DS 4400

Machine Learning and Data Mining I

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Topics for Exam

- Linear regression (simple, multiple)
- Gradient descent
- Regularization (Lasso, ridge)
- Learning challenges
  - Overfitting, generalization, bias-variance tradeoff
- Linear classifiers
  - Perceptron, logistic regression
- Evaluation metrics
  - Confusion matrix, ROC curves
  - Cross-validation

Topics for Exam, cont.

- Generative models
  - LDA, Naïve Bayes
- Decision trees
  - Entropy, Information Gain
- Ensemble learning
  - Bagging (Random Forest), Boosting (AdaBoost)
- SVM
  - Linear and kernel, support vectors
- Neural networks
  - Feed-Forward NN (activation, architecture)
  - Convolutional NN (convolution, max pool)
- Compare different techniques (list pros and cons)

Outline

- Feed-Forward architectures
  - Multi-class classification (softmax unit)
  - Representing Boolean functions
  - Lab in Keras
- Convolutional Neural Networks
  - Convolution layer
  - Max pooling layer
  - Examples of famous architectures

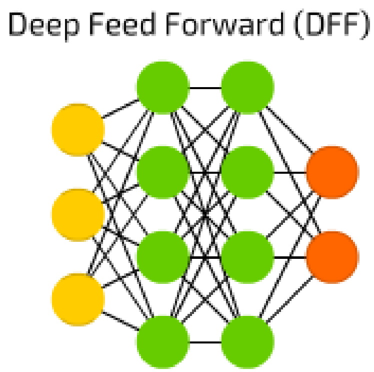
References

- Deep Learning books
  - https://www.deeplearningbook.org/
  - http://d2l.ai/
- Stanford notes on deep learning
  - http://cs229.stanford.edu/notes/cs229-notes-deep_learning.pdf
- History of Deep Learning
  - https://beamandrew.github.io/deeplearning/2017/02/23/deep_learning_101_part1.html

Neural Network Architectures

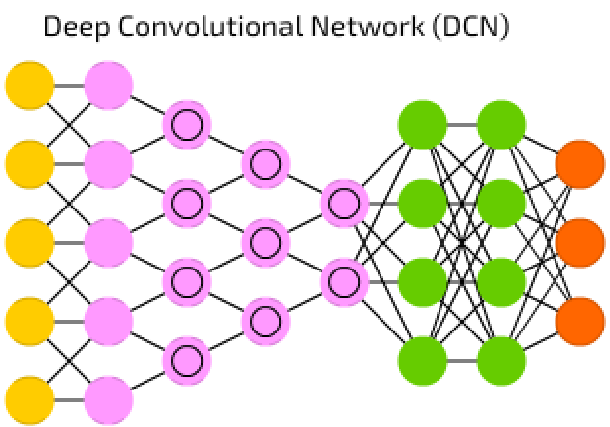
Feed-Forward Networks

- Neurons from each layer connect to neurons from next layer



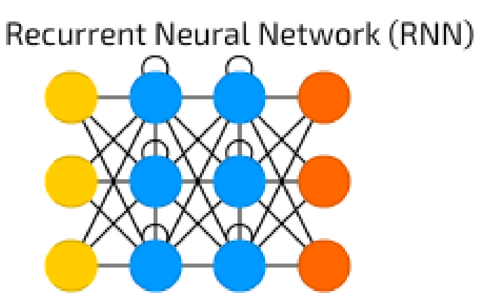
Convolutional Networks

- Includes convolution layer for feature reduction
- Learns hierarchical representations

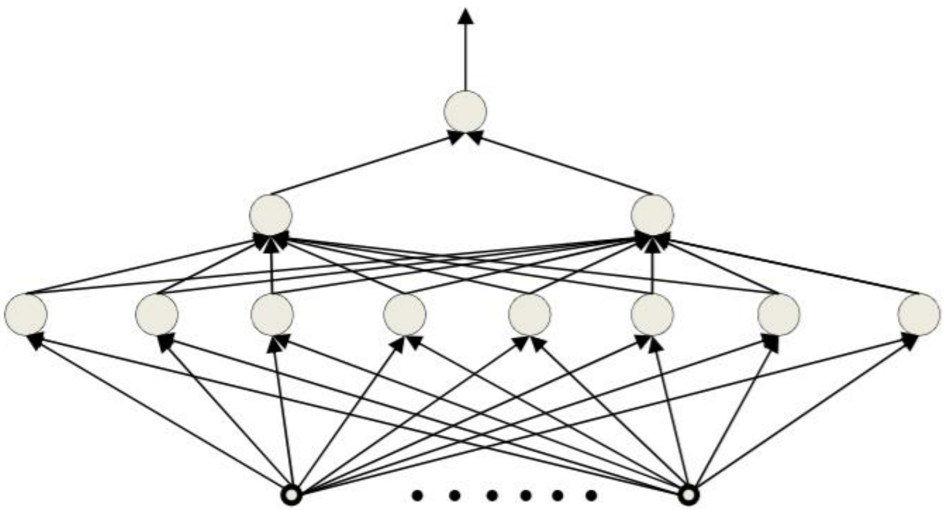


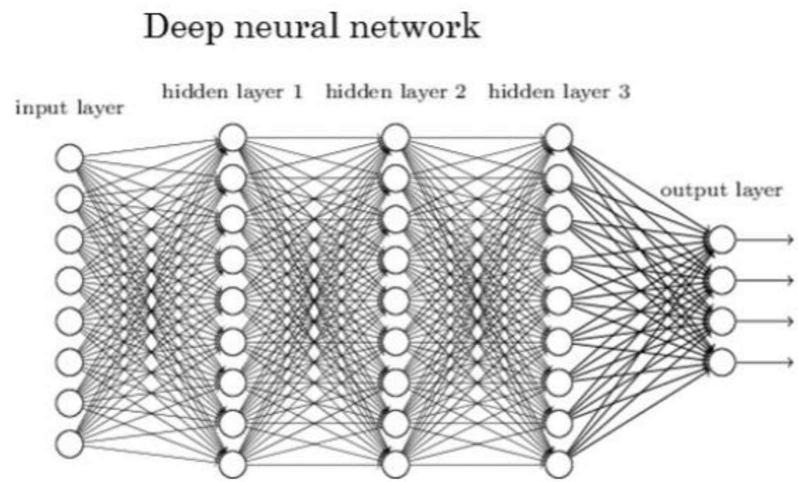
Recurrent Networks

- Keep hidden state
- Have cycles in computational graph



Multi-Layer Perceptron

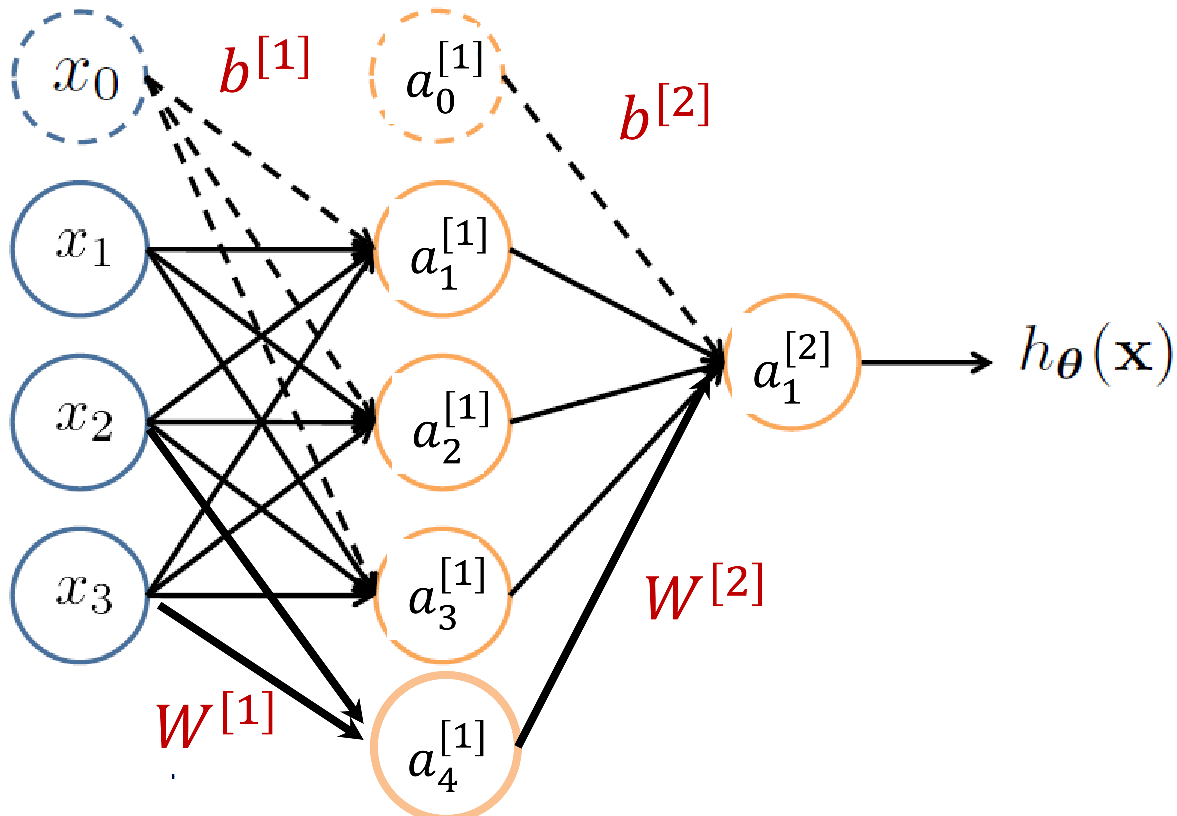




- A network of perceptrons
  - Generally "layered"

Feed-Forward Neural Network

bias units



Training example
$x = (x_1, x_2, x_3)$

(Input Layer) (Hidden Layer) (Output Layer)

Layer 0 Layer 1 Layer 2

No cycles

$\theta = (b^{[1]}, W^{[1]}, b^{[2]}, W^{[2]})$

Vectorization

$$z_1^{[1]} = W_1^{[1]T} x + b_1^{[1]} \quad \text{and} \quad a_1^{[1]} = g(z_1^{[1]})$$

$$\vdots \qquad\qquad \vdots \qquad\qquad \vdots$$

$$z_4^{[1]} = W_4^{[1]T} x + b_4^{[1]} \quad \text{and} \quad a_4^{[1]} = g(z_4^{[1]})$$

$$\underbrace{\begin{bmatrix} z_1^{[1]} \\ \vdots \\ \vdots \\ z_4^{[1]} \end{bmatrix}}_{z^{[1]} \in \mathbb{R}^{4\times 1}} = \underbrace{\begin{bmatrix} — & W_1^{[1]T} & — \\ — & W_2^{[1]T} & — \\ & \vdots & \\ — & W_4^{[1]T} & — \end{bmatrix}}_{W^{[1]} \in \mathbb{R}^{4\times 3}} \underbrace{\begin{bmatrix} x_1 \\ x_2 \\ x_3 \end{bmatrix}}_{x \in \mathbb{R}^{3\times 1}} + \underbrace{\begin{bmatrix} b_1^{[1]} \\ b_2^{[1]} \\ \vdots \\ b_4^{[1]} \end{bmatrix}}_{b^{[1]} \in \mathbb{R}^{4\times 1}}$$

$$z^{[1]} = W^{[1]} x + b^{[1]}$$

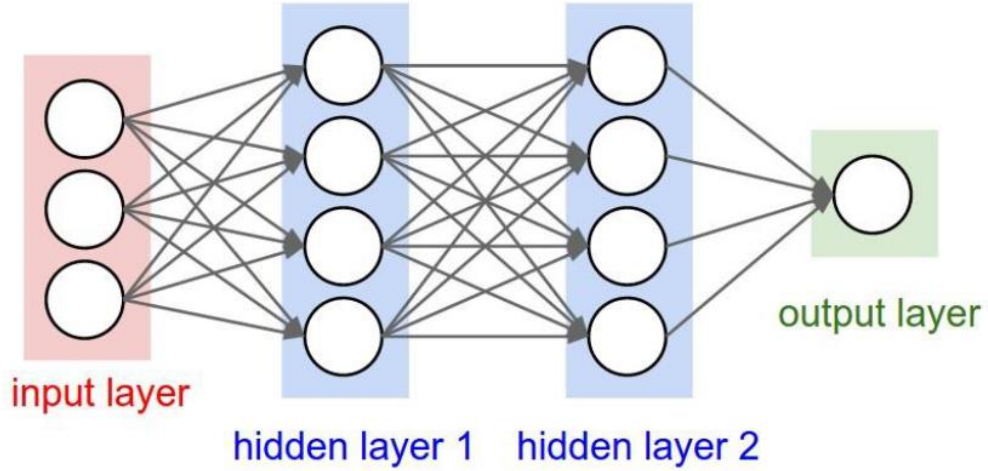
$$a^{[1]} = g(z^{[1]})$$

Linear

Non-Linear

Forward Propagation

- The input neurons first receive the data features of the object. After processing the data, they send their output to the first hidden layer.
- The hidden layer processes this output and sends the results to the next hidden layer.
- This continues until the data reaches the final output layer, where the output value determines the object's classification.
- This entire process is known as Forward Propagation, or Forward prop.

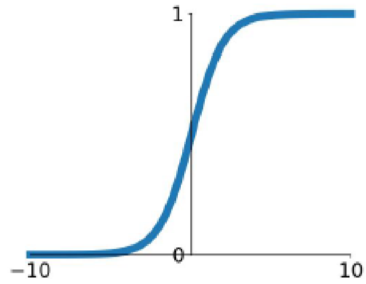


$x \longrightarrow$ *Prediction*

Activation Functions

Sigmoid

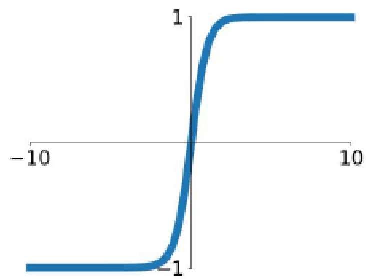
$\sigma(x) = \frac{1}{1+e^{-x}}$



Binary Classification

tanh

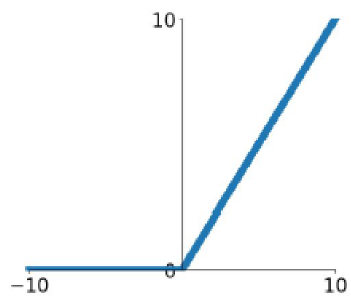
$\tanh(x)$



Regression

ReLU

$\max(0, x)$



Intermediary layers

Non-Linear Activations

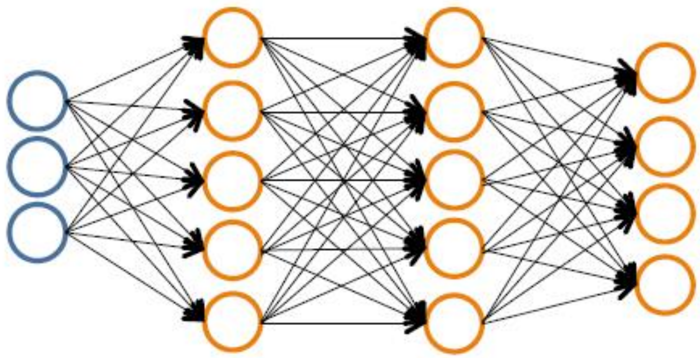
Multiple Output Units: One-vs-Rest

Pedestrian

Car

Motorcycle

Truck



$$h_\Theta(\mathbf{x}) \in \mathbb{R}^K$$

We want:

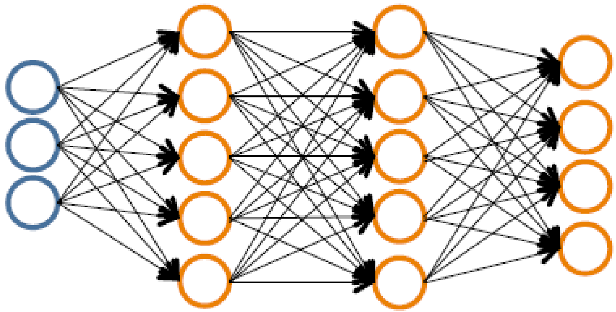
$$h_\Theta(\mathbf{x}) \approx \begin{bmatrix}1\\0\\0\\0\end{bmatrix}$$
when pedestrian

$$h_\Theta(\mathbf{x}) \approx \begin{bmatrix}0\\1\\0\\0\end{bmatrix}$$
when car

$$h_\Theta(\mathbf{x}) \approx \begin{bmatrix}0\\0\\1\\0\end{bmatrix}$$
when motorcycle

$$h_\Theta(\mathbf{x}) \approx \begin{bmatrix}0\\0\\0\\1\end{bmatrix}$$
when truck

Multiple Output Units: One-vs-Rest



$$h_\Theta(\mathbf{x}) \in \mathbb{R}^K$$

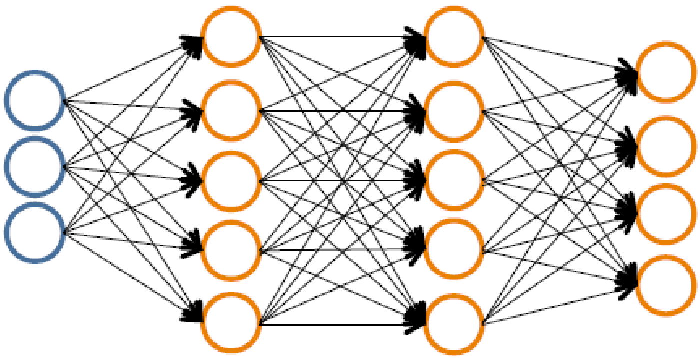
We want:

$h_\Theta(\mathbf{x}) \approx \begin{bmatrix} 1 \\ 0 \\ 0 \\ 0 \end{bmatrix}$ when pedestrian $\quad h_\Theta(\mathbf{x}) \approx \begin{bmatrix} 0 \\ 1 \\ 0 \\ 0 \end{bmatrix}$ when car $\quad h_\Theta(\mathbf{x}) \approx \begin{bmatrix} 0 \\ 0 \\ 1 \\ 0 \end{bmatrix}$ when motorcycle $\quad h_\Theta(\mathbf{x}) \approx \begin{bmatrix} 0 \\ 0 \\ 0 \\ 1 \end{bmatrix}$ when truck

- Given $\{(\mathbf{x}_1, y_1), (\mathbf{x}_2, y_2), ..., (\mathbf{x}_n, y_n)\}$
- Must convert labels to 1-of-K representation
  - e.g., $\mathbf{y}_i = \begin{bmatrix} 0 \\ 0 \\ 1 \\ 0 \end{bmatrix}$ when motorcycle, $\mathbf{y}_i = \begin{bmatrix} 0 \\ 1 \\ 0 \\ 0 \end{bmatrix}$ when car, etc.

Based on slide by Andrew Ng

Neural Network Classification



Given:

$\{(\mathbf{x}_1,y_1), (\mathbf{x}_2,y_2), \ldots, (\mathbf{x}_n,y_n)\}$

$\mathbf{s} \in \mathbb{N}^{+L}$ contains # nodes at each layer

- $s_0 = d$ (# features)

<u>Binary classification</u>

y = 0 or 1

1 output unit $(s_{L-1} = 1)$

Sigmoid

<u>Multi-class classification</u> (K classes)

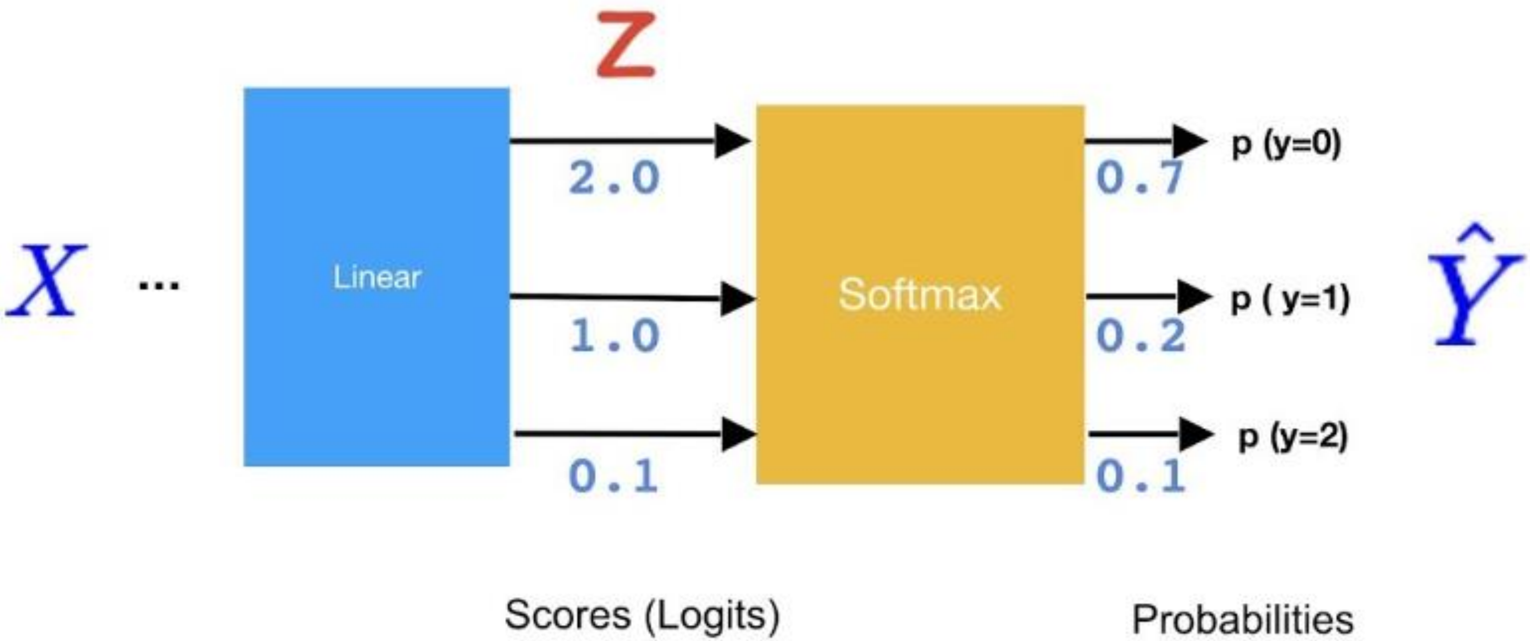
$\mathbf{y} \in \mathbb{R}^K$ e.g. $\begin{bmatrix}1\\0\\0\\0\end{bmatrix}$, $\begin{bmatrix}0\\1\\0\\0\end{bmatrix}$, $\begin{bmatrix}0\\0\\1\\0\end{bmatrix}$, $\begin{bmatrix}0\\0\\0\\1\end{bmatrix}$

pedestrian car motorcycle truck

K output units $(s_{L-1} = K)$

Softmax

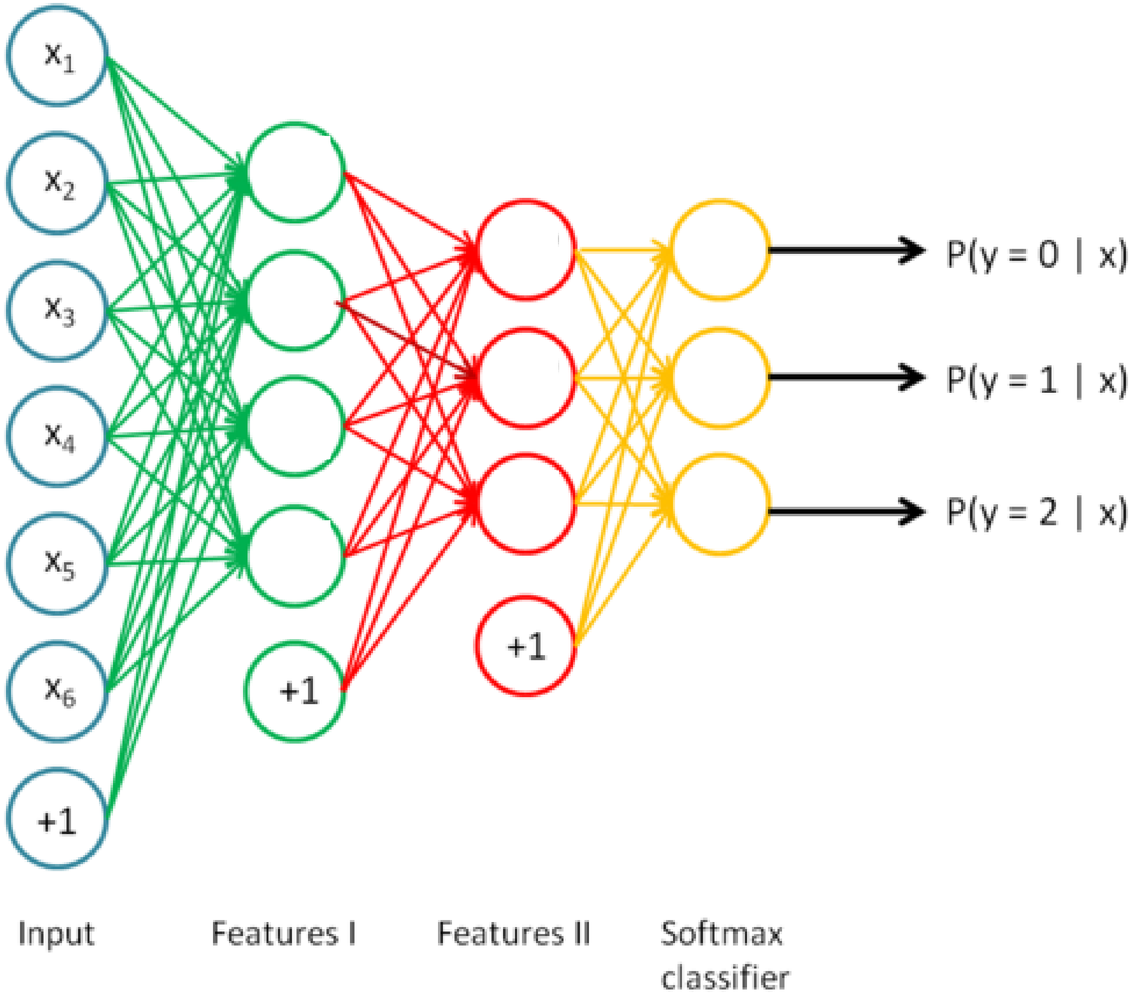
Softmax classifier



$$\sigma(\mathbf{z})_j = \frac{e^{z_j}}{\sum_{k=1}^{K} e^{z_k}} \quad \text{for } j = 1, \ldots, K.$$

- Predict the class with highest probability
- Generalization of sigmoid/logistic regression to multi-class

Multi-class classification

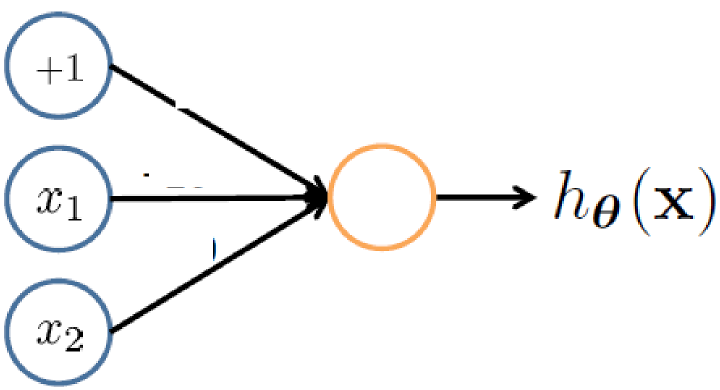


Representing Boolean Functions

Simple example: AND

$x_1, x_2 \in \{0, 1\}$

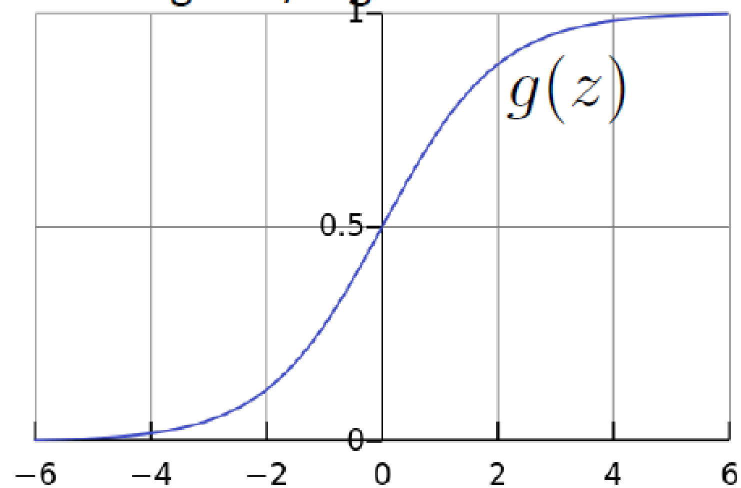
$y = x_1 \text{ AND } x_2$



$h_\Theta(\mathbf{x}) = g(\ ? \ + \ ? \ x_1 + \ ? \ x_2)$

Logistic unit

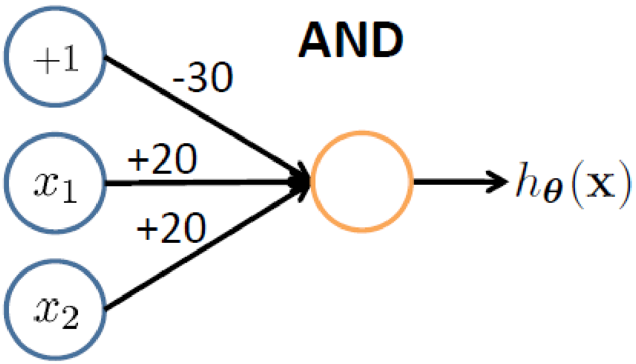
Logistic / Sigmoid Function



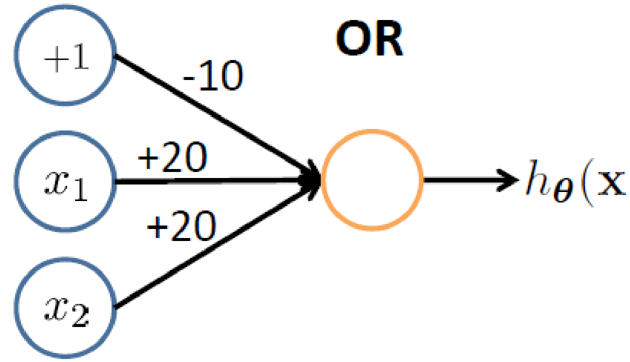
x_1	x_2	$h_\Theta(\mathbf{x})$
0	0	0
0	1	0
1	0	0
1	1	1

Representing Boolean Functions

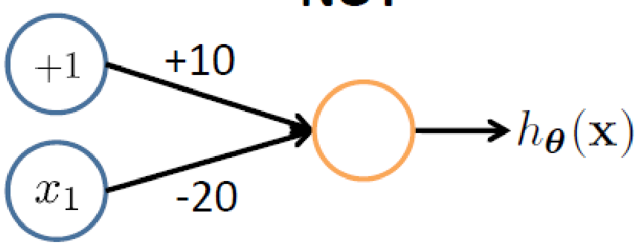
AND



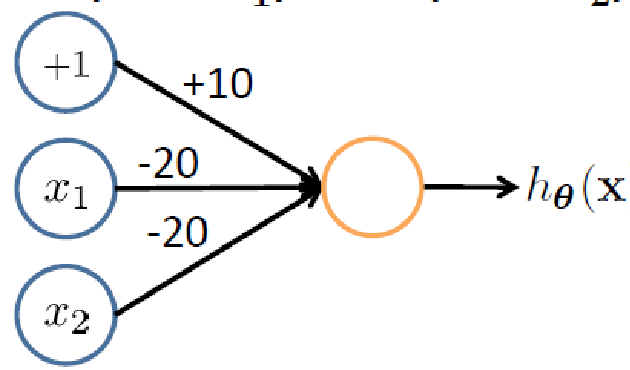
OR



NOT

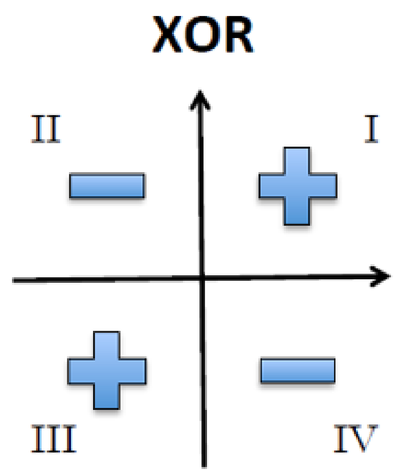


(NOT x_1) AND (NOT x_2)



XOR

- Need at least one hidden layer to compute XOR!

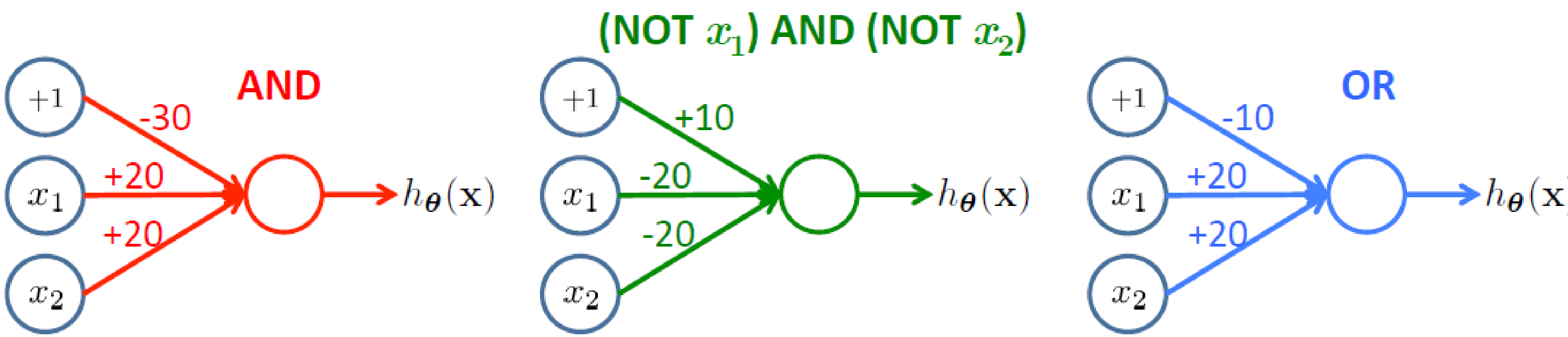


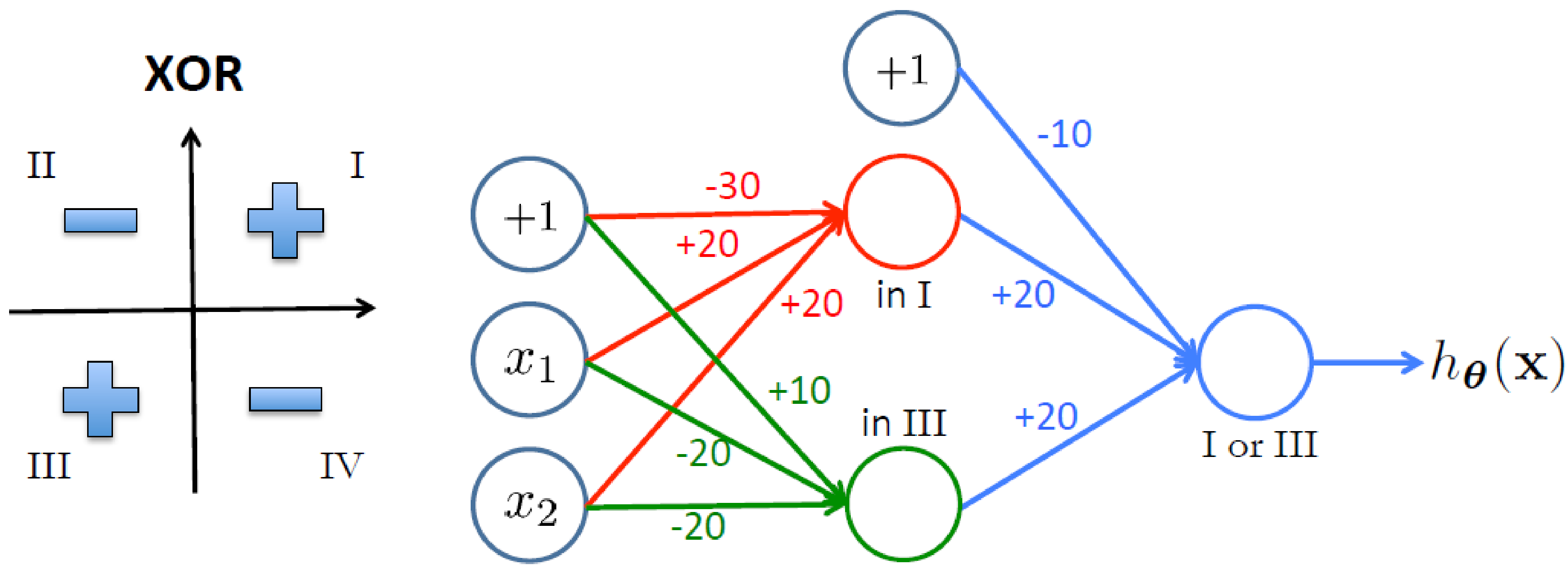
Non-linearly separable

- NOT[X1 XOR X2]=

(X1 AND X2) OR ((NOT X1) AND (NOT X2))

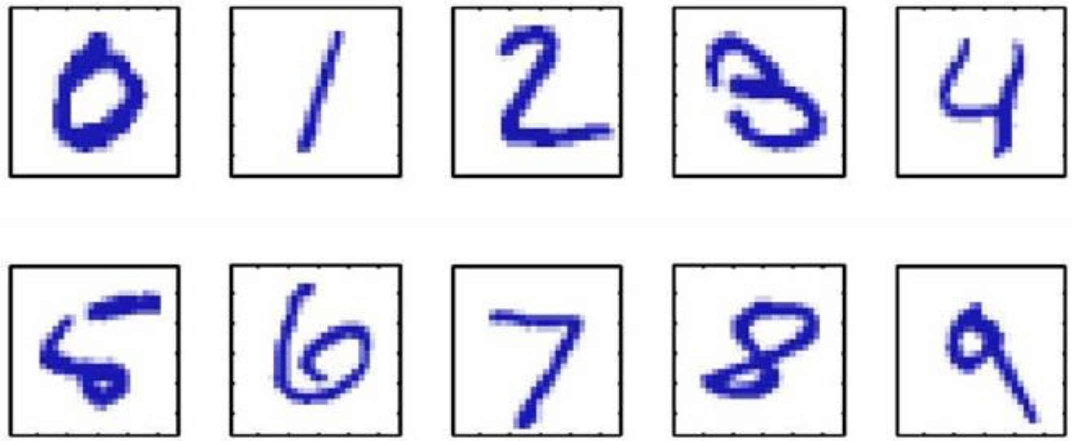
Combining Representations





XOR is non-linear!

MNIST: Handwritten digit recognition



Images are 28 x 28 pixels

Represent input image as a vector $\mathbf{x} \in \mathbb{R}^{784}$

Learn a classifier $f(\mathbf{x})$ such that,

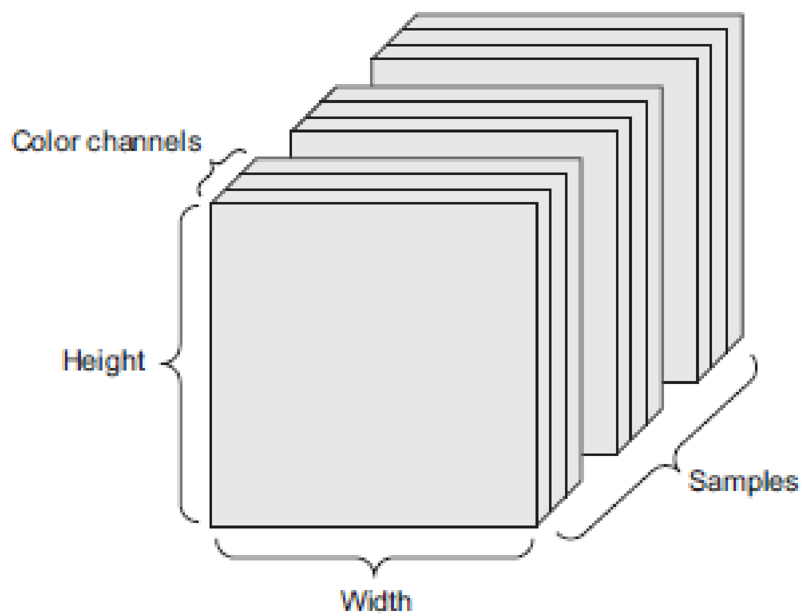
$$f : \mathbf{x} \rightarrow \{0, 1, 2, 3, 4, 5, 6, 7, 8, 9\}$$

Predict the digit

Multi-class classifier

Image Representation

- Image is 3D "tensor": height, width, color channel (RGB)
- Black-and-white images are 2D matrices: height, width
  - Each value is pixel intensity



Lab – Feed Forward NN

```python
import time
import numpy as np
from keras.utils import np_utils
import keras.callbacks as cb
from keras.models import Sequential
from keras.layers.core import Dense, Dropout, Activation
from keras.optimizers import RMSprop
from keras.datasets import mnist

import matplotlib
matplotlib.use('agg')
import matplotlib.pyplot as plt
```

Import modules

```python
def load_data():
    print("Loading data")
    (X_train, y_train), (X_test, y_test) = mnist.load_data()

    X_train = X_train.astype('float32')
    X_test = X_test.astype('float32')

    # Normalize
    X_train /= 255
    X_test /= 255

    y_train = np_utils.to_categorical(y_train, 10)
    y_test = np_utils.to_categorical(y_test, 10)

    X_train = np.reshape(X_train, (60000, 784))
    X_test = np.reshape(X_test, (10000, 784))

    print("Data Loaded")
    return [X_train, X_test, y_train, y_test]
```

Load MNIST data Processing

Vector representation

Neural Network Architecture

```python
def init_model():
    start_time = time.time()

    print("Compiling Model")
    model = Sequential()
    model.add(Dense(10, input_dim=784))
    model.add(Activation('relu'))

    model.add(Dense(10))
    model.add(Activation('softmax'))

    rms = RMSprop()
    model.compile(loss='categorical_crossentropy', optimizer=rms, metrics=['accuracy'])

    print("Model finished"+format(time.time() - start_time))
    return model
```

10 hidden units
ReLU activation

Output Layer
Softmax activation

Loss function

Optimizer

Feed-Forward Neural Network Architecture

- 1 Hidden Layer ("Dense" or Fully Connected)
- 10 neurons
- Output layer uses softmax activation

Train and evaluate

```python
def run_network(data=None, model=None, epochs=10, batch=256):
    try:
        start_time = time.time()
        if data is None:
            X_train, X_test, y_train, y_test = load_data()
        else:
            X_train, X_test, y_train, y_test = data

        if model is None:
            model = init_model()

        print("Training model")
        history = model.fit(X_train, y_train, nb_epoch=epochs, batch_size=batch,
                  validation_data=(X_test, y_test), verbose=2)

        print("Training duration:"+format(time.time() - start_time))
        score = model.evaluate(X_test, y_test, batch_size=16)

        print("\nNetwork's test loss and accuracy:"+format(score))
        return model, history
    except KeyboardInterrupt:
        print("KeyboardInterrupt")
        return model, history
```

Training/testing results

```
2s - loss: 0.9114 - acc: 0.7649 - val_loss: 0.4499 - val_acc: 0.8819
Epoch 2/10
0s - loss: 0.3935 - acc: 0.8907 - val_loss: 0.3378 - val_acc: 0.9049
Epoch 3/10
0s - loss: 0.3296 - acc: 0.9063 - val_loss: 0.3042 - val_acc: 0.9128
Epoch 4/10
0s - loss: 0.3036 - acc: 0.9132 - val_loss: 0.2889 - val_acc: 0.9181
Epoch 5/10
0s - loss: 0.2888 - acc: 0.9189 - val_loss: 0.2874 - val_acc: 0.9185
Epoch 6/10
0s - loss: 0.2785 - acc: 0.9210 - val_loss: 0.2703 - val_acc: 0.9257
Epoch 7/10
0s - loss: 0.2705 - acc: 0.9241 - val_loss: 0.2718 - val_acc: 0.9239
Epoch 8/10
0s - loss: 0.2649 - acc: 0.9257 - val_loss: 0.2694 - val_acc: 0.9240
Epoch 9/10
0s - loss: 0.2601 - acc: 0.9264 - val_loss: 0.2616 - val_acc: 0.9261
Epoch 10/10
0s - loss: 0.2561 - acc: 0.9277 - val_loss: 0.2607 - val_acc: 0.9274
Training duration:10.31288456916809
 9840/10000 [============================>.] - ETA: 0s
Network's test loss and accuracy:[0.26067940444946291, 0.9274]
```

Epoch Output

Metrics

- Loss
- Accuracy

Reported on both training and testing

Changing Number of Neurons

```
def init_model():
    start_time = time.time()

    print("Compiling Model")
    model = Sequential()
    model.add(Dense(500, input_dim=784))
    model.add(Activation('relu'))

    model.add(Dense(10))
    model.add(Activation('softmax'))

    rms = RMSprop()
    model.compile(loss='categorical_crossentropy', optimizer=rms, metrics=['accuracy'])

    print("Model finished"+format(time.time() - start_time))
    return model
```

500 hidden units

```
2s - loss: 0.3169 - acc: 0.9088 - val_loss: 0.1652 - val_acc: 0.9502
Epoch 2/10
0s - loss: 0.1277 - acc: 0.9626 - val_loss: 0.1071 - val_acc: 0.9679
Epoch 3/10
0s - loss: 0.0847 - acc: 0.9749 - val_loss: 0.0861 - val_acc: 0.9731
Epoch 4/10
0s - loss: 0.0607 - acc: 0.9822 - val_loss: 0.0746 - val_acc: 0.9767
Epoch 5/10
0s - loss: 0.0471 - acc: 0.9863 - val_loss: 0.0655 - val_acc: 0.9796
Epoch 6/10
0s - loss: 0.0359 - acc: 0.9895 - val_loss: 0.0636 - val_acc: 0.9813
Epoch 7/10
0s - loss: 0.0280 - acc: 0.9920 - val_loss: 0.0599 - val_acc: 0.9810
Epoch 8/10
0s - loss: 0.0223 - acc: 0.9937 - val_loss: 0.0678 - val_acc: 0.9795
Epoch 9/10
0s - loss: 0.0174 - acc: 0.9952 - val_loss: 0.0607 - val_acc: 0.9815
Epoch 10/10
0s - loss: 0.0134 - acc: 0.9964 - val_loss: 0.0672 - val_acc: 0.9806
Training duration:10.4581892490386 96
 9456/10000 [===========================>..] - ETA: 0s
Network's test loss and accuracy:[0.067179036217656543, 0.98060000000000003]
```

Two Layers

```python
def init_model():
    start_time = time.time()

    print("Compiling Model")
    model = Sequential()

    # Hidden Layer 1
    model.add(Dense(500, input_dim=784))
    model.add(Activation('relu'))

    # Hidden Layer 2
    model.add(Dense(300))
    model.add(Activation('relu'))

    model.add(Dense(10))
    model.add(Activation('softmax'))

    rms = RMSprop()
    model.compile(loss='categorical_crossentropy', optimizer=rms, metrics=['accuracy'])

    print("Model finished"+format(time.time() - start_time))
    return model
```

Layer 1

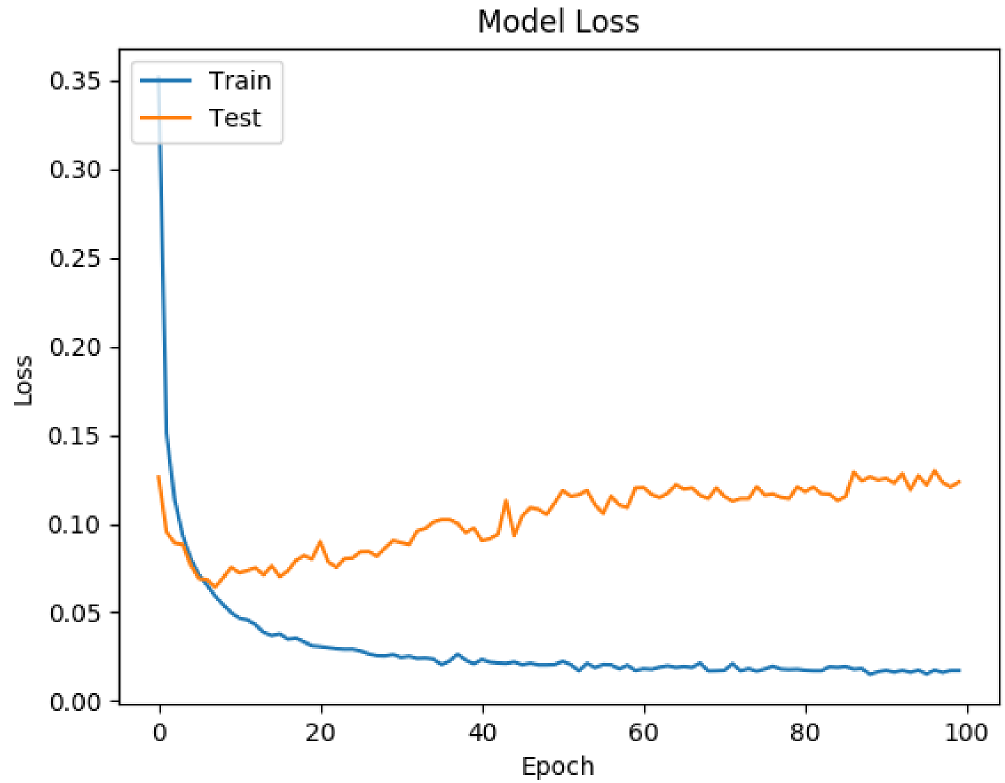
Layer 2

Output Softmax Layer

```
2s - loss: 0.2800 - acc: 0.9132 - val_loss: 0.1821 - val_acc: 0.9409
Epoch 2/10
1s - loss: 0.0974 - acc: 0.9699 - val_loss: 0.0951 - val_acc: 0.9703
Epoch 3/10
0s - loss: 0.0616 - acc: 0.9803 - val_loss: 0.0843 - val_acc: 0.9754
Epoch 4/10
0s - loss: 0.0429 - acc: 0.9862 - val_loss: 0.0670 - val_acc: 0.9809
Epoch 5/10
0s - loss: 0.0303 - acc: 0.9904 - val_loss: 0.0820 - val_acc: 0.9777
Epoch 6/10
0s - loss: 0.0233 - acc: 0.9922 - val_loss: 0.0794 - val_acc: 0.9783
Epoch 7/10
0s - loss: 0.0180 - acc: 0.9941 - val_loss: 0.0866 - val_acc: 0.9792
Epoch 8/10
0s - loss: 0.0137 - acc: 0.9956 - val_loss: 0.0788 - val_acc: 0.9814
Epoch 9/10
0s - loss: 0.0116 - acc: 0.9963 - val_loss: 0.0901 - val_acc: 0.9795
Epoch 10/10
1s - loss: 0.0100 - acc: 0.9966 - val_loss: 0.0812 - val_acc: 0.9827
Training duration:11.816290140151978
 9744/10000 [============================>.] - ETA: 0s
```

Monitor Loss

```
def plot_losses(history):
    plt.plot(history.history['loss'])
    plt.plot(history.history['val_loss'])
    plt.title('Model Loss')
    plt.ylabel('Loss')
    plt.xlabel('Epoch')
    plt.legend(['Train', 'Test'], loc='upper left')
    plt.show()
    plt.savefig('output.png')
```



Acknowledgements

- Slides made using resources from:
  - Yann LeCun
  - Andrew Ng
  - Eric Eaton
  - David Sontag
  - Andrew Moore
- Thanks!