way of approximately training a generative model.
- It also provides a different reason for why the features learned by the autoencoder are useful: they describe the latent variables that explain the input.

Denoising Autoencoders

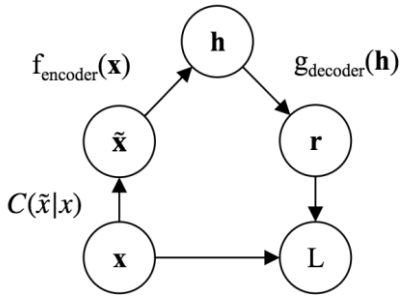
- The denoising autoencoder (DAE) is an autoencoder that receives a **corrupted** data point as input and is trained to predict the original, uncorrupted data point as its output.
- A denoising autoencoder or DAE minimizes

$$L\left(\boldsymbol{x}, g\left(f\left(\tilde{\boldsymbol{x}}\right)\right)\right)$$

where $\tilde{\boldsymbol{x}}$ is a copy of **x** that has been corrupted by some form of noise.

Denoising Autoencoders

- $C(\tilde{x}|x)$ represents a conditional distribution over corrupted samples $\tilde{x}$, given a data sample x.



Denoising Autoencoders

- So long as the encoder is deterministic, the denoising autoencoder is a feedforward network minimizing the loss

$$L = -\log p_{decoder}(x|h = f(\tilde{x}))$$

- We can view the DAE as performing stochastic gradient descent on the following expectation:

$$-\mathbb{E}_{x\sim\hat{p}_{data}(x)}\mathbb{E}_{\tilde{x}\sim C(\tilde{x}|x)} \log p_{decoder}(x|h = f(\tilde{x}))$$

where $\hat{p}_{data}(x)$ is the training distribution.

Contractive Autoencoders

- The contractive autoencoder introduces an explicit regularizer on the code h = f(x), encouraging the derivatives of f to be as small as possible:

$$L\left(\boldsymbol{x}, g\left(f(\boldsymbol{x})\right)\right) + \Omega(\boldsymbol{h}, \boldsymbol{x})$$

$$\Omega(\boldsymbol{h}, \boldsymbol{x}) = \lambda \sum_i ||\nabla_{\boldsymbol{x}} h_i||^2$$

- The penalty Ω(h) is the squared Frobenius norm (sum of squared elements) of the Jacobian matrix of partial derivatives associated with the encoder function.

Contractive Autoencoders

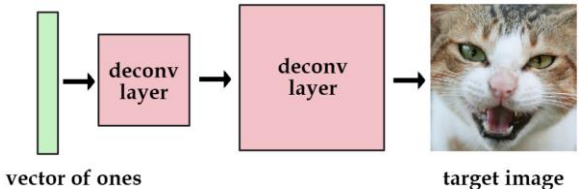
- The name **contractive** arises from the way that the CAE warps space. Specifically, because the CAE is trained to resist perturbations of its input, it is encouraged to map a neighborhood of input points to a smaller neighborhood of output points.

Variational Autoencoders

- Variational autoencoders are **generative models**.
- An common way of describing a neural network is an approximation of some function. However, they can also be thought of as a data structure that **holds information**.
- Assume a network with a few **deconvolution layers**.
- Set the input to be a vector of ones.

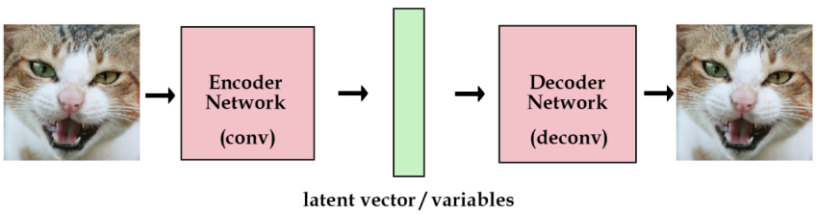
Variational Autoencoders

- Train the network to reduce the mean squared error between the deconvoluted image and the target image.
- The "data" for that image is now contained within the network's parameters.



Variational Autoencoders

- Use real vector (**latent variable**) to remember more images
- Choosing the latent variables randomly is a bad idea.
- In an autoencoder, we add in another component that takes in the original images and encodes them into vectors for us.



Variational Autoencoders

- To generate images, we add a constraint on the encoding network, that forces it to generate latent vectors that roughly follow **some distribution** q(z | x), e.g. unit Gaussian.
- Generating new images is now easy:
  - Get the encoded feature
  - Based on it, sample a latent vector from the unit Gaussian
  - Pass it to the decoder

Variational Autoencoders

- The key insight behind variational autoencoders is that they may be trained by maximizing the **variational lower bound** L(q) associated with data point x:

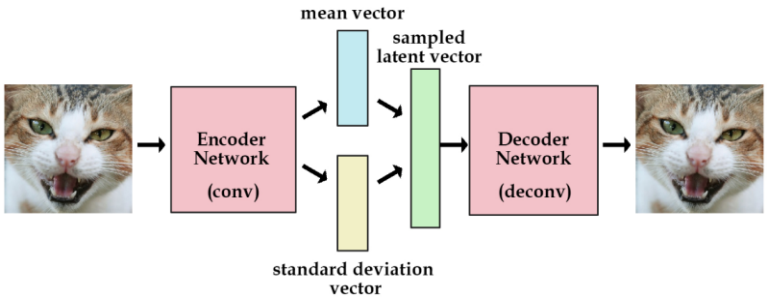
$$
\begin{aligned}
L(q) &= \mathbb{E}_{z\sim q(z|x)} \log p_{model}(z,x) + H\big(q(z|x)\big) \\
&= \mathbb{E}_{z\sim q(z|x)} \log p_{model}(x|z) + D_{KL}(q(z|x)||p_{model}(z)) \\
&\leq \log p_{model}(x)
\end{aligned}
$$

Variational Autoencoders

- In first line, the first term is the **joint** log-likelihood of the visible and hidden variables. The second term is entropy of the approximate posterior, which encourages the variational posterior to place **high probability mass** on many z values that could have generated x, rather than collapsing to a single point estimate of the most likely value.
- In second, the first term is the **reconstruction** log-likelihood. The second term tries to make the approximate posterior distribution $q(z \mid x)$ and the model prior $p_{model}(z)$ **approach each other**.

Variational Autoencoders

- In order to optimize the KL divergence, we need to apply a simple reparameterization trick:
  - Instead of the encoder generating a vector of real values
  - It will generate a vector of means and a vector of standard deviations.



Training of Autoencoders

- Depth can exponentially reduce the **computational** cost of representing some functions.
- Depth can also exponentially decrease the amount of **training data** needed to learn some functions.
- A common strategy for training a deep autoencoder is to greedily pretrain the deep architecture by training a stack of shallow autoencoders.

Software for Autoencoders

- Tensorflow
- Caffe
- Torch
- MXNet
- Keras
- Theano
- CNTK
- Chainer

Example for Autoencoders

- MNIST dataset overview
  - 60,000 examples for training
  - 10,000 examples for testing
  - Size-normalized digits
  - Centered in a fixed-size image (28x28 pixels)
  - Values from 0 to 1

Example for Autoencoders

- Define parameters to be learned

```
# tf Graph input (only pictures)
X = tf.placeholder("float", [None, num_input])

weights = {
    'encoder_h1': tf.Variable(tf.random_normal([num_input, num_hidden_1])),
    'encoder_h2': tf.Variable(tf.random_normal([num_hidden_1, num_hidden_2])),
    'decoder_h1': tf.Variable(tf.random_normal([num_hidden_2, num_hidden_1])),
    'decoder_h2': tf.Variable(tf.random_normal([num_hidden_1, num_input])),
}
biases = {
    'encoder_b1': tf.Variable(tf.random_normal([num_hidden_1])),
    'encoder_b2': tf.Variable(tf.random_normal([num_hidden_2])),
    'decoder_b1': tf.Variable(tf.random_normal([num_hidden_1])),
    'decoder_b2': tf.Variable(tf.random_normal([num_input])),
}
```

Example for Autoencoders

- Define network structure

```
# Building the encoder
def encoder(x):
    # Encoder Hidden layer with sigmoid activation #1
    layer_1 = tf.nn.sigmoid(tf.add(tf.matmul(x, weights['encoder_h1']),
                                   biases['encoder_b1']))
    # Encoder Hidden layer with sigmoid activation #2
    layer_2 = tf.nn.sigmoid(tf.add(tf.matmul(layer_1, weights['encoder_h2']),
                                   biases['encoder_b2']))
    return layer_2


# Building the decoder
def decoder(x):
    # Decoder Hidden layer with sigmoid activation #1
    layer_1 = tf.nn.sigmoid(tf.add(tf.matmul(x, weights['decoder_h1']),
                                   biases['decoder_b1']))
    # Decoder Hidden layer with sigmoid activation #2
    layer_2 = tf.nn.sigmoid(tf.add(tf.matmul(layer_1, weights['decoder_h2']),
                                   biases['decoder_b2']))
    return layer_2

# Construct model
encoder_op = encoder(X)
decoder_op = decoder(encoder_op)
```

Example for Autoencoders

- Define loss and optimizer

```
# Prediction
y_pred = decoder_op
# Targets (Labels) are the input data.
y_true = X

# Define loss and optimizer, minimize the squared error
loss = tf.reduce_mean(tf.pow(y_true - y_pred, 2))
optimizer = tf.train.RMSPropOptimizer(learning_rate).minimize(loss)

# Initialize the variables (i.e. assign their default value)
init = tf.global_variables_initializer()
```

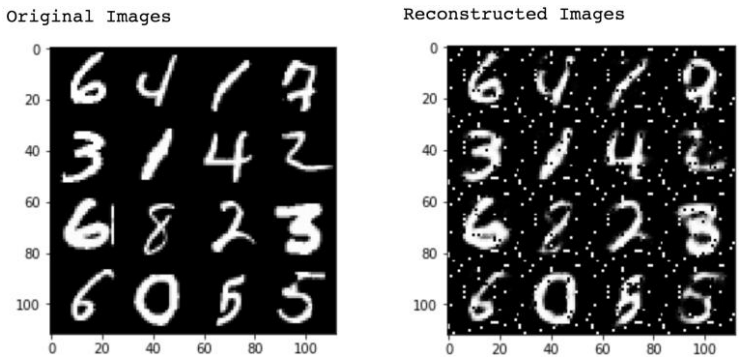
Example for Autoencoders

- Training

```
# Start Training
# Start a new TF session
sess = tf.Session()

# Run the initializer
sess.run(init)

# Training
for i in range(1, num_steps+1):
    # Prepare Data
    # Get the next batch of MNIST data (only images are needed, not labels)
    batch_x, _ = mnist.train.next_batch(batch_size)

    # Run optimization op (backprop) and cost op (to get loss value)
    _, l = sess.run([optimizer, loss], feed_dict={X: batch_x})
    # Display logs per step
    if i % display_step == 0 or i == 1:
        print('Step %i: Minibatch Loss: %f' % (i, l))
```

Example for Autoencoders

- Result



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