DS 4400

Machine Learning and Data Mining I

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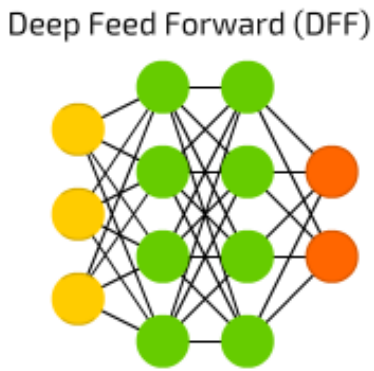
Outline

- Feed Forward Neural Networks
  - Forward Propagation
  - Hyper-parameters
  - Activations
- Multi-class classification
  - The softmax classifier
- Example
- Lab in Keras

Neural Network Architectures

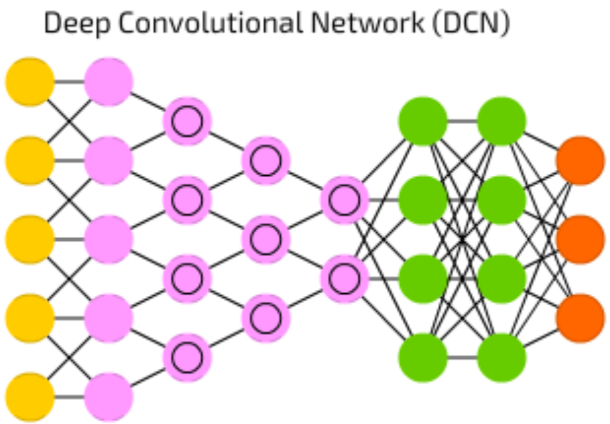
Feed-Forward Networks

- Neurons from each layer connect to neurons from next layer



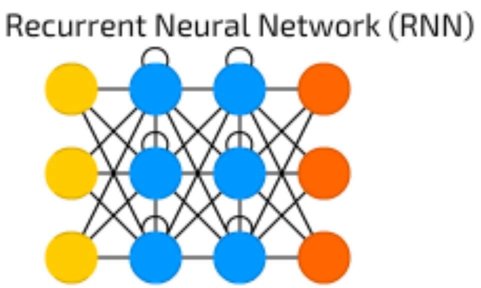
Convolutional Networks

- Includes convolution layer for feature reduction
- Learns hierarchical representations



Recurrent Networks

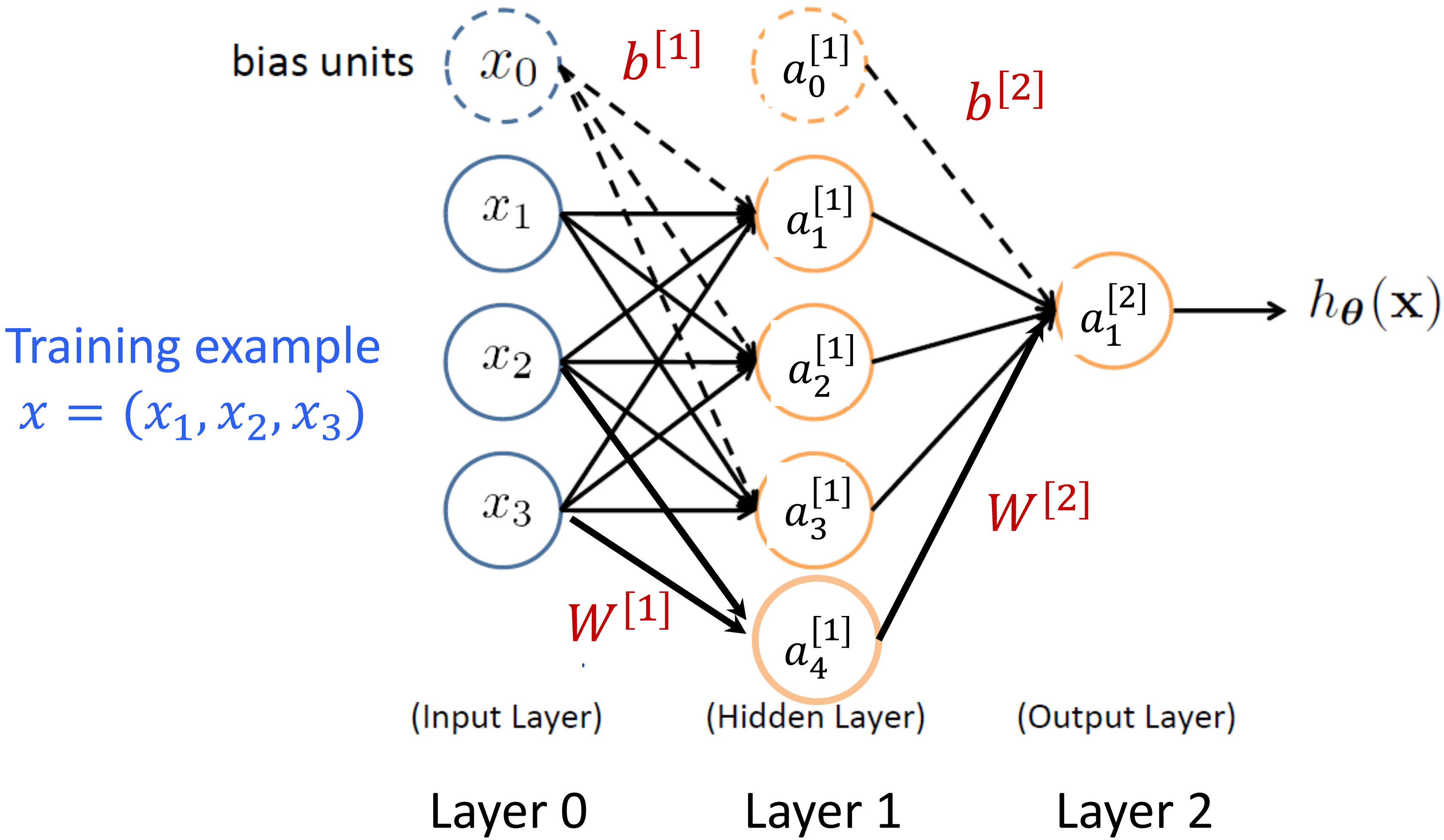
- Keep hidden state
- Have cycles in computational graph



Feed-Forward NN

- Hyper-parameters
  – Number of layers
  – Architecture (how layers are connected)
  – Number of hidden units per layer
  – Number of units in output layer
  – Activation functions
- Other
  – Initialization
  – Regularization

Feed-Forward Neural Network



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

Vectorization

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

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

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

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

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

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

Vectorization

Output layer

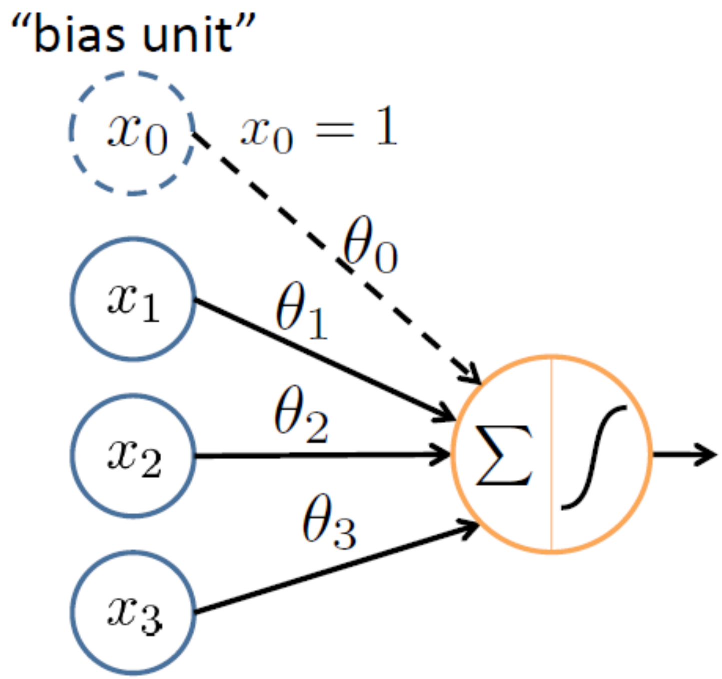
$$z_1^{[2]} = W_1^{[2]} \ a^{[1]} + b_1^{[2]} \quad \text{and} \quad a_1^{[2]} = g(z_1^{[2]})$$

$$\underbrace{z^{[2]}}_{1\times1} = \underbrace{W^{[2]}}_{1\times4}\underbrace{a^{[1]}}_{4\times1} + \underbrace{b^{[2]}}_{1\times1} \quad \text{and} \quad \underbrace{a^{[2]}}_{1\times1} = g(\underbrace{z^{[2]}}_{1\times1})$$

Terminology

- Layer 1
  - First hidden unit:
    - Linear: $z_1^{[1]} = \mathrm{W}_1^{[1]\,\mathrm{T}} x + \mathrm{b}_1^{[1]}$
    - Non-linear: $a_1^{[1]} = \mathrm{g}(\mathrm{z}_1^{[1]})$
  - …
  - Fourth hidden unit:
    - Linear: $z_4^{[1]} = \mathrm{W}_4^{[1]\,\mathrm{T}} x + \mathrm{b}_4^{[1]}$
    - Non-linear: $a_4^{[1]} = \mathrm{g}(\mathrm{z}_4^{[1]})$
- Terminology
  - $a_i^{[j]}$ - Activation of unit i in layer j
  - g - Activation function
  - $W^{[j]}$ - Weight vector controlling mapping from layer j-1 to j
  - $b^{[j]}$ - Bias vector from layer j-1 to j

Logistic Unit: A simple NN



$$\mathbf{x} = \begin{bmatrix} x_0 \\ x_1 \\ x_2 \\ x_3 \end{bmatrix} \qquad \boldsymbol{\theta} = \begin{bmatrix} \theta_0 \\ \theta_1 \\ \theta_2 \\ \theta_3 \end{bmatrix}$$

$$h_{\boldsymbol{\theta}}(\mathbf{x}) = g\left(\boldsymbol{\theta}^\intercal \mathbf{x}\right) = g(w^T x + b)$$

$$= \frac{1}{1 + e^{-\boldsymbol{\theta}^\intercal \mathbf{x}}}$$

Sigmoid (logistic) activation function: $g(z) = \frac{1}{1 + e^{-z}}$

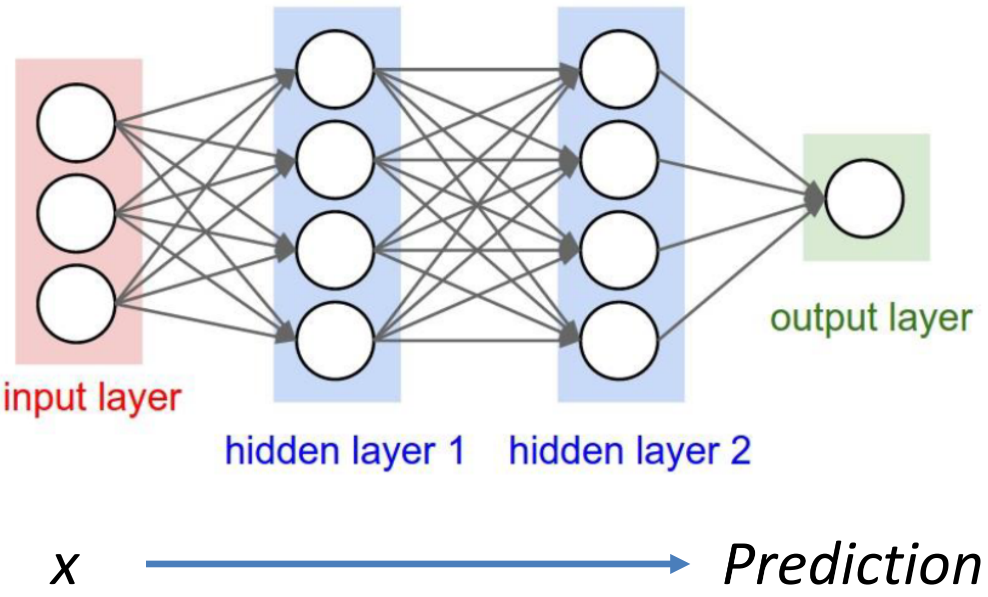
No hidden layers

Training Neural Networks

- Input training dataset D
  - Number of features: d
  - Labels from K classes
- First layer has d+1 units (one per feature and bias)
- Output layer has K units
- Training procedure determines parameters that optimize loss function
  - Backpropagation
  - Learn optimal $W^{[i]}, b^{[i]}$ at layer *i*
- Evaluation of a point done by forward propagation

Forward Propagation

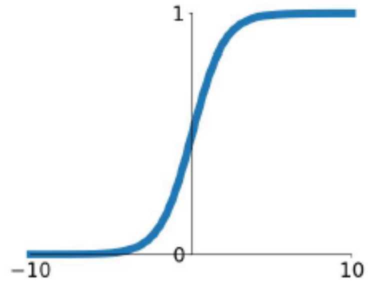
- The input neurons first receive the data features of the object. After processing the data, they send their output to the first hidden layer.
- The hidden layer processes this output and sends the results to the next hidden layer.
- This continues until the data reaches the final output layer, where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



Activation Functions

Sigmoid

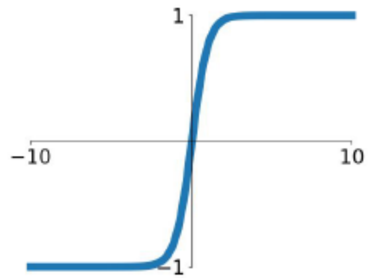
$\sigma(x) = \frac{1}{1+e^{-x}}$



Binary Classification

tanh

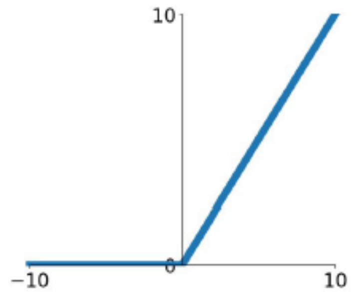
$\tanh(x)$



Regression

ReLU

$\max(0, x)$



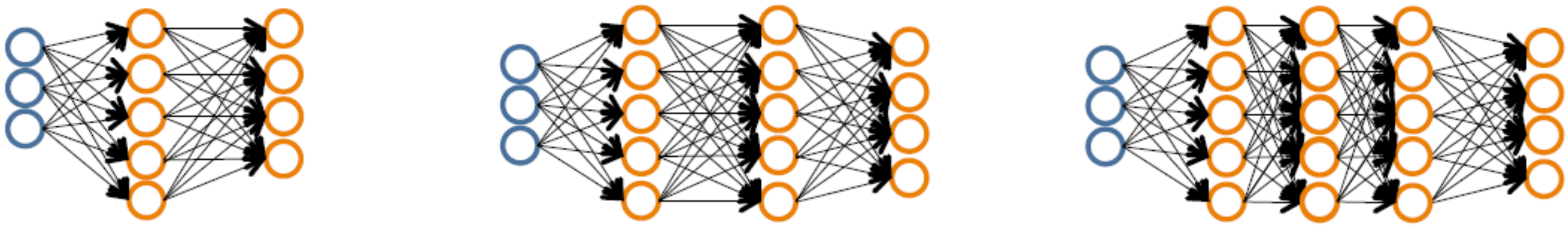
Intermediary layers

Why Non-Linear Activations?

- Assume g is linear: $\mathrm{g}(z) = Uz$

How to pick architecture?

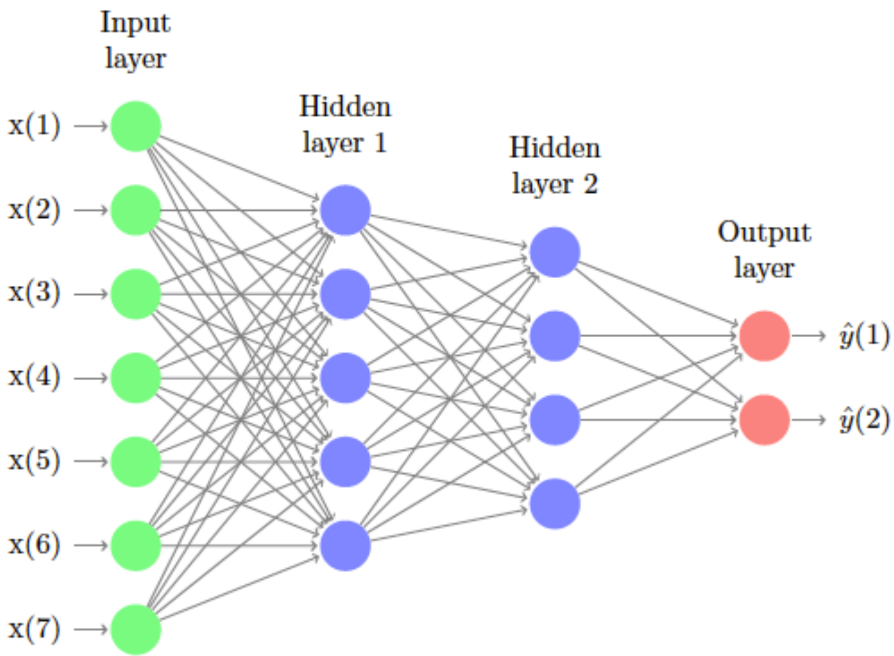
Pick a network architecture (connectivity pattern between nodes)



- # input units = # of features in dataset
- # output units = # classes

Reasonable default: 1 hidden layer

FFNN Architectures



- Input and Output Layers are completely specified by the problem domain
- In the Hidden Layers, number of neurons in Layer i+1 is usually smaller or equal to the number of neurons in Layer i

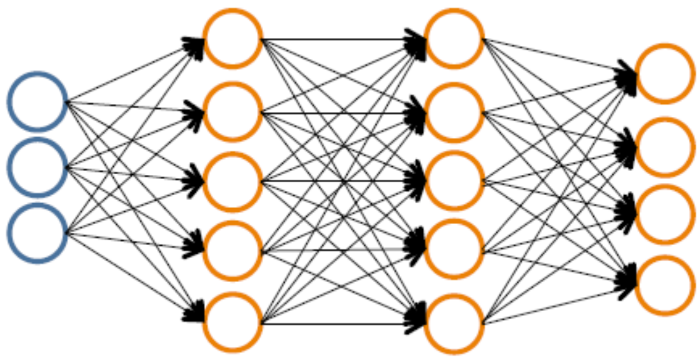
Multi-Class Classsification


Pedestrian


Car


Motorcycle


Truck



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

We want:

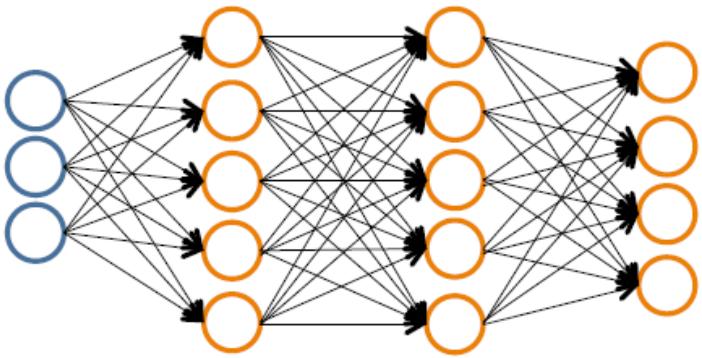
$$h_\Theta(\mathbf{x}) \approx \begin{bmatrix} 1 \\ 0 \\ 0 \\ 0 \end{bmatrix}$$
when pedestrian

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

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)

Binary classification

y = 0 or 1

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

Sigmoid

Multi-class classification (K classes)

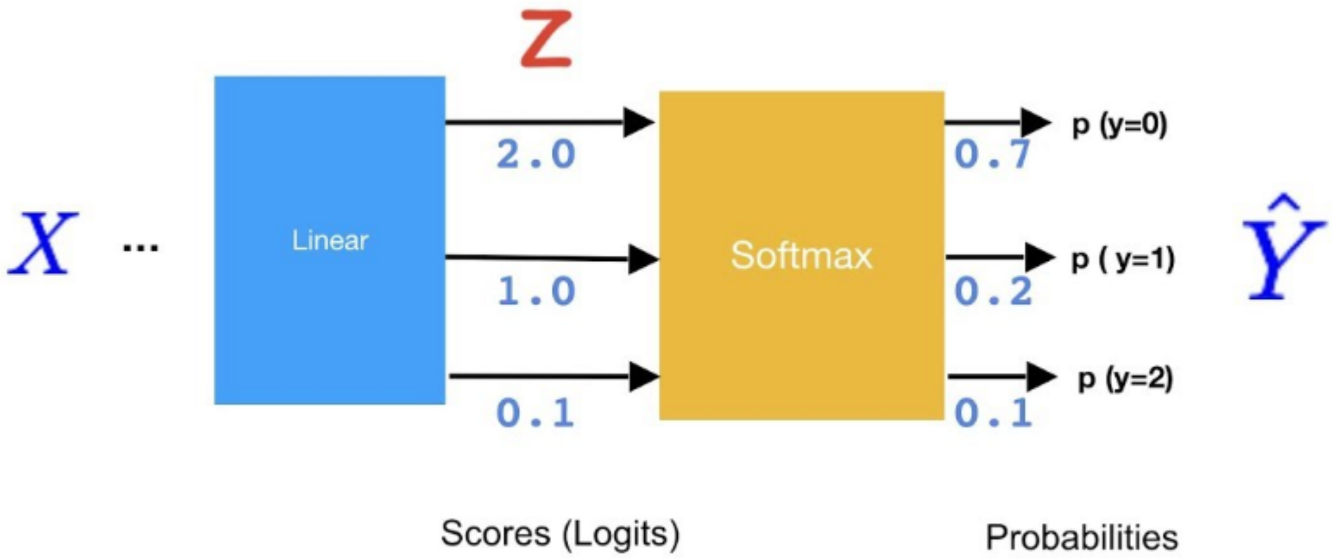
$\mathbf{y} \in \mathbb{R}^K$ e.g. $\begin{bmatrix}1\\0\\0\\0\end{bmatrix}$, $\begin{bmatrix}0\\1\\0\\0\end{bmatrix}$, $\begin{bmatrix}0\\0\\1\\0\end{bmatrix}$, $\begin{bmatrix}0\\0\\0\\1\end{bmatrix}$

pedestrian car motorcycle truck

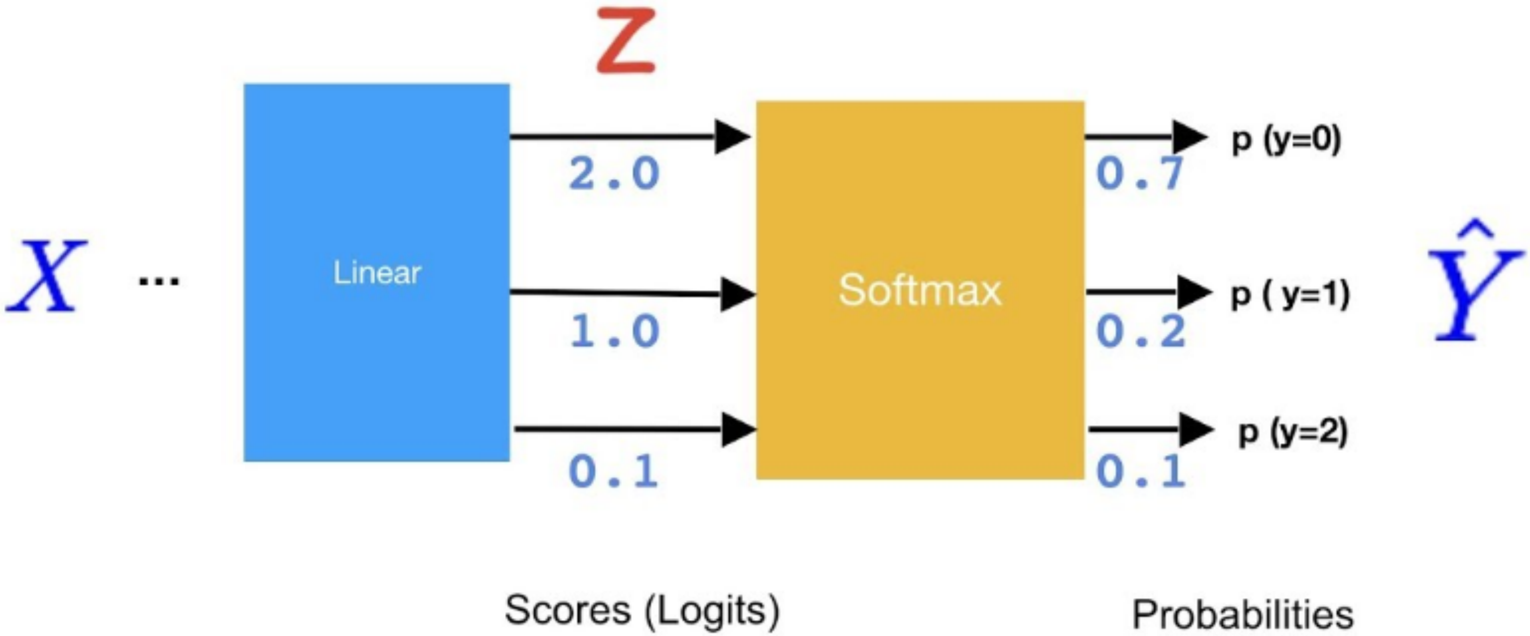
K output units $(s_{L-1} = K)$

Softmax

Softmax classifier



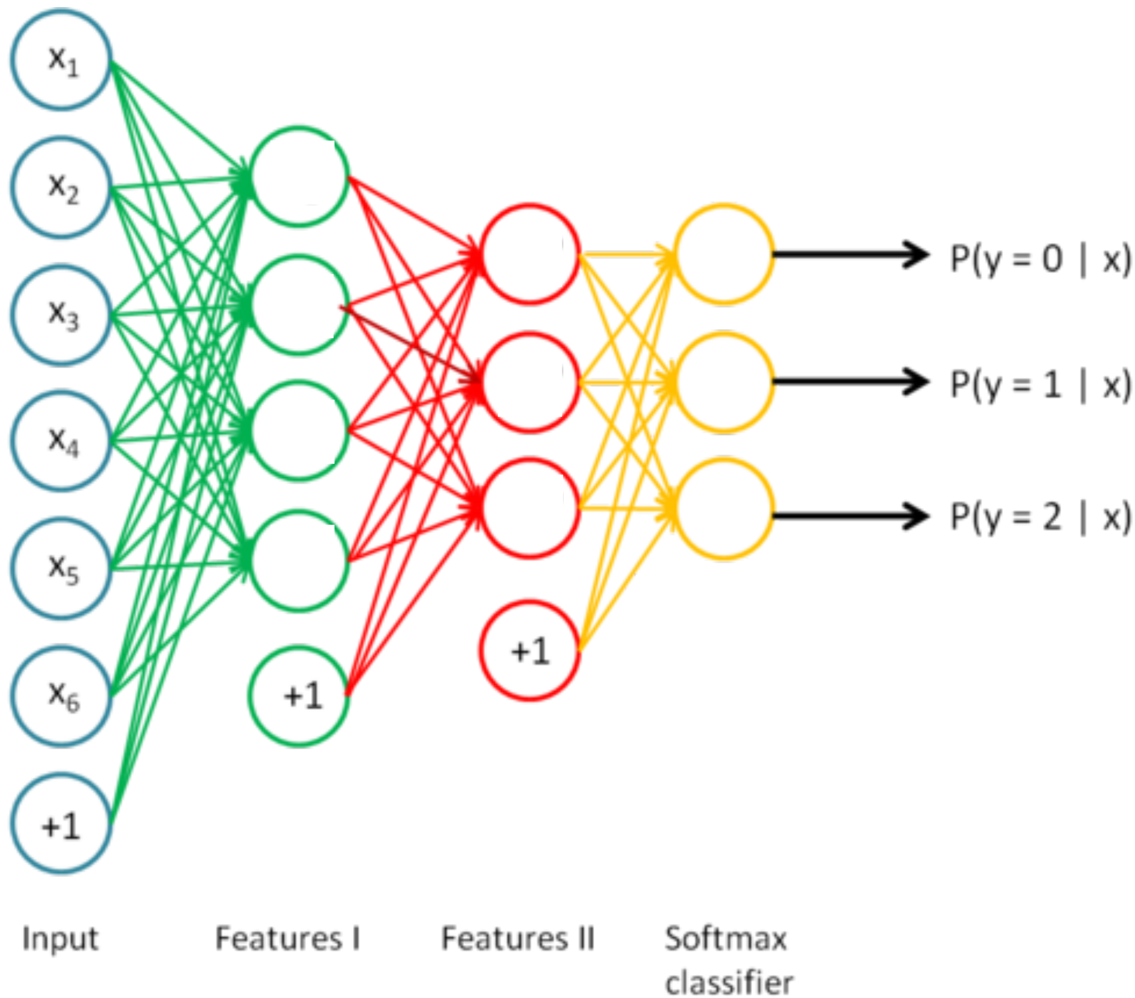
Softmax classifier



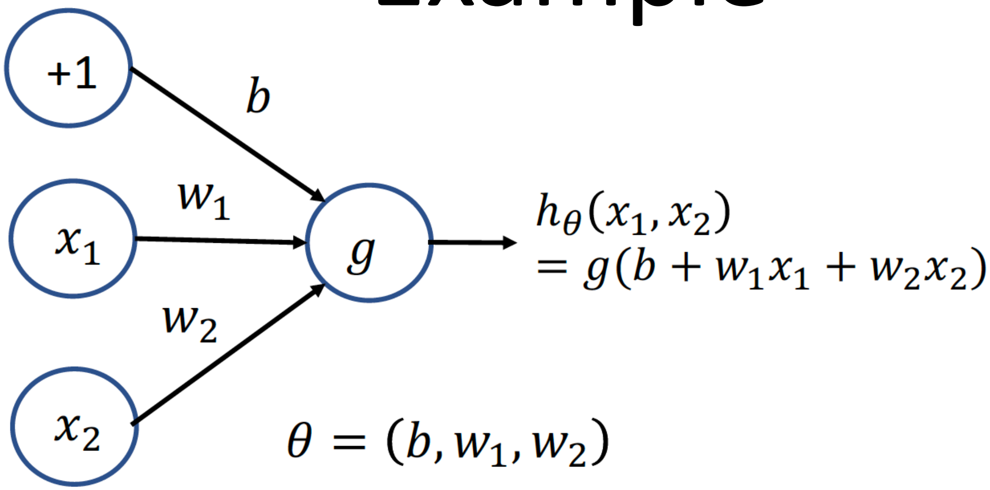
$$\sigma(\mathbf{z})_j = \frac{e^{z_j}}{\sum_{k=1}^{K} e^{z_k}} \quad \text{for } j = 1, \ldots, K.$$

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

Multi-class classification



Example



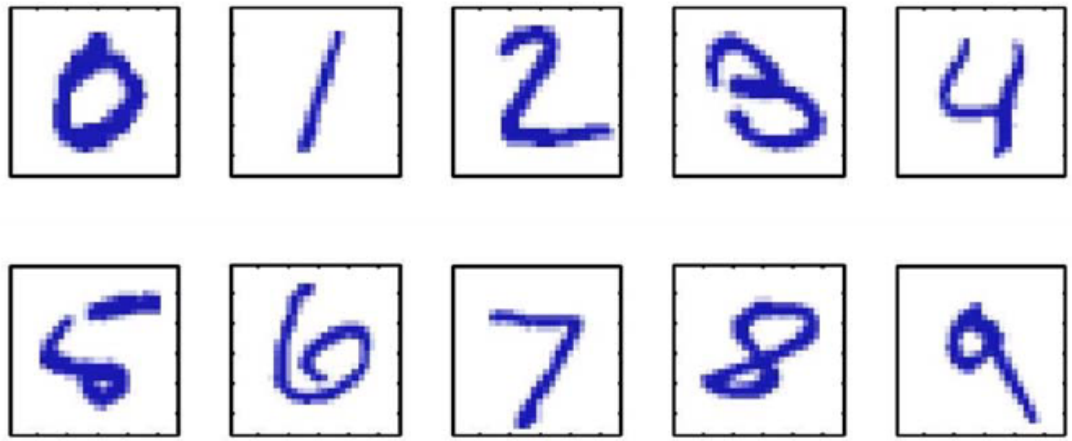
1. Given $b = -10, w_1 = 12, w_2 = 5$
Activation $g(z) = sign(z)$
Compute the output:

x_1	x_2	$h(x_1, x_2)$
0	0	
0	1	
1	0	
1	1	

2. Find out the weights $b,\ w_1, w_2$ and activation function to get the following output:

x_1	x_2	$h(x_1, x_2)$
0	0	1
0	1	1
1	0	1
1	1	0

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,

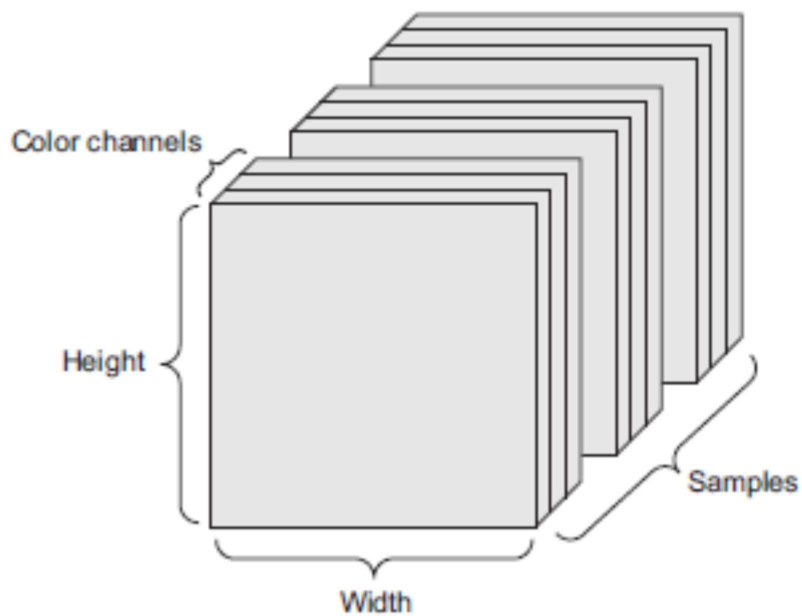
$$f : \mathbf{x} \rightarrow \{0, 1, 2, 3, 4, 5, 6, 7, 8, 9\}$$

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

```
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 validation

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:[0.06717903621765654 3, 0.98060000000000003]
```

Two Layers

```
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
```

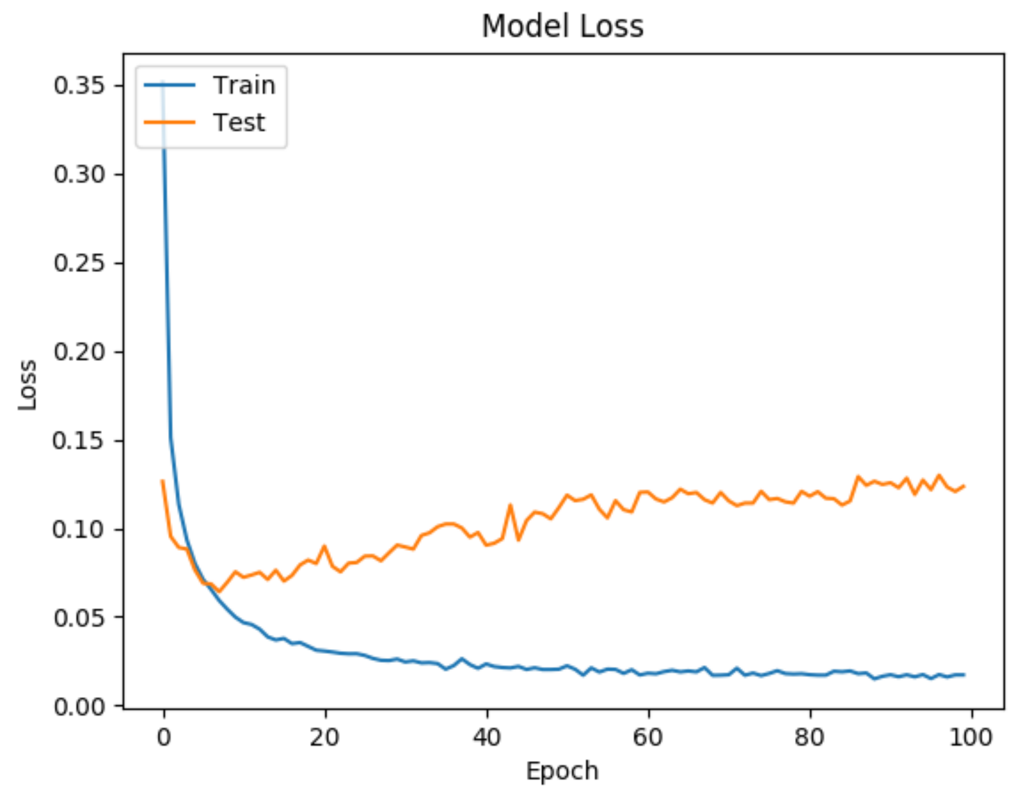
Model Parameters

```
model.summary()
```

```
Using TensorFlow backend.
Loading data
Data loaded
Compiling Model
_________________________________________________________________
Layer (type)                 Output Shape              Param #
=================================================================
dense_1 (Dense)              (None, 500)               392500
_________________________________________________________________
activation_1 (Activation)    (None, 500)               0
_________________________________________________________________
dense_2 (Dense)              (None, 300)               150300
_________________________________________________________________
activation_2 (Activation)    (None, 300)               0
_________________________________________________________________
dense_3 (Dense)              (None, 10)                3010
_________________________________________________________________
activation_3 (Activation)    (None, 10)                0
=================================================================
Total params: 545,810
Trainable params: 545,810
Non-trainable params: 0
```

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')
```



Review Feed-Forward Neural Networks

- Simplest architecture of NN
- Neurons from one layer are connected to neurons from next layer
  - Input layer has feature space dimension
  - Output layer has number of classes
  - Hidden layers use linear operations, followed by non-linear activation function
  - Multi-Layer Perceptron (MLP): fully connected layers
- Activation functions
  - Sigmoid for binary classification in last layer
  - Softmax for multi-class classification in last layer
  - ReLU for hidden layers
- Forward propagation is the computation of the network output given an input
- Back propagation is the training of a network
  - Determine weights and biases at every layer

Acknowledgements

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