BST 261: Data Science II
Lecture 3
Feedforward networks in Python with Keras

Heather Mattie
Harvard T.H. Chan School of Public Health
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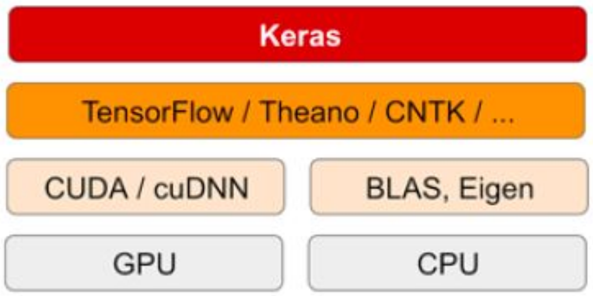
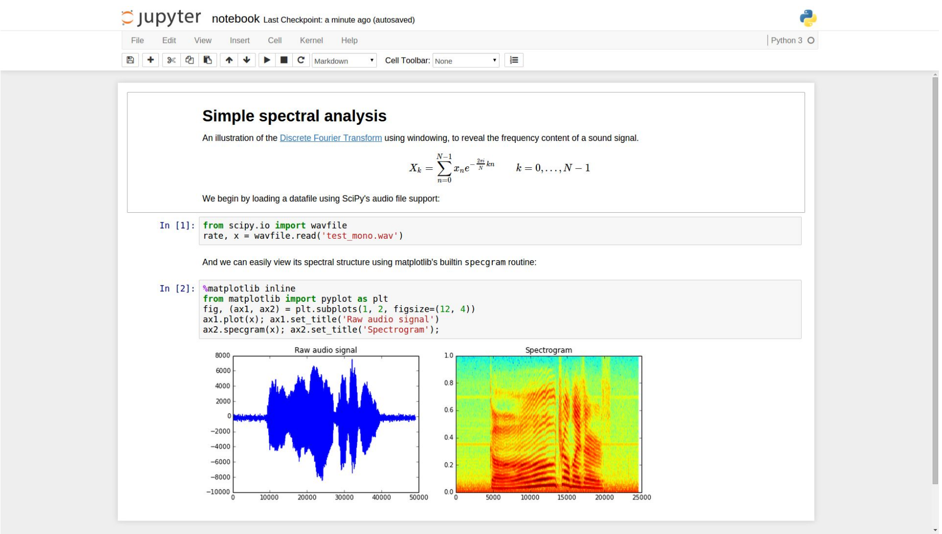
Keras and Tensorflow



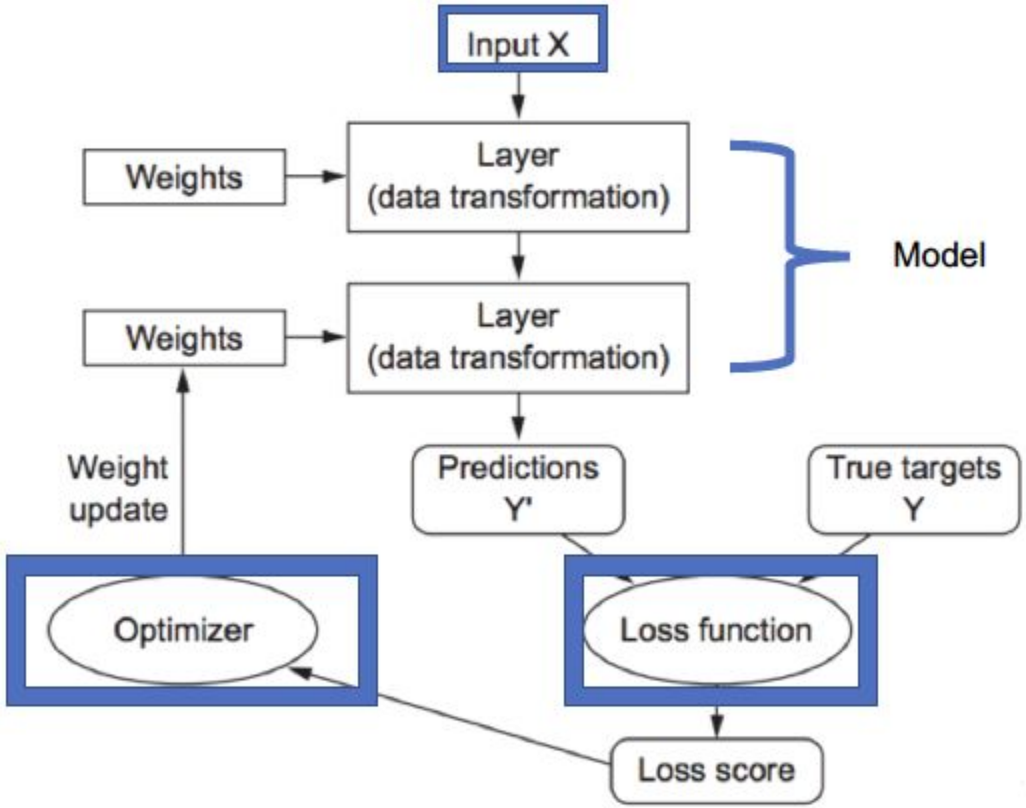
- Keras is a model-level library that provides high-level building blocks for developing deep learning models
- It doesn’t handle low-level operations like matrix and tensor (n-dimensional matrix) multiplication and differentiation
  - It uses TensorFlow or Theano or CNTK (Microsoft Cognitive Toolkit) backends for this
  - We will be using TensorFlow
    - It is the most widely adopted, scalable and production ready
- Keras can run on both CPUs and GPUs
  - When running on CPUs, uses a Eigen for tensor operations
  - When running on GPUs, uses the NVIDIA CUDA Deep Neural Network library (cuDNN)

Jupyter Notebooks

- Jupyter notebooks are the Python equivalent of R RMarkdown files
  - You can blend text, pictures, links and code in the same file
- We will be using them for all examples shown in class and in the labs, and the homework assignment templates will be Jupyter notebooks
  - We encourage you to use Jupyter notebooks, but if you are more comfortable using something else, feel free to use that
- For today's examples you will need the following libraries:
  - NumPy
  - TensorFlow*
  - Keras
  - Matplotlib
  - * TensorFlow must be installed before Keras



Neural Network Architecture



Generic Feedforward Network

```
# Format data to be fed into the network
(train_data, train_labels), (test_data, test_labels) = load_data()
# This tells keras you want a linear stack of layers
network = models.Sequential()
# Layer 1 (Hidden layer)
network.add(layers.Dense(c, activation='activation function', input_shape=( n, )))
# Layer 2 (Output layer)
network.add(layers.Dense(d, activation='activation function'))

# Create (compile) the network
network.compile(optimizer='optimizing algorithm',
# Include optimizing function, loss
                loss='loss function',
# function and performance measure
                metrics=['performance measure'])

# Train (learn) the network, specify batch size and number of epochs
network.fit(train_data, train_labels, epochs=e, batch_size=b)
# Save loss and performance measure values
test_loss, test_acc = network.evaluate(test_data, test_labels)
```

Generic Feedforward Network

train_data: training examples (matrix of feature vectors; $\mathbf{X}_{train}$)

train_labels: training labels ($\mathbf{y}_{train}$)

test_data: test examples used to measure performance of network ($\mathbf{X}_{test}$)

test_labels: test set labels ($\mathbf{y}_{test}$)

Optimizing algorithms: rmsprop, sgd, adagrad, adam, etc.

Loss function options: mse, mae, categorical_crossentropy, etc.

Performance measure options: accuracy, mae, etc.

Here:

- ***c*** = the number of hidden units (neurons) in a hidden layer
- ***d*** = the number of units (neurons) in the output layer
- ***e*** = the number of epochs (iterations) over entire training data set
- ***b*** = the batch size (how many training examples to optimize at once)

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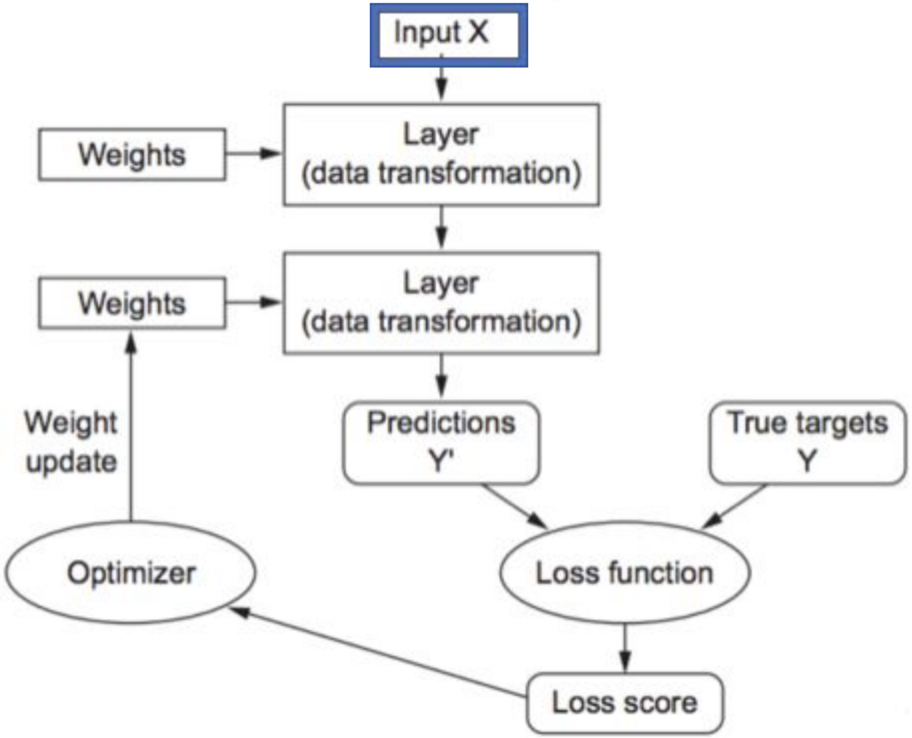

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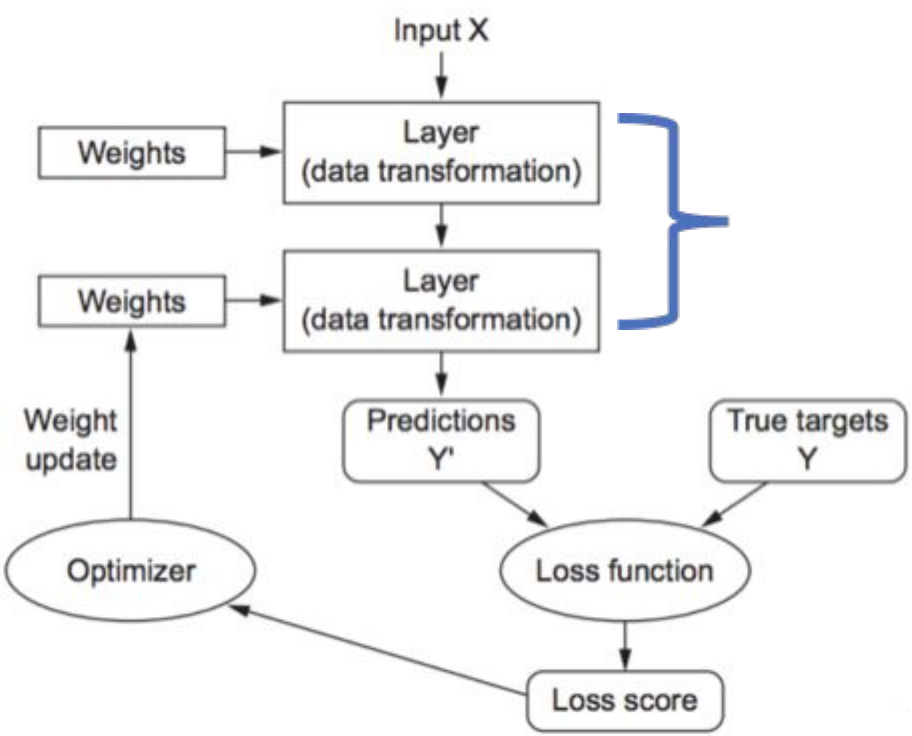

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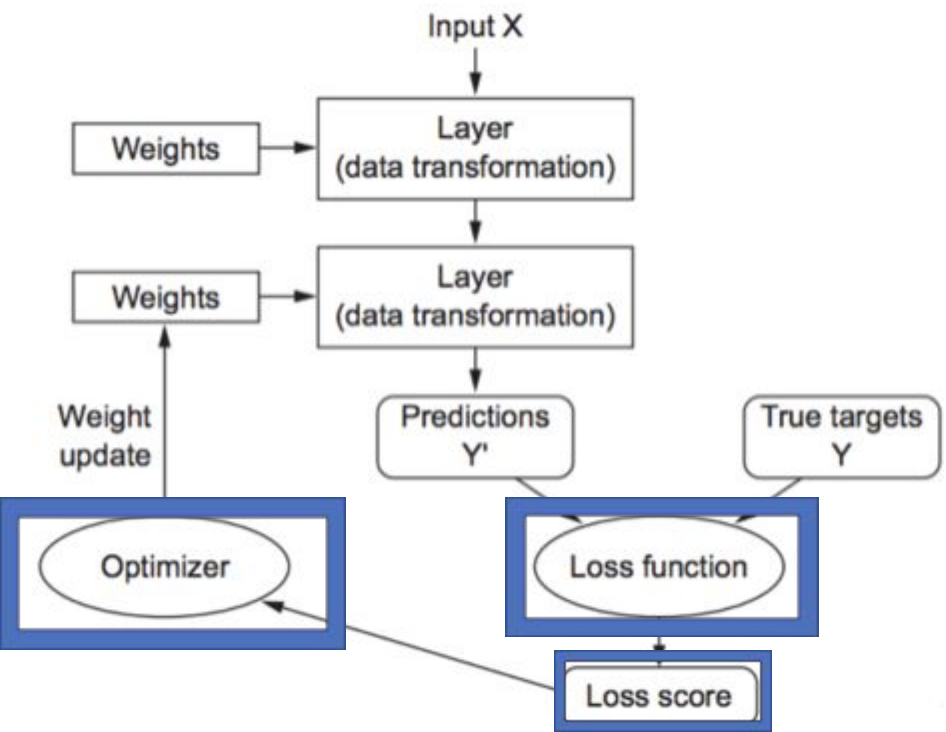

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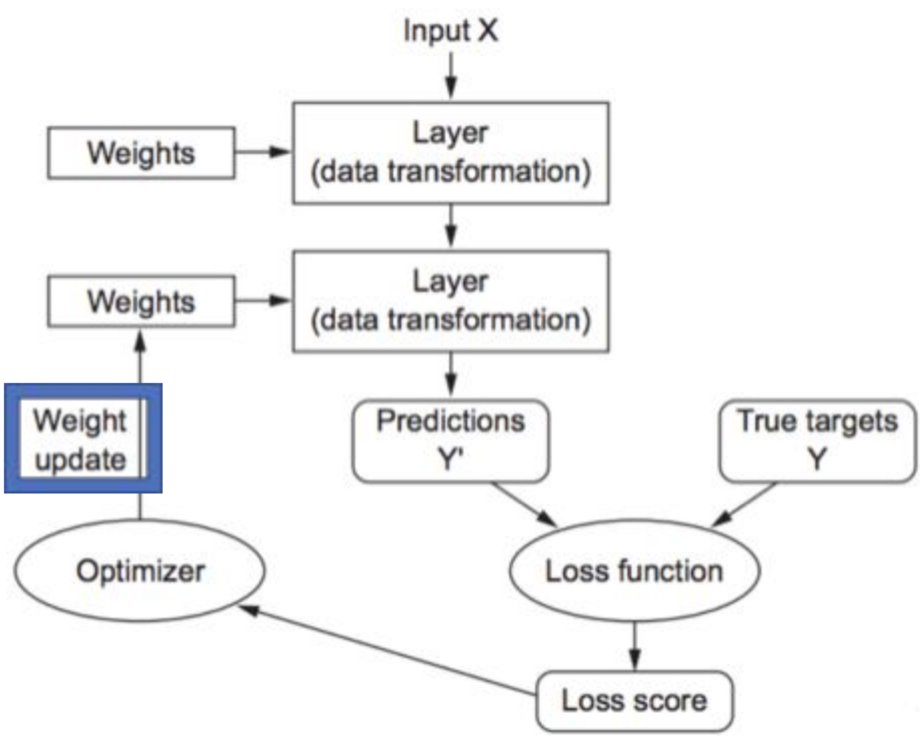
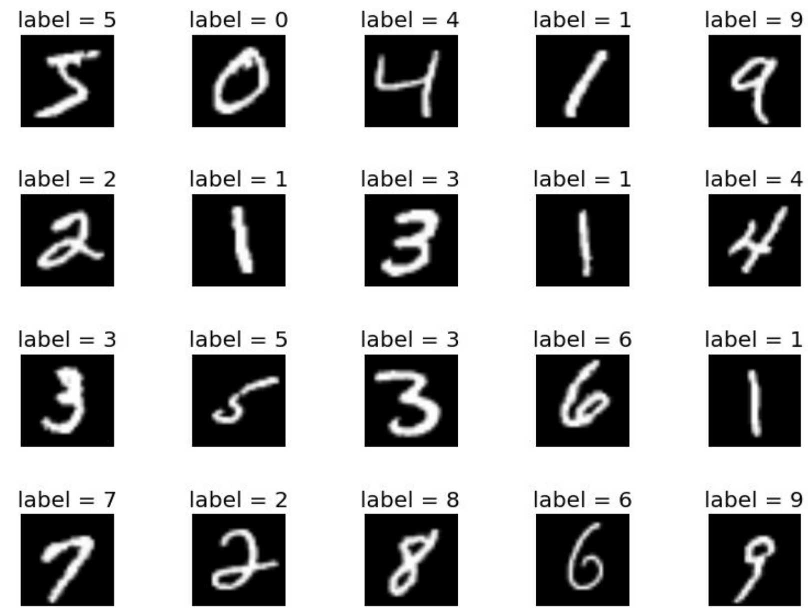
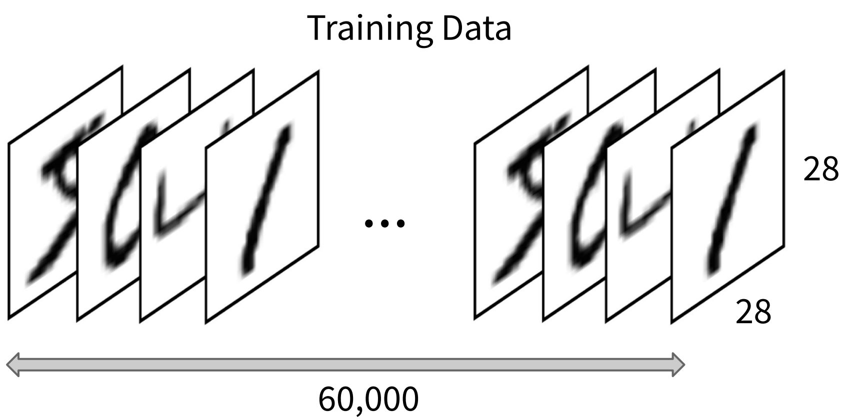


MNIST Data Example

- The MNIST data set includes handwritten digits with corresponding labels
- Training set: 60,000 images of handwritten digits and corresponding labels
    - Each digit is represented as a 28 x 28 matrix of grayscale values 0 - 255
    - The entire training set is stored in a 3D tensor of shape (60000, 28, 28)
    - The corresponding image values are stored as a 1D tensor of values 0 - 9
- Testing set: 10,000 images with the same set up as the training set





MNIST Data Example

Data wrangling

- We'll get into RGB images later, but for grayscale images, we need to first transform the matrix of values into a vector of values, and then normalize them to be between 0 and 1. It is not strictly necessary to normalize your inputs, but smaller numbers help speed up training and avoid getting stuck in local minima. This also ensures the gradients don't "explode" or "vanish"
  - Reshape each image from a 28 x 28 matrix of grayscale values 0 - 255 to a vector of length 28*28 = 784 of values 0 - 1 (divide each by 255)

- We now have 10 classes (categories; the digits 0-9)
  - We need to have multiclass labels that tell the network which digit the example is
  - Reshape each corresponding image label to a vector of length 10 of values 0 or 1
  - Example: the digit 3 would be represented as [0, 0, 0, 1, 0, 0, 0, 0, 0, 0]
  - You can think of this as "dummy coding" the labels

Activation and Loss Function Choices

Task	Last-layer activation	Loss function
Binary classification	sigmoid	Binary cross-entropy
Multiclass, single-label classification	softmax	Categorical cross-entropy
Multiclass, multilabel classification	sigmoid	Binary cross-entropy
Regression to arbitrary values	None	Mean square error (MSE)
Regression to values between 0 and 1	sigmoid	MSE or binary cross-entropy

Softmax function

$$\text{softmax}(\boldsymbol{z})_i = \frac{\exp(z_i)}{\sum_j \exp(z_j)}$$

- Softmax units are used as outputs when predicting a discrete variable *y* with *k* possible values
- In this setting, which can be seen as a generalization of the Bernoulli distribution, we need to produce a vector $\hat{\mathbf{y}}$ with $\hat{y}_i = P(y = i|x)$
- We require that each $\hat{y}_i$ lie in the [0, 1] interval and that the entire vector sums to 1
- We first compute $z = w^T x + b$ as usual
- Here, $z_i = log[\tilde{P}(y = i|x)]$ represents an unnormalized log probability for class *i*
- The softmax function then exponentiates and normalizes *z* to obtain $\hat{\mathbf{y}}$

Softmax function

- In this case we want to maximize

$$log[P(y = i; z)] = log[\text{softmax}(z)_i] = z_i - log \sum_j exp(z_j)$$

- The first term shows that the input always has a direct contribution to the loss function

- Because $log \sum_j exp(z_j) \approx max_j z_j$, the negative log-likelihood loss function always strongly penalizes the most active incorrect prediction

MNIST Data Example

Network Architecture

- Let's start with 2 layers:
  - 1 hidden and 1 output layer
  - Hidden layer will have 512 hidden units and the **relu activation function**
  - Output layer with 10 units (one for each possible digit) and the **softmax activation function** (this produces a vector of length 10, where each element is a probability between 0 and 1 of the image being classified as that digit)
  - Example: [0, 0.3, 0, 0, 0, 0, 0, 0.7, 0, 0] - the highest probability corresponds to a label of 7, so the network would classify this image as a 7
  - **rmsprop optimization algorithm**
  - **categorical_crossentropy loss function**
  - **accuracy performance measure** (the proportion of times the correct class is chosen)

MNIST Data Example

```
(train_data, train_labels), (test_data, test_labels) = mnist.load_data()

network = models.Sequential()
# Layer 1 (Hidden layer)
network.add(layers.Dense(512, activation='relu', input_shape=(28 * 28, )))
# Layer 2 (Output layer)
network.add(layers.Dense(10, activation='softmax'))

network.compile(optimizer='rmsprop',
                loss='categorical_crossentropy',
                metrics=['accuracy'])

train_data = train_data.reshape((60000, 28 * 28))
train_data = train_data.astype('float32') / 255

test_data = test_data.reshape((10000, 28 * 28))
test_data = test_data.astype('float32') / 255

train_labels = to_categorical(train_labels)
test_labels = to_categorical(test_labels)

network.fit(train_data, train_labels, epochs=5, batch_size=128)
test_loss, test_acc = network.evaluate(test_data, test_labels)
print('test accuracy:', test_acc)
```

MNIST Data Example

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train_labels = to_categorical(train_labels)
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network.fit(train_data, train_labels, epochs=5, batch_size=128)
test_loss, test_acc = network.evaluate(test_data, test_labels)
print('test accuracy:', test_acc)
```

If the input is a vector, no second number is needed. If we had kept the images as matrices, we would put (28, 28, 1). The 1 is for how many matrices are needed to represent each digit. Here, we have grayscale images that can be represented with 1 matrix. Once we have RGB color images, the 1 will be replaced by a 3; one matrix each for R, B, and G. We'll see this when we start CNNs.

MNIST Data Example

```
Epoch 1/5
60000/60000 [==============================] - 8s 135us/step - loss: 0.2576 - acc: 0.9244
Epoch 2/5
60000/60000 [==============================] - 7s 119us/step - loss: 0.1030 - acc: 0.9695
Epoch 3/5
60000/60000 [==============================] - 8s 131us/step - loss: 0.0678 - acc: 0.9798
Epoch 4/5
60000/60000 [==============================] - 8s 130us/step - loss: 0.0493 - acc: 0.9852
Epoch 5/5
60000/60000 [==============================] - 7s 123us/step - loss: 0.0370 - acc: 0.9892
10000/10000 [==============================] - 1s 54us/step
test accuracy: 0.9778
```

MNIST Data Example

```
Epoch 1/5
60000/60000 [==============================] - 8s 135us/step - loss: 0.2576 - acc: 0.9244
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10000/10000 [==============================] - 1s 54us/step
test accuracy: 0.9778
```

Training set accuracy

IMDb Data Example

The IMDb data set is a set of movie reviews that have been labeled as either positive or negative, based on the text content of the reviews

- Training set: 25,000 either positive or negative movie reviews that have each been turned into a vector of integers
  - We'll see how to actually do this later in the course
  - Each review can be of any length
  - Only the top 10,000 most frequently occurring words are kept i.e. rare words are discarded
  - Each review includes a label: 0 = negative review and 1 = positive review

- Testing set: 25,000 either positive or negative movie reviews, similar to the training set

IMDb Data Example

Data Wrangling

- Each review is of a varying length and is a list of integers - we need to turn this into a tensor with a common length for each review
- Create a 2D tensor of shape 25,000 x 10,000
  - 25,000 reviews and 10,000 possible words
- Use the **vectorize_sequences** function to turn a movie review list of integers into a vector of length 10,000 with 1s for each word that appears in the review and 0s for words that do not
- The labels are already 0s and 1s, so the only thing we need to do is make them float numbers

Activation and Loss Function Choices

Task	Last-layer activation	Loss function
Binary classification	sigmoid	Binary cross-entropy
Multiclass, single-label classification	softmax	Categorical cross-entropy
Multiclass, multilabel classification	sigmoid	Binary cross-entropy
Regression to arbitrary values	None	Mean square error (MSE)
Regression to values between 0 and 1	sigmoid	MSE or binary cross-entropy

IMDb Data Example

Network Architecture

- 3 layers
  - 2 hidden layers and 1 output layer
  - Hidden layers have 16 hidden units each and a **relu activation function**
  - Output layer has 1 unit (the probability a review is positive)
- **Sigmoid activation function**
- **rmsprop optimization algorithm**
- **binary_crossentropy loss function**
- **accuracy performance measure** (proportion of times the correct class is chosen)

IMDb Data Example

```
import keras
from keras.datasets import imdb
import numpy as np
from keras import models
from keras import layers

(train_data, train_labels), (test_data, test_labels) = imdb.load_data(num_words=10000)

def vectorize_sequences(sequences, dimension=10000):
    results = np.zeros((len(sequences), dimension))
    for i, sequence in enumerate(sequences):
        results[i, sequence] = 1.
    return results

x_train = vectorize_sequences(train_data)
x_test = vectorize_sequences(test_data)

y_train = np.asarray(train_labels).astype('float32')
y_test = np.asarray(test_labels).astype('float32')

model = models.Sequential()
model.add(layers.Dense(16, activation='relu', input_shape=(10000,)))
model.add(layers.Dense(16, activation='relu'))
model.add(layers.Dense(1, activation='sigmoid'))

model.compile(optimizer='rmsprop',
              loss='binary_crossentropy',
              metrics=['accuracy'])
```

IMDb Data Example

```
x_val = x_train[:10000]
partial_x_train = x_train[10000:]

y_val = y_train[:10000]
partial_y_train = y_train[10000:]

history = model.fit(partial_x_train,
                    partial_y_train,
                    epochs=20,
                    batch_size=512,
                    validation_data=(x_val, y_val))

train_acc = history.history['acc']
val_acc = history.history['val_acc']
train_loss = history.history['loss']
val_loss = history.history['val_loss']
```

history is a dictionary that contains data about what happened during training.

It contains 4 entries: the training loss and accuracy and the validation loss and accuracy

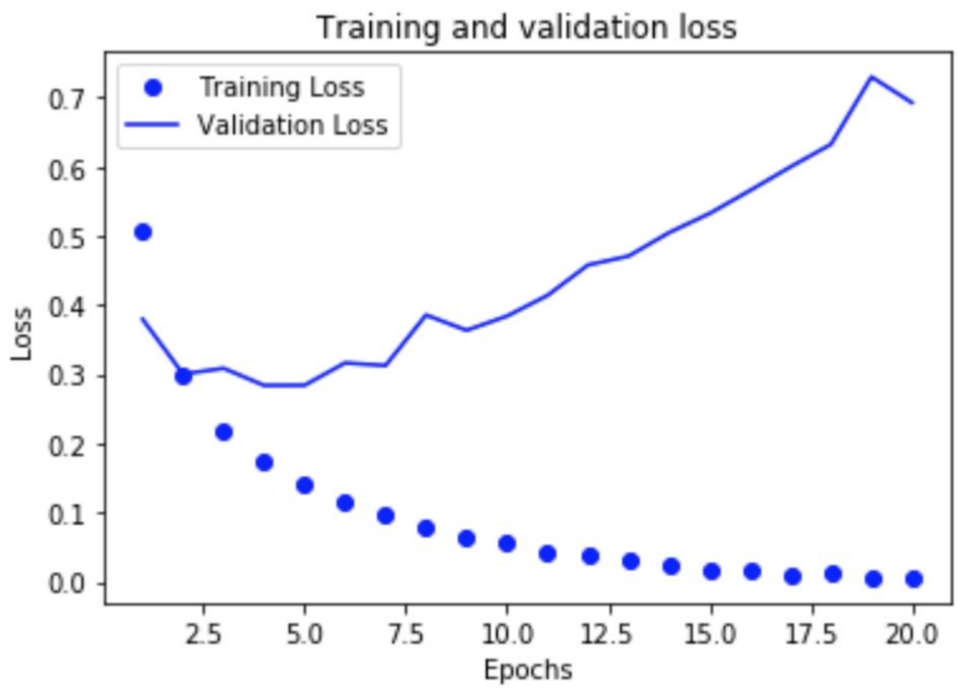
IMDb Data Example

```
Train on 15000 samples, validate on 10000 samples
Epoch 1/20
15000/15000 [==============================] - 5s 363us/step - loss: 0.5084 - acc: 0.7813 - val_loss: 0.3797 - val_acc: 0.8684
Epoch 2/20
15000/15000 [==============================] - 3s 170us/step - loss: 0.3004 - acc: 0.9047 - val_loss: 0.3003 - val_acc: 0.8897
Epoch 3/20
15000/15000 [==============================] - 2s 109us/step - loss: 0.2179 - acc: 0.9285 - val_loss: 0.3087 - val_acc: 0.8711
Epoch 4/20
15000/15000 [==============================] - 1s 98us/step - loss: 0.1751 - acc: 0.9438 - val_loss: 0.2839 - val_acc: 0.8832
Epoch 5/20
15000/15000 [==============================] - 1s 96us/step - loss: 0.1427 - acc: 0.9542 - val_loss: 0.2841 - val_acc: 0.8871
Epoch 6/20
15000/15000 [==============================] - 1s 95us/step - loss: 0.1150 - acc: 0.9650 - val_loss: 0.3171 - val_acc: 0.8773
Epoch 7/20
15000/15000 [==============================] - 1s 99us/step - loss: 0.0980 - acc: 0.9705 - val_loss: 0.3126 - val_acc: 0.8846
Epoch 8/20
15000/15000 [==============================] - 2s 118us/step - loss: 0.0807 - acc: 0.9763 - val_loss: 0.3858 - val_acc: 0.8650
Epoch 9/20
15000/15000 [==============================] - 2s 102us/step - loss: 0.0661 - acc: 0.9820 - val_loss: 0.3634 - val_acc: 0.8783
Epoch 10/20
15000/15000 [==============================] - 2s 104us/step - loss: 0.0563 - acc: 0.9850 - val_loss: 0.3840 - val_acc: 0.8796
Epoch 11/20
15000/15000 [==============================] - 2s 104us/step - loss: 0.0435 - acc: 0.9899 - val_loss: 0.4146 - val_acc: 0.8784
Epoch 12/20
15000/15000 [==============================] - 2s 105us/step - loss: 0.0380 - acc: 0.9921 - val_loss: 0.4548 - val_acc: 0.8684
Epoch 13/20
15000/15000 [==============================] - 1s 99us/step - loss: 0.0300 - acc: 0.9929 - val_loss: 0.4702 - val_acc: 0.8726
Epoch 14/20
15000/15000 [==============================] - 2s 118us/step - loss: 0.0247 - acc: 0.9943 - val_loss: 0.5041 - val_acc: 0.8716
Epoch 15/20
15000/15000 [==============================] - 1s 94us/step - loss: 0.0190 - acc: 0.9967 - val_loss: 0.5314 - val_acc: 0.8705
Epoch 16/20
15000/15000 [==============================] - 1s 97us/step - loss: 0.0169 - acc: 0.9967 - val_loss: 0.5644 - val_acc: 0.8685
Epoch 17/20
15000/15000 [==============================] - 1s 93us/step - loss: 0.0115 - acc: 0.9987 - val_loss: 0.5989 - val_acc: 0.8667
Epoch 18/20
15000/15000 [==============================] - 2s 103us/step - loss: 0.0123 - acc: 0.9977 - val_loss: 0.6313 - val_acc: 0.8677
Epoch 19/20
15000/15000 [==============================] - 2s 106us/step - loss: 0.0063 - acc: 0.9997 - val_loss: 0.7389 - val_acc: 0.8518
Epoch 20/20
15000/15000 [==============================] - 2s 108us/step - loss: 0.0062 - acc: 0.9996 - val_loss: 0.6937 - val_acc: 0.8657
```

Training and Validation Loss

```
plt.plot(epochs, train_loss, 'bo', label = 'Training Loss')
plt.plot(epochs, val_loss, 'b', label = 'Validation Loss')
plt.title('Training and validation loss')
plt.xlabel('Epochs')
plt.ylabel('Loss')
plt.legend()
```

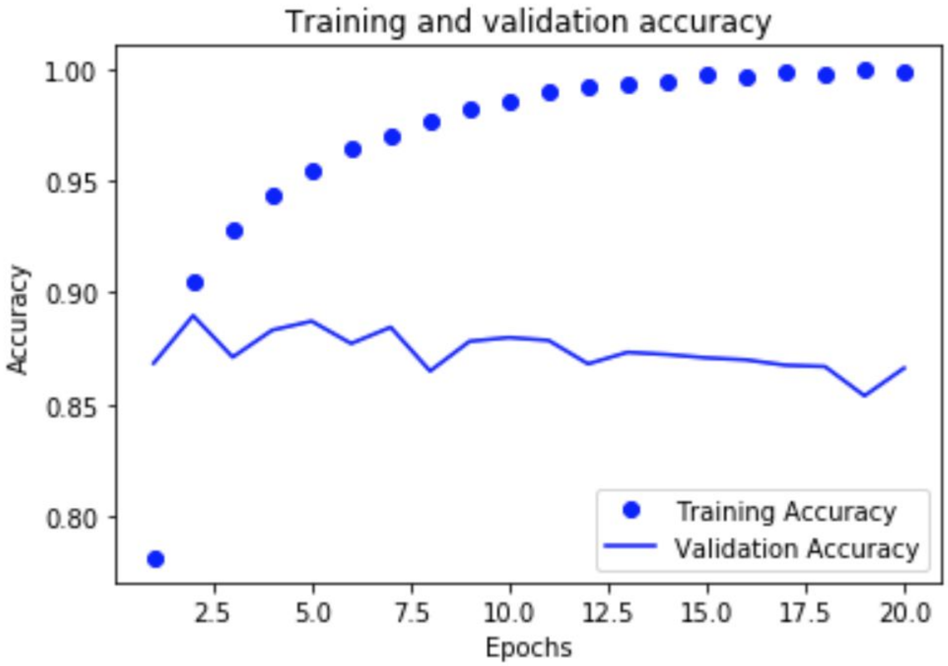
```
<matplotlib.legend.Legend at 0xb2c30f2b0>
```



Training and Validation Accuracy

```
plt.plot(epochs, train_acc, 'bo', label = 'Training Accuracy')
plt.plot(epochs, val_acc, 'b', label = 'Validation Accuracy')
plt.title('Training and validation accuracy')
plt.xlabel('Epochs')
plt.ylabel('Accuracy')
plt.legend()
```

```
<matplotlib.legend.Legend at 0xb209d0b70>
```



Test Set Accuracy

```
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model.add(layers.Dense(16, activation='relu', input_shape=(10000,)))
model.add(layers.Dense(16, activation='relu'))
model.add(layers.Dense(1, activation='sigmoid'))

model.compile(optimizer='rmsprop',
              loss='binary_crossentropy',
              metrics=['accuracy'])

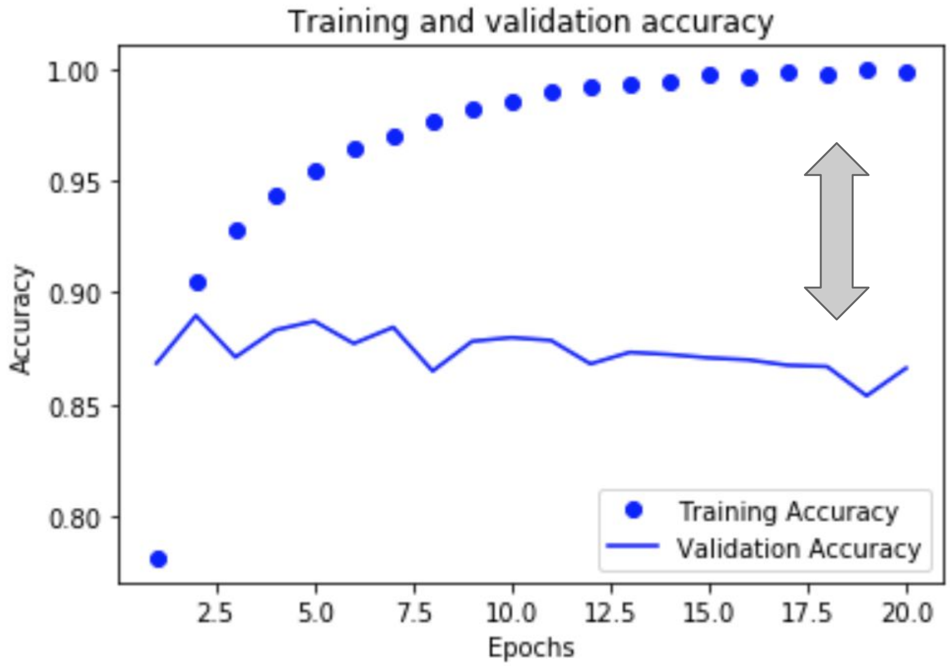
model.fit(x_train, y_train, epochs=4, batch_size=512)
results = model.evaluate(x_test, y_test)
print(results)
```

```
Epoch 1/4
25000/25000 [==============================] - 2s 70us/step - loss: 0.4584 - acc: 0.8133
Epoch 2/4
25000/25000 [==============================] - 2s 61us/step - loss: 0.2630 - acc: 0.9095
Epoch 3/4
25000/25000 [==============================] - 1s 59us/step - loss: 0.2005 - acc: 0.9282
Epoch 4/4
25000/25000 [==============================] - 1s 59us/step - loss: 0.1685 - acc: 0.9388
25000/25000 [==============================] - 1s 45us/step
[0.298845004286766, 0.88256]
```

How do we make this model better?

```
plt.plot(epochs, train_acc, 'bo', label = 'Training Accuracy')
plt.plot(epochs, val_acc, 'b', label = 'Validation Accuracy')
plt.title('Training and validation accuracy')
plt.xlabel('Epochs')
plt.ylabel('Accuracy')
plt.legend()
```

```
<matplotlib.legend.Legend at 0xb209d0b70>
```



There is a big difference in the training accuracy and validation set accuracy - a sign of overfitting.

How do we combat this?

Regularization: reducing network size

When we are battling overfitting, one option is to simplify the model. Let’s compare the performance we get from a simpler model. Here we have simplified the model by reducing the number of hidden units in each hidden layer.

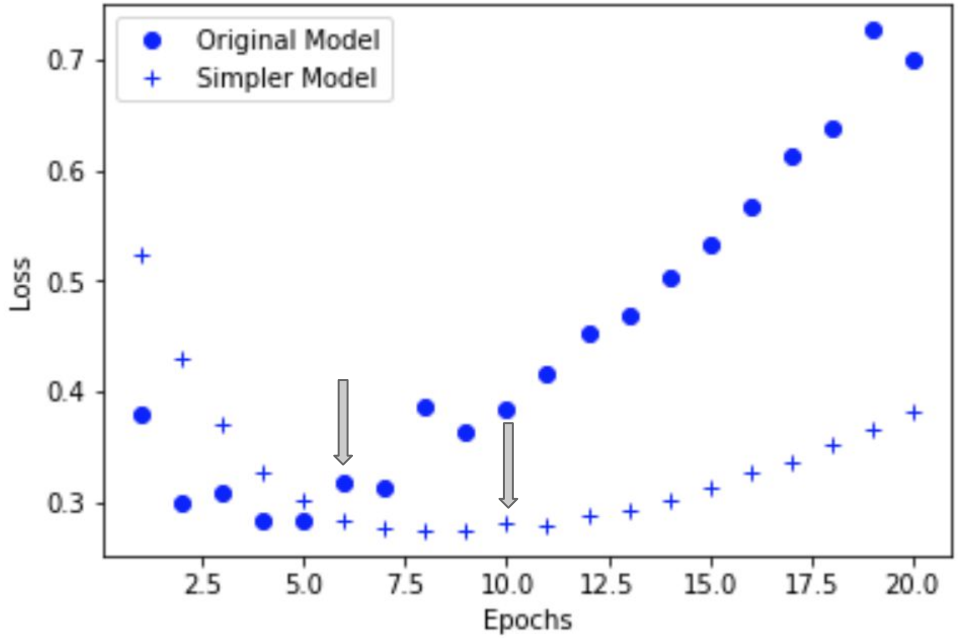
```
# Original Model
model = models.Sequential()
model.add(layers.Dense(16, activation='relu', input_shape=(10000,)))
model.add(layers.Dense(16, activation='relu'))
model.add(layers.Dense(1, activation='sigmoid'))

# Simpler, lower capaciy model
model = models.Sequential()
model.add(layers.Dense(4, activation='relu', input_shape=(10000,)))
model.add(layers.Dense(4, activation='relu'))
model.add(layers.Dense(1, activation='sigmoid'))
```

Regularization: reducing network size

```
plt.plot(epochs, val_loss, 'bo', label = 'Original Model')
plt.plot(epochs, val_loss2, 'b+', label = 'Simpler Model')
plt.title('')
plt.xlabel('Epochs')
plt.ylabel('Loss')
plt.legend()
```

```
<matplotlib.legend.Legend at 0xb2ebcc240>
```



The smaller network performs better than the original model - it starts to overfit at epoch 10 rather than epoch 6. These values are when the validation loss starts to increase.

What happens if we make the model more complex?

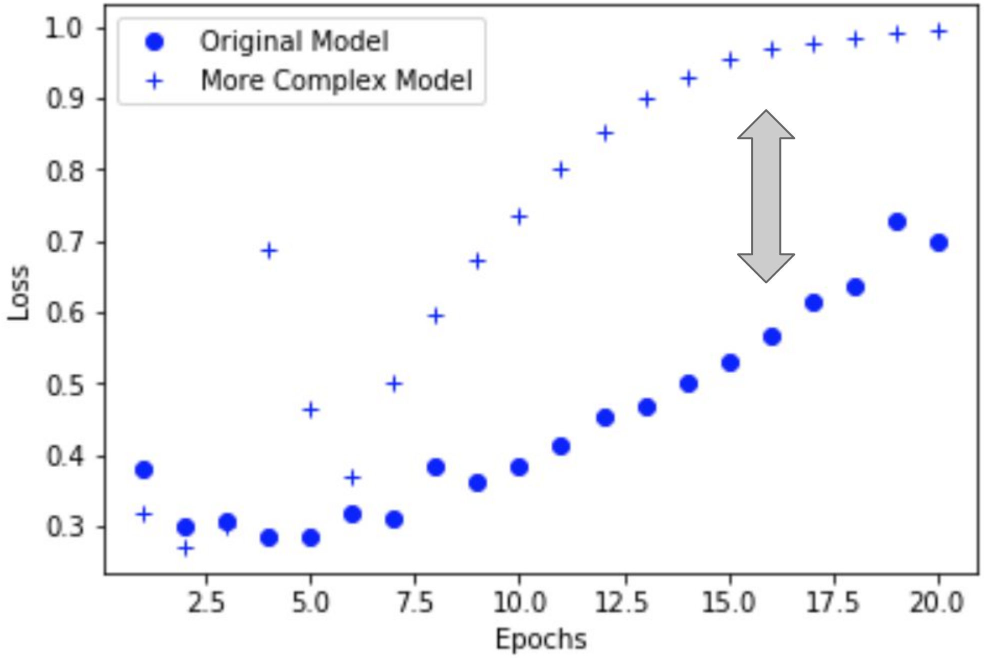
```
# Original Model
model = models.Sequential()
model.add(layers.Dense(16, activation='relu', input_shape=(10000,)))
model.add(layers.Dense(16, activation='relu'))

model.add(layers.Dense(1, activation='sigmoid'))
# More complex, higher capaciy model
model3 = models.Sequential()
model3.add(layers.Dense(512, activation='relu', input_shape=(10000,)))
model3.add(layers.Dense(512, activation='relu'))
model3.add(layers.Dense(1, activation='sigmoid'))

model3.compile(optimizer='rmsprop',
              loss='binary_crossentropy',
              metrics=['accuracy'])
```

```
plt.plot(epochs, val_loss, 'bo', label = 'Original Model')
plt.plot(epochs, val_loss3, 'b+', label = 'More Complex Model')
plt.title('')
plt.xlabel('Epochs')
plt.ylabel('Loss')
plt.legend()
```

```
<matplotlib.legend.Legend at 0xb2ef71b38>
```



The original model performs better than the more complex model with many more hidden nodes

Regularization: weight regularization

```
from keras import regularizers

l2_model = models.Sequential()
l2_model.add(layers.Dense(16, kernel_regularizer=regularizers.l2(0.001),
                          activation='relu', input_shape=(10000,)))
l2_model.add(layers.Dense(16, kernel_regularizer=regularizers.l2(0.001),
                          activation='relu'))
l2_model.add(layers.Dense(1, activation='sigmoid'))
```

```
l2_model.compile(optimizer='rmsprop',
                 loss='binary_crossentropy',
                 metrics=['acc'])
```

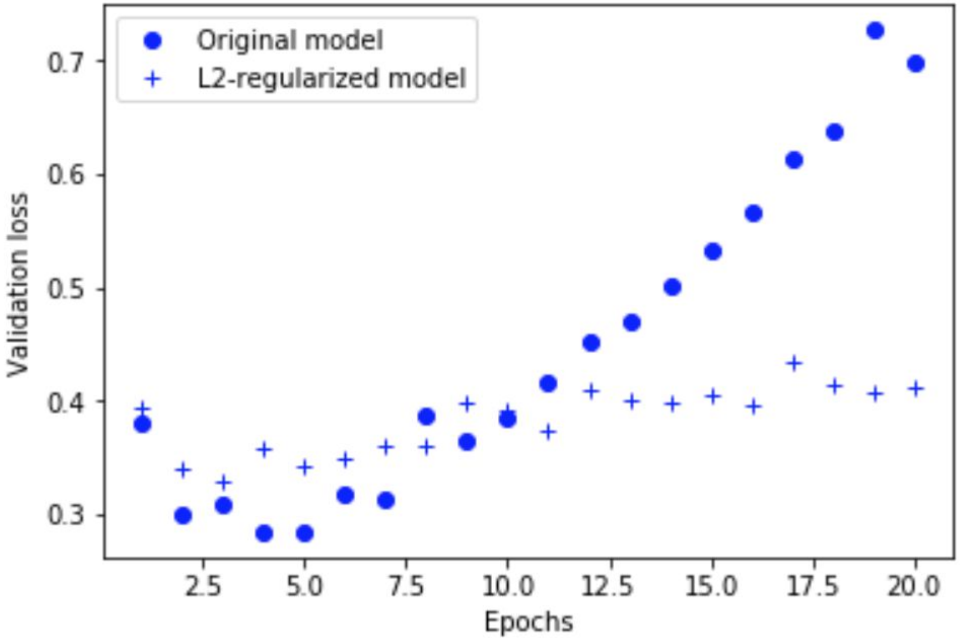
```
l2_model_hist = l2_model.fit(x_train, y_train,
                             epochs=20,
                             batch_size=512,
                             validation_data=(x_test, y_test))
```

Regularization: weight regularization

```
l2_model_val_loss = l2_model_hist.history['val_loss']

plt.plot(epochs, val_loss, 'bo', label='Original model')
plt.plot(epochs, l2_model_val_loss, 'b+', label='L2-regularized model')
plt.xlabel('Epochs')
plt.ylabel('Validation loss')
plt.legend()
```

```
<matplotlib.legend.Legend at 0xc3c607588>
```



The L2-regularized model is much more resistant to overfitting - the validation loss starts to increase at a much slower rate

Regularization: adding dropout

```
dpt_model = models.Sequential()
dpt_model.add(layers.Dense(16, activation='relu', input_shape=(10000,)))
dpt_model.add(layers.Dropout(0.5))
dpt_model.add(layers.Dense(16, activation='relu'))
dpt_model.add(layers.Dropout(0.5))
dpt_model.add(layers.Dense(1, activation='sigmoid'))

dpt_model.compile(optimizer='rmsprop',
                  loss='binary_crossentropy',
                  metrics=['acc'])
```

```
dpt_model_hist = dpt_model.fit(x_train, y_train,
                               epochs=20,
                               batch_size=512,
                               validation_data=(x_test, y_test))
```

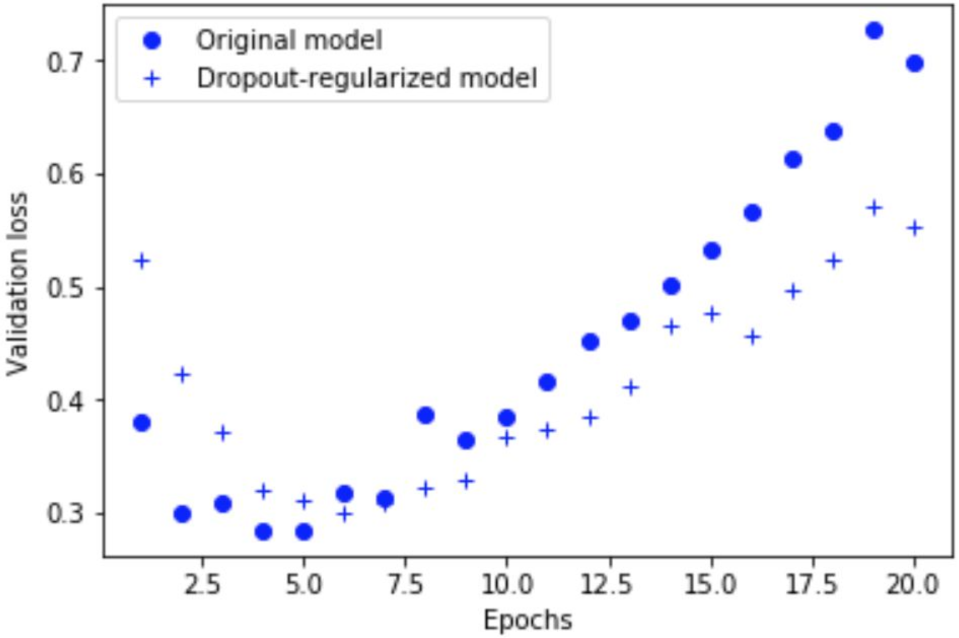
The 0.5 indicates a 50% probability of dropping out a unit. Typically, 20% is used in practice, but you can try different values and see what performs best.

Regularization: adding dropout

```
dpt_model_val_loss = dpt_model_hist.history['val_loss']

plt.plot(epochs, val_loss, 'bo', label='Original model')
plt.plot(epochs, dpt_model_val_loss, 'b+', label='Dropout-regularized model')
plt.xlabel('Epochs')
plt.ylabel('Validation loss')
plt.legend()
```

```
<matplotlib.legend.Legend at 0xc3af9acc0>
```



The dropout model is slightly better than the original model but does not control for overfitting as well as the L2 network