Deep Learning Specialization

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1 Neural Networks and Deep Learning

1.1 Introduction to Deep Learning

• Takes input x to a "neuron" and gives some output y



- Simple neural network has a single input, neuron and output
- -x: size of the house
- -y: price of the house
- Hypothesis (blue line) is a ReLU (Rectified Linear Unit)
- More complex neural networks can be formed by "stacking" neurons



- Every input layer feature is interconnected with every hidden layer feature
 - The neural network will decide what the intermediate features will be
- Most useful in supervised learning settings

1.1.1 Supervised Learning

- Aims to learn a function to map an input x to an output y
 - Real estate: predicting house prices from the house features
 - Online advertising: showing ads based on probability of user clicking on ad
 - Photo tagging: tagging images based on objects in the image
 - Speech recognition: generating a text transcript from audio
 - Machine translation: translating from one language to another
 - Autonomous driving: returning the positions of other cars from images and radar info
- Different types of neural network used for different tasks
 - Standard neural network: real estate and online advertising
 - Convolutional neural network (CNN): image data
 - Recurrent neural network (RNN): audio and language data (sequenced data)
 - Hybrid neural network: Autonomous driving (more complex input)



- Supervised learning can be applied to structured and unstructured data
 - Structured data has features with well defined meanings
 - Unstructured data has more abstract features (images, audio, text)
- Deep learning has only recently started to become more widespread
 - Given large amounts of data and a large NN, deep learning will outperform more traditional learning algorithms
 - For small amounts of data, any performance of the algorithm depends on specific implementation
- "Scale drives deep learning progress"
 - Both the scale of the data and the NN
- Recent algorithmic innovations with increase scale of computation



- Idea to switch from sigmoid activation function to ReLu function increased NN performance
- Ends of sigmoid function have close to 0 gradient so and therefore result in small changes in θ
- ReLu function has gradient of 1 for positive values
- Neural network process is iterative
 - Increasing speed at which a NN can be trained allows different ideas to be tried

1.2 Neural Network Basics

1.2.1 Logistic Regression as a Neural Network

- Logistic regression used for binary classification
- For a colour image, of 64×64 pixels, will have total 12288 input features
 - Image is stored as 3 separate matrices for each colour channel
 - All pixel intensities should be unrolled into a single feature vector

$$n = 12288$$

$$x \in \mathbb{R}^{12288}$$

- For a matrix X of shape (a, b, c, d), want a matrix X_flatten of shape (b * c * d, 1)

Notation

$$\{(x^{(1)}, y^{(1)}), (x^{(2)}, y^{(2)}), ..., (x^{(m)}, y^{(m)})\}$$

- (x,y): single training example
 - $-x \in \mathbb{R}^{n_x}$ $(n_x = \text{number of features})$
 - $-y \in \{0,1\}$

- $(x^{(i)}, y^{(i)})$: i^{th} training example
- $m = m_{train}$
- $m_{test} = \#$ of test examples

•
$$X = \begin{bmatrix} | & | & | \\ x^{(1)} & x^{(2)} & \dots & x^{(3)} \\ | & | & & | \end{bmatrix}$$

- $X \in \mathbb{R}^{n_x \times n}$

•
$$Y = \begin{bmatrix} y^{(1)} & y^{(2)} & \dots & y^{(m)} \end{bmatrix}$$

- $Y \in \mathbb{R}^{1 \times m}$

Logistic Regression

• Given x, want $\hat{y} = P(y = 1|x)$

– Since \hat{y} is a probability, want $0 \le \hat{y} \le 1$

• Parameters: $w \in \mathbb{R}^{n_x}, b \in \mathbb{R}$

• Output: $\hat{y} = \sigma(w^T x + b)$



$$\sigma(z) = \frac{1}{1 + e^{-z}}$$
$$z = w^{T}x + b$$

• Aim is to learn parameters w and b such that \hat{y} is a good estimate of the probability

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- \bullet Previous convention had θ vector with an additional θ_0 parameter
 - Keeping θ_0 (b) separate from the rest of the parameters is easier to implement

Cost Function

- Given $\{(x^{(1)},y^{(1)}),(x^{(2)},y^{(2)}),...,(x^{(m)},y^{(m)})\}$, want $\hat{y}^{(i)}\approx y^{(i)}$
- Squared error function not used for logistic regression loss function

- Optimization problem becomes non convex and will have local optima

$$\mathcal{L}(\hat{y}, y) = -(y \log(\hat{y}) + (1 - y) \log(1 - \hat{y}))$$

- If y = 1:
 - $\mathcal{L}(\hat{y}, y) = -\log(\hat{y})$
 - Want large $\log(\hat{y})$: want large \hat{y}
 - $-\hat{y}$ has a max of 1: want $\hat{y} = 1$
- If y = 0:
 - $\mathcal{L}(\hat{y}, y) = -log(1 \hat{y})$
 - Want large $\log(1-\hat{y})$ ∴ want small \hat{y}
 - $-\hat{y}$ has a min of 0: want $\hat{y} = 0$
- Cost function:

$$J(w,b) = \frac{1}{m} \sum_{i=1}^{m} \mathcal{L}(\hat{y}^{(i)}, y^{(i)})$$
$$= -\frac{1}{m} \sum_{i=1}^{m} [y^{(i)} \log(\hat{y}^{(i)}) + (1 - y^{(i)}) \log(1 - \hat{y}^{(i)})]$$

- Average loss function over all training examples

Gradient Descent

- Want to find values of w and b that minimize the cost function J(w,b)
 - For logistic regression, w and b usually initialized to 0
- One iteration of gradient descent will take a step in the direction of steepest descent

$$\begin{array}{llll} \texttt{Repeat} & \{ & & \\ & \texttt{w} & := & \texttt{w} & - & \alpha \frac{\partial J(w,b)}{\partial w} \\ & \texttt{b} & := & \texttt{b} & - & \alpha \frac{\partial J(w,b)}{\partial b} \\ \} & & \end{array}$$

• Using the computation graph:

$$\frac{\partial \mathcal{L}(a,y)}{\partial a} = -\frac{y}{a} + \frac{1-y}{1-a}$$

$$x_1 \\ w_1 \\ x_2 \\ w_2 \\ b$$

$$z = w_1 x_1 + w_2 x_2 + b$$

$$a = \sigma(z)$$

$$\mathcal{L}(a, y)$$

$$\frac{\partial \mathcal{L}(a,y)}{\partial z} = \frac{\partial \mathcal{L}}{\partial a} \times \frac{\partial a}{\partial z}$$

$$= (-\frac{y}{a} + \frac{1-y}{1-a}) \times a(1-a)$$

$$= a - y$$

$$\frac{\partial \mathcal{L}}{\partial w_1} = x_1 \times \frac{\partial \mathcal{L}}{\partial z}$$

$$\frac{\partial \mathcal{L}}{\partial w_2} = x_2 \times \frac{\partial \mathcal{L}}{\partial z}$$

$$\frac{\partial \mathcal{L}}{\partial b} = \frac{\partial \mathcal{L}}{\partial z}$$

• Partial derivative over all training examples calculated by taking the average dw1

$$\frac{\partial}{\partial w_1} J(w, b) = \frac{1}{m} \sum_{i=1}^{m} \frac{\partial}{\partial w_1} \mathcal{L}(a^{(i)}, y^{(i)})$$

Initialize J = 0,
$$dw1 = 0$$
, $dw2 = 0$, $db = 0$

For $i = 1$ to m :
$$z^{(i)} = w^T x^{(i)} + b$$

$$a^{(i)} = \sigma(z^{(i)})$$

$$J += -[y^{(i)} \log(a^{(i)}) + (1-y^{(i)})\log(1-a^{(i)})]$$

$$dz^{(i)} = a^{(i)} - y^{(i)}$$

$$dw1 += x_1^{(i)} dz^{(i)}$$

$$dw2 += x_2^{(i)} dz^{(i)}$$

$$db += dz^{(i)}$$

$$J /= m$$

db /= m
w1 := w1 -
$$\alpha$$
 dw1
w2 := w2 - α dw2
b := b - α db

dw1 /= mdw2 /= m

- Above implementation requires for loop over all features for all training examples
 - Vectorization can be used to remove explicit for loops
 - Vectorization required for deep learning to be efficient

1.2.2 Vectorisation in Python

- Deep learning performs best on large data sets
 - Code must be able to run quickly to be effective on large data sets

$$z = w^T x + b$$
$$w \in \mathbb{R}^{n_x} \quad x \in \mathbb{R}^{n_x}$$

• Non vectorized implementation:

- GPUs and CPUs both have parallelization instructions (SIMD: Single Instruction Multiple Data)
 - If built in functions are used, numpy will use parallelism to perform computations faster
- For logistic regression, need to calculate z and a values for each training example

$$z^{(i)} = w^T x^{(i)} + b$$

$$a^{(i)} = \sigma(z^{(i)})$$

$$X = \begin{bmatrix} | & | & | \\ x^{(1)} & x^{(2)} & \dots & x^{(m)} \\ | & | & | \end{bmatrix}$$

$$w \in \mathbb{R}^{n_x} \quad X \in \mathbb{R}^{n_x \times m}$$

• In Python:

$$Z = np.dot(w.T, X) + b$$

- Python will broadcast the value b so it can be added to the matrix
- Vectorized implementation of sigmoid function can be used on Z to calculate A

$$A = \begin{bmatrix} a^{(1)} & a^{(2)} & \dots & a^{(m)} \end{bmatrix}$$

$$dz^{(i)} = a^{(i)} - y^{(i)}$$
$$dz = A - Y$$
$$db = \frac{1}{m} \sum_{i=1}^{m} dz^{(i)}$$
$$dw = \frac{1}{m} X (dz)^{T}$$

```
Z = np.dot(w.T,X) + b
A = sigmoid(Z)
dz = A - Y
dw = 1/m * np.dot(X, dz.T)
db = 1/m * np.sum(dz)

# Gradient descent update
w = w - alpha * dw
b = b - alpha * db
```

• for loop is required to run multiple iterations of gradient descent

1.3 Shallow Neural Networks

- A neural network will have stacked logistic regression units in each layer
 - Logistic regression output from one layer will be fed to another layer



- Input layer of the neural network contains the feature x_1, x_2, x_3
 - $a^{[0]} = X$
- Intermediate layers in the network are hidden layers
 - Hidden layers do not have "true" values in the training set
- Final layer in the network is the output layer
 - Generates the predicted value \hat{y}
- Above diagram is a 2 layer NN
 - Input layer is layer 0
- \bullet Each layer will have parameters w and b associated with them
- Each node in the NN will perform logistic regression with its inputs

$$z_i^{[l]} = w_i^{[l]T} x + b_i^{[l]} \rightarrow a_i^{[l]} = \sigma(z_i^{[l]})$$

$$W^{[1]} = \begin{bmatrix} - & w_1^{[1]T} & - \\ - & w_2^{[1]T} & - \\ - & w_3^{[1]T} & - \\ - & w_4^{[1]T} & - \end{bmatrix}$$

$$a^{[0]} = \begin{bmatrix} x_1 \\ x_2 \\ x_3 \end{bmatrix}$$

$$b^{[1]} = \begin{bmatrix} b_1^{[1]} \\ b_2^{[1]} \\ b_3^{[1]} \\ b_4^{[1]} \end{bmatrix}$$

$$\begin{split} z^{[1]} &= \begin{bmatrix} z_1^{[1]} \\ z_2^{[1]} \\ z_3^{[1]} \\ z_4^{[1]} \end{bmatrix} \\ &= \begin{bmatrix} w_1^{[1]T} a^{[0]} + b_1^{[1]} \\ w_2^{[1]T} a^{[0]} + b_1^{[1]} \\ w_3^{[1]T} a^{[0]} + b_1^{[1]} \\ w_4^{[1]T} a^{[0]} + b_1^{[1]} \end{bmatrix} \\ &= w^{[1]} a^{[0]} + b^{[1]} \end{split}$$

$$\begin{split} a^{[1]} &= \begin{bmatrix} a_1^{[1]} \\ a_2^{[1]} \\ a_3^{[1]} \\ a_4^{[1]} \end{bmatrix} \\ &= \sigma(z^{[1]}) \\ z^{[2]} &= W^{[2]} a^{[1]} + b^{[2]} & \rightarrow \quad a^{[2]} = \sigma(z^{[2]}) \end{split}$$

- Vectorized method should be able to work on all training examples at one time
 - Vector for each training example can be stacked horizontally in a matrix
 - Vertical dimension will be the number of units in a layer (n_x) for the input layer

$$X = \begin{bmatrix} | & | & | & | \\ x^{(1)} & x^{(2)} & x^{(m)} \end{bmatrix}$$

$$Z^{[1]} = \begin{bmatrix} | & | & | & | & | \\ z^{1} & z^{[1](2)} & \dots & z^{[1](m)} \end{bmatrix}$$

$$A^{[1]} = \begin{bmatrix} | & | & | & | & | & | \\ a^{1} & a^{[1](2)} & \dots & a^{[1](m)} \end{bmatrix}$$

$$Z^{[1]} = W^{[1]}X + b^{[1]}$$

$$A^{[1]} = \sigma(Z^{[1]})$$

$$Z^{[2]} = W^{[2]}A^{[1]} + b^{[2]}$$

$$A^{[2]} = \sigma(Z^{[2]})$$

1.3.1 Activation Functions

ullet After z values are calculated, activation function must be run to get the activation value a

$$a_{sigmoid} = \frac{1}{1 + e^{-z}}$$

- \bullet Alternatively $a^{[1]}=g(z^{[1]})$ where g is a non linear function
- tanh function almost always performs better than the sigmoid function
 - Equivalent to a transformed version of the sigmoid function
 - tanh function is odd and is "centered" around the origin
 - The mean of the data will be closer to 0 and will help with learning in the next layer

$$a_{\text{tanh}} = \frac{e^z - e^{-z}}{e^z + e^{-z}}$$



- For binary classification, the final output layer can use the sigmoid function
 - Want the value of \hat{y} to be between 0 and 1
- \bullet For both the sigmoid and tanh functions, when z is large, the gradient is very small
 - Results in a slower gradient descent
- ullet ReLU function has a gradient of 1 when z is positive



- Gradient is 0 when z is negative
- For majority of the ReLU function, gradient is very different from 0
 - Will typically allow NN to learn much faster than sigmoid or tanh function
- ReLU function should be used as the default activation function
- The leaky ReLu function has a slight positive gradient when z is negative

$$a_{leakyReLU} = \max(0.01z, z)$$



- For a NN to compute more complex functions, activation function must be non linear
 - If a linear activation function is used, final output of the NN can only be a linear function
 - Multiple linear activation neurons with a sigmoid as the output neuron is equivalent to standard logistic regression
- Linear activation function can be used in the output layer if output is a real number
- Derivative of the activation function must be calculated for backpropagation
 - Sigmoid function

$$g(z) = \frac{1}{1 + e^{-z}}$$

$$\frac{d}{dz}g(z) = \frac{1}{1 + e^{-z}} \left(1 - \frac{1}{1 + e^{-z}} \right)$$
$$= g(z)(1 - g(z))$$

- tanh function

$$g(z) = \tanh(z)$$
$$= \frac{e^z - e^{-z}}{e^z + e^{-z}}$$

$$\frac{d}{dz}g(z) = 1 - \left(\frac{e^z - e^{-z}}{e^z + e^{-z}}\right)^2$$
$$= 1 - g(z)^2$$

- ReLU function

$$g(z) = \max(0, z)$$

$$\frac{d}{dz}g(z) = \begin{cases} 0 & \text{if } z < 0\\ 1 & \text{if } z \ge 0 \end{cases}$$

Leaky ReLU function

$$g(z) = \max(0.01z, z)$$

$$\frac{d}{dz}g(z) = \begin{cases} 0.01 & \text{if } z < 0\\ 1 & \text{if } z \ge 0 \end{cases}$$

1.3.2 Gradient Descent for Neural Networks

- \bullet For a single hidden layer NN, parameters are: $w^{[1]}, b^{[1]}, w^{[2]}, b^{[2]}$
 - $w^{[1]} \in \mathbb{R}^{n_1 \times n_0}$
 - $-b^{[1]} \in \mathbb{R}^{n_1 \times 1}$
 - $w^{[2]} \in \mathbb{R}^{n_2 \times n_1}$
 - $-b^{[2]} \in \mathbb{R}^{n_2 \times 1}$
- Cost function: $J(w^{[1]}, b^{[1]}, w^{[2]}, b^{[2]}) = \frac{1}{m} \sum_{i=1}^{n} \mathcal{L}(\hat{y}, y)$
- For one iteration of gradient descent:

$$w^{[1]} := w^{[1]} - \alpha dw^{[1]}, \ b^{[1]} := b^{[1]} - \alpha db^{[1]}$$

$$w^{[2]} := w^{[2]} - \alpha dw^{[2]}, \ b^{[2]} := b^{[2]} - \alpha db^{[2]}$$

- Gradient descent step will take place after backpropagation calculates the derivatives
- Forward propagation:

$$Z^{[1]} = W^{[1]}X + b^{[1]}$$

$$A^{[1]} = g^{[1]}(Z^{[1]})$$

$$Z^{[2]} = W^{[2]}A^{[1]} + b^{[2]}$$

$$A^{[2]} = g^{[2]}(Z^{[2]})$$

• Backpropagation:

$$\begin{split} dz^{[2]} &= A^{[2]} - Y \\ dw^{[2]} &= \frac{1}{m} dz^{[2]} A^{[1]T} \\ db^{[2]} &= \frac{1}{m} \mathrm{np.sum}(dz^{[2]}, \mathrm{axis} = \mathrm{1, keepdims} = \mathrm{True}) \\ dz^{[1]} &= w^{[2]T} dz^{[2]} \times g^{[1]'}(z^{[1]}) \\ dw^{[1]} &= \frac{1}{m} dz^{[1]} X^T \\ db^{[1]} &= \frac{1}{m} \mathrm{np.sum}(dz^{[1]}, \mathrm{axis} = \mathrm{1, keepdims} = \mathrm{True}) \end{split}$$

1.3.3 Random Initialization

- Weights must be initialized randomly for a NN
 - Weights can be initialized to 0 for logistic regression
 - The bias terms b can be initialized
- If weights are initialized to 0, all neurons in a layer will compute the same hypothesis

```
W1 = np.random.randn((2,2)) * 0.01
b1 = np.zero((2,1))
```

- Weights should be initialized to small random values
 - If weight is too large, activation value $z^{[1]}$ will be large
 - If sigmoid or tanh function is used, derivative will be very small and learning will be very slow
- Different constant for np.random.randn should be used for deeper neural networks

1.4 Deep Neural Networks

- Logistic regression is equivalent to a 1-layer NN
- Deep NN have more hidden layers
 - Number of hidden layers in the network can be a parameter for the ML problem



- Above network has 4 layers, L=4
- $-n^{[l]} = \text{number of units in layer } l$
- $-a^{[l]} = activations in layer l$
- The inputs x are the activations of the first layer, $x=a^{[0]}$
 - Prediction \hat{y} will be the activations of the last layer, $\hat{y} = a^{[L]}$
- Forward propagation for a deep NN will follow the same pattern for all layers

$$z^{[l]} = w^{[l]}a^{[l-1]} + b^{[l]}$$

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

 \bullet For a vectorized implementation

$$Z^{[l]} = W^{[l]}A^{[l-1]} + b^{[l]}$$

$$A^{[l]} = g^{[l]}(z^{[l]})$$

- Explicit for loop will be used to loop over the layers in the network
- $-\ b$ will still be a column vector but will apply correctly due to broadcasting
- When working with W and A matrices, A will be for the previous layer so the dimensions will fit
- When debugging NN, can look at dimensions of all the matrices
- For a non vectorized implementation:

$$-W^{[l]}:(n^{[l]},n^{[l-1]})$$

$$-b^{[l]}:(n^{[l]},1)$$

– Dimensions of dw and db should be the same as the dimensions of W and b

$$-a^{[l]}, z^{[l]}: (n^{[l]}, 1)$$

ullet For a vectorized implementation, z vectors and a vectors will be stacked horizontally for all training examples

$$-Z^{[l]}, A^{[l]}: (n^{[l]}, m)$$

- Deep NN tend to work better as each layer can compute increasingly complex functions
 - Face recognition: edge detection \rightarrow individual features \rightarrow large parts of the face
 - Audio: low level waveforms \rightarrow phonemes \rightarrow words \rightarrow sentences
- Functions that can be computed with a "small" deep neural network require exponentially more hidden units in a shallower network
- ullet For each forward propagation step, the value of $z^{[l]}$ should be cached for backpropagation
 - Values of $w^{[l]}$ and $b^{[l]}$ can also be stored in the cache so they can be accessed for backpropagation



- All forward propagation steps will carried out until the hypothesis, \hat{y} is found
 - Using cached values, all backpropagation steps will be carried out until $dz^{[1]}$
 - Parameters $W^{[l]}$ and $b^{[l]}$ can be updated accordingly

$$W^{[l]} := W^{[l]} - \alpha dw^{[l]}$$

$$b^{[l]} := b^{[l]} - \alpha db^{[l]}$$

• Backpropagation will also follow a pattern for all layers in the NN

$$- dz^{[l]} = da^{[l]} * g^{[l]'}(z^{[l]})$$

$$-dW^{[l]} = dz^{[l]}a^{[l-1]T}$$

$$- db^{[l]} = dz^{[l]}$$
$$- da^{[l-1]} = W^{[l]T} dz^{[l]}$$

• For a vectorized implementation:

$$\begin{split} &-dZ^{[l]} = dA^{[l]} * g^{[l]'}(Z^{[l]}) \\ &-dW^{[l]} = \frac{1}{m} dZ^{[l]} A^{[l-1]T} \\ &-db^{[l]} = \frac{1}{m} \text{np.sum} (dZ^{[l]}\text{, axis=1, keepdims=True}) \\ &-dA^{[l-1]} = W^{[l]T} dZ^{[l]} \end{split}$$

1.4.1 Parameters vs Hyperparameters

- ullet Parameters of the NN are the W and b matrices
- NN also has a number of associated hyperparameters:
 - Learning rate α
 - Number of iterations z'
 - Number of layers in the network
 - Number of hidden units
 - Choice of activation function
- ullet Hyperparameters will control the values of W and b
- Deep learning has many more hyperparameters than earlier eras of machine learning
 - Applying deep learning becomes an empirical process
- Intuitions about hyperparameters may be different across different applications

2 Improving Deep Neural Networks: Hyperparameter Tuning, Regularization and Optimization

2.1 Practical Aspects of Deep Learning

- Applying ML is a highly iterative process
 - Very hard to choose "correct" values for hyperparameters



- Deep learning used in many different areas
 - NLP
 - Computer vision
 - Speech analysis
 - Structured data
 - * Advertisement
 - * Search engines
 - * Computer security
 - * Logistics
- Intuitions from one subject area often don't transfer to another application
- Success of deep learning can depend on speed of iteration
 - Choice of split of the data can influence speed of iteration
- Whole dataset should be split into training, development and test set
 - Dev set should be used rate performance of different models
 - Final model should be evaluated on the test set
 - Split will allow better evaluation of bias and variance of the model
- Previous eras of ML had a 60/20/20 split between dataset

- For the big data era, a smaller percentage of data is given to the dev and test sets
 - For 1,000,000 examples, can allocate just 10,000 examples each to dev and test set
 - 10,000 examples is enough to run the algorithm and get a good idea about the algorithm performance
- Recent trends also show mismatched training and test set distributions
 - For images, training set may have very high quality images while test set may have lower quality
 - Dev and test set should come from the same distribution
- Dataset might be split to not include a test set
 - Dev set can be used to get to a "good" model
 - Since data is fit to the dev set, there is no unbiased estimate of performance
 - When data doesn't include a test set, dev set is usually referred to as "test" set
 - Resulting model may overfit to the dev set

2.1.1 Bias and Variance

- In the deep learning era, there tends to be less of a discussion about the bias/variance trade off
- In 2 dimensions, data can be plotted to look for high bias or variance
 - High bias classifiers underfit the data
 - High variance classifiers overfit the data
- For higher dimensions, training set error and dev set error can be used
 - High variance classifier has low training error and high dev set error
 - High bias classifier has high training error and high dev set error
 - Classifier with high bias and high variance will have high training error and even higher dev set error
- Above ideas only work with the assumption that the optimal error is 0%
 - Training and dev set must also come from the same distribution

2.1.2 Basic Recipe for Machine Learning

- Train initial algorithm and reduce bias of algorithm to an "acceptable value"
 - Use a larger network
 - Train algorithm for longer

- Reduce variance of the algorithm by getting more data
 - Add regularization terms to the cost function
- Bias and variance can also be reduced by using a more appropriate NN architecture
- In the big data era, bias and variance can be reduced without affecting each other
 - Training a bigger network typically reduce the bias
 - Getting more training data will typically reduce the variance
- Using regularization will have a bias variance trade off

2.1.3 Regularization

- Adding regularization will usually help in reducing variance and prevent overfitting
 - Regularization will only affect how the weights change during backpropagation
 - For forward propagation, regularization has no effect
- For logistic regression:

$$J(w,b) = \frac{1}{m} \sum_{i=1}^{m} \mathcal{L}(\hat{y}^{(i)}, y^{(i)}) + \frac{\lambda}{2m} ||w||_{2}^{2}$$

$$||w||_2^2 = \sum_{j=1}^{n_x} w_j^2$$
$$= w^T w$$

- Above method is L_2 regularization after the L_2 norm (Euclidean norm) of w
- b values can also be regularized but will have a much smaller effect than w
- L_1 regularization adds the term:

$$\frac{\lambda}{m} \sum_{i=1}^{n_x} |w| = \frac{\lambda}{m} ||w||_1$$

- Using L_1 regularization will result in w being sparse
- Can be seen to compressing the model
- L_2 regularization is more common for deep learning
- Regularization parameter λ will be set using the cross validation set
 - lambda is a reserved keyword in Python

• For a neural network:

$$J(w^{[1]}, b^{[1]}, ..., w^{[l]}, b^{[l]}) = \frac{1}{m} \sum_{i=1}^{m} \mathcal{L}(\hat{y}^{(i)}, y^{(i)}) + \frac{\lambda}{2m} \sum_{l=1}^{L} ||w^{[l]}||^2$$
$$||w^{[L]}||^2 = \sum_{i=1}^{n^{[l]}} \sum_{i=1}^{n^{[l-1]}} (w^{[l]}_{i,j})^2$$

- $-||W^{[l]}||_F^2$ known as the Frobenius norm of the matrix
- Since new term added to cost function, $\frac{\partial J}{\partial W^{[l]}}$ will be different

$$dW^{[l]} = \dots + \frac{\lambda}{m}W^{[l]}$$

$$W^{[l]} = W^{[l]} - \frac{\alpha \lambda}{m} W^{[l]} - \alpha(...)$$

- Also known as weight decay as value of W will decrease on every iteration

$$W^{[l]} - \frac{\alpha \lambda}{m} W^{[l]} = \left(1 - \frac{\alpha \lambda}{m}\right) W^{[l]}$$

- Value of $\left(1 \frac{\alpha \lambda}{m}\right)$ will be slightly less than 1
- ullet Adding regularization term will penalize the weight matrix from being too large
 - As the value of λ is increased, the weights in w will get closer to 0
 - Each hidden unit will have a smaller effect and the resulting NN will be simpler
- When using the tanh function, penalizing w will make $z^{[l]}$ smaller
 - For a small $z^{[l]}$, tanh function is roughly linear
 - If all hidden units in the network are roughly linear, the result of the NN will also be roughly linear

Dropout Regularization

- Each layer in the NN has a probability of eliminating a node
 - When a node is eliminated, all outgoing links from the node are also deleted
 - Each example will be trained on a smaller network so will have less chance of overfitting
- For each different training example, the NN is reset and randomly eliminates nodes again
- Inverted dropout:

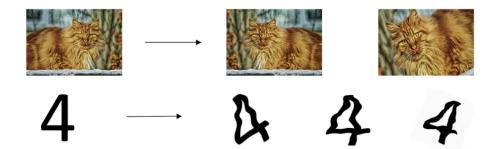
```
d3 = np.random.rand(a3.shape[0], a3.shape[1]) < keep_prob
a3 = np.multiply(a3, d3)
a3 /= keep_prob</pre>
```

- For keep_prob = 0.8 each node has a 0.2 chance of being removed
- Activation values should be scaled by $keep_prob$ so the expected value of z can stay constant
- On each pass through the training set, a different set of units should be zeroed out
- At test time, dropout should not be used as it will create noise in the predictions
- A single hidden unit cannot rely on a specific feature as it may not be used on each iteration
 - Weights for the unit will be spread out between the units
 - Has the same effect as shrinking the weights like L2 regularization
 - The equivalent L2 penalty on different weights depends on the size of the activations being used for the weight
- keep_prob can be varied between the layers
 - Larger layers may be more prone to overfitting and can have a larger keep_prob
 - For small layers with a very small chance of overfitting, keep_prob can be set to
- Many dropout implementations started with computer vision
 - Input size for computer vision is extremely large
- Cost function is not well defined when dropout is used
 - Can set keep_prob to 1 and check for monotonically decreasing J
 - When J is decreasing, then can reduce the value of keep_prob to use dropout

Other Regularization Methods

- Getting more training data will almost always help overfitting
 - May not be possible to get more training data or very expensive
- Data augmentation will create new examples and can help reduce overfitting
- For an image dataset:
 - Flipping the image horizontally

- Randomly cropping and distorting the image
- Magnitude of image transformation depends on classifier
 - For a cat dataset, image should not be flipped vertically
 - For OCR, distortions and rotations can be slightly more extreme



- Early stopping can be used to prevent overfitting from happening
 - If the NN is overfitting the data, the dev set error will initially decrease before increasing
 - Training of the NN can be stopped when the dev set error is lowest and the data has not been overfit
- ullet Using early stopping links the task of optimizing J and not overfitting the data
 - Early stopping will prevent the cost function from being optimized
- L2 regularization is a better method to prevent overfitting
 - Requires a choice for the value of λ and is much more computationally expensive

2.1.4 Setting up the Optimization Problem

- Normalization can be used to speed up the training of a NN
 - Subtract the mean:

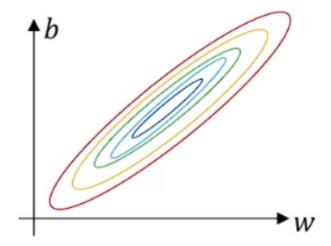
$$\mu = \frac{1}{m} \sum_{i=1}^{m} x^{(i)}$$
$$x := x = \mu$$

– Normalize the variance:

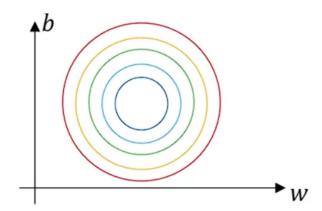
$$\sigma^2 = \frac{1}{m} \sum_{i=1}^m x^{(i)} * *2$$
$$x/ = \sigma$$

• When normalizing a training set, test set and training set should be processed together

- All the data must go through the same transformation
- For data that is not normalized, the cost function will be very elongated
 - The gradient will be quite shallow and will take longer to converge
 - Algorithm will require a smaller learning rate



- \bullet On average, normalized data will have a cost function that is more symmetric
 - Gradient descent will converge faster and can use a larger learning rate



Vanishing/Exploding Gradients

- For very deep neural networks, the derivatives can get exponentially big or small
- If the weights of a NN are all the same, the prediction \hat{y} will x to the Lth power
 - For $W^{[l]} > I$ the gradient will explode
 - For $W^{[l]} < I$ the gradient will vanish

- Some modern applications use 152 layer NN
 - Require careful initialization of the weights to ensure correct training
- For a single neuron:
 - The output \hat{y} will be the sum of all $w_i x_i$

$$z = w_1 x_1 + w_2 x_2 + \dots + w_n x_n$$

- For a large n, want a smaller w_i
- Want $Var(w_i) = \frac{1}{n}$

$$W^{[l]} = \text{np.random.randn(shape)} * \text{np.sqrt}\left(\frac{1}{n^{[l-1]}}\right)$$

- Variance of Gaussian random variable can be set by multiplying by sqrt tem
- For ReLU activation function, the variance should be set to $\frac{2}{n}$
 - tanh activation uses Xavier initialization $\frac{1}{n^{[l-1]}}$
 - Yoshua Bengio multiplied random variable by $\sqrt{\frac{2}{n^{[l-1]}+n^{[l]}}}$
- Initialization of weights aims to set weight matrices close to 1
 - Helps to prevent \hat{y} from vanishing or exploding too quickly
- Variance parameter can be tuned as another hyperparameter

Gradient Checking

- Can be used to ensure implementation of backpropagation is correct
- Requires numerical approximations of gradients
 - For a function f at a point θ , gradient can be approximated by looking at $\theta + \epsilon$ and $\theta \epsilon$
 - Approximation is closer when double sided estimate is used
- If g is the derivative of f:

$$g(\theta) \approx \frac{f(\theta + \epsilon) - f(\theta - \epsilon)}{2\epsilon}$$

• Using the 2 sided difference will give a much better estimate but is more computationally expensive

• The derivative of a function at a point is the limit of the numerical approximation

$$f'(\theta) = \lim_{\epsilon \to 0} \frac{f(\theta + \epsilon) - f(\theta - \epsilon)}{2\epsilon}$$

- For a non 0 value of ϵ , the error of the approximation is $O(\epsilon^2)$
- For the single sided numerical approximation, the error is $O(\epsilon)$
- To perform gradient checking on a NN:
 - 1. Reshape $W^{[1]}, b^{[1]}, ..., W^{[L]}, b^{[L]}$ into a single vector θ
 - 2. Reshape $dW^{[1]}, db^{[1]}, ..., W^{[L]}, b^{[L]}$ into a single vector $d\theta$
 - 3. For every i in θ , calculate:

$$d\theta_{approx}[i] = \frac{J(\theta_1, \theta_2, ..., \theta_i + \epsilon) - J(\theta_1, \theta_2, ..., \theta_i - \epsilon)}{2\epsilon}$$

4. Check if $d\theta_{approx}$ and $d\theta$ are reasonably close to each other

For
$$\epsilon = 10^{-7}$$
:

$$\frac{||d\theta_{approx} - d\theta||_2}{||d\theta_{approx}||_2 + ||d\theta||_2} \approx 10^{-7}$$

- Grad check should be only be used when debugging
 - Calculating $d\theta_{approx}$ is very computationally expensive
- If regularization is used, correct cost function must be used to calculate the gradient
- If dropout is used, J is not well defined and cannot use grad check
 - Cost function J that is optimized by dropout is defined by summing over all subsets of nodes that could be eliminated on each iteration
 - Can implement grad check with a keep_prob of 1 before turning on dropout
- Implementation of gradient descent may be correct when W and b are close to 0
 - Can run grad check just after random initialization
 - After training the network for a number of iterations, can run grad check again

2.2 Optimization Algorithms

2.2.1 Mini Batch Gradient Descent

- For gradient descent, vectorization will allow computation over all m training examples
 - If m is very large, then vectorization will still be very slow
- Gradient descent requires the whole training set to be processed for a single step of gradient descent

• Data from training set can be split into mini batches

$$X^{\{1\}} = [x^{(1)}, x^{(2)}, ..., x^{(1000)}]$$

$$Y^{\{1\}} = [y^{(1)}, y^{(2)}, ..., y^{(1000)}]$$

- Mini batch gradient descent looks at one mini batch on each iteration of gradient descent
- For each mini batch in the training set:
 - Run forward propagation on $X^{\{t\}}$

$$Z^{[1]} = W^{[1]}X^{\{t\}} + b^{[1]}$$

$$A^{[1]} = q^{[1]}(Z^{[1]})$$

...

$$A^{[l]} = q^{[l]}(Z^{[l]})$$

- Compute cost: $J^{\{t\}} = \frac{1}{1000} \sum_{i=1}^{l} \mathcal{L}(\hat{y}^{(i)}, y^{(i)}) + \frac{\lambda}{2 \times 1000} \sum_{l} ||W^{[l]}||_F^2$
- Use backpropagation to calculate gradients wrt $J^{\{t\}}$
- Update weights

$$W^{[l]} := W^{[l]} - \alpha dW^{[l]}$$

$$b^{[l]} := b^{[l]} - \alpha db^{[l]}$$

- A single pass through the training set is known as an epoch
- Algorithm can continue to run for multiple passes through the training set until an optimal solution is found
- For batch gradient descent, the cost should decrease on each iteration
 - If the cost doesn't decrease per iteration, then the algorithm has a bug
- For mini batch gradient descent, the cost will trend downwards but will be more noisy
 - Algorithm is being trained on a different batch of results on each iteration
- When running mini batch gradient descent, must choose the size of the mini batch
 - For mini batch size = m: Batch gradient descent
 - For mini batch size = 1: Stochastic gradient descent
- For stochastic gradient descent, each example may be good or bad for gradient descent
 - On average the cost function will be minimized for gradient descent
 - Path taken by gradient descent will be very noisy

- Stochastic gradient descent will never converge and just oscillate around the minimum
- Choice of mini batch size should be between 1 and m
 - Batch gradient descent will take very long for a single iteration
 - Stochastic gradient descent will lose all the speed from vectorization
- For a small training set $(m \le 2000)$, can just use gradient descent
- Otherwise can try a mini batch size from 64-512
 - Code may run faster if the mini batch size is a power of 2
- A single mini batch should be able to fit in the whole CPU/GPU memory

Advanced Optimization Algorithms

- Some advanced algorithms require the use of exponentially weighted averages
- Moving averages can be calculated for data such as daily temperature

$$V_0 = 0$$

$$V_t = \beta V_{t-1} + (1 - \beta)\theta_t$$

- V_t is the approximated average temperature over the last $\frac{1}{1-\beta}$ days
- If β is larger than the average will adapt slower to changes in the data
- Exponentially weighted average can be found by summing the daily temperature with an exponentially decaying function
- If $\beta = 0.9$:

$$V_{100} = 0.1\theta_{100} + (0.1)(0.9)\theta_{99} + (0.1)(0.9)^2\theta_{98} + (0.1)(0.9)^3\theta_{97} + \dots$$

- ullet When calculating the exponentially weighted average, the same variable v should be used and overwritten each time
 - Implementation will be much more efficient than calculating average manually from the past 10 values
- For large values of β , initial average will be much lower than they should be

$$\frac{V_t}{1-\beta^t}$$

- Bias correction can be used to ensure initial values are correct estimations of the averages
 - As t becomes larger, denominator becomes closer to 1

Momentum

- Gradient descent with momentum uses an exponentially weighted average of the gradients to update the weights
 - Almost always performs better than standard gradient descent

$$V_{dW} = \beta V_{dW} + (1 - \beta)dW$$

$$V_{db} = \beta V_{db} + (1 - \beta)db$$

$$W = W - \alpha V_{dw}$$

$$b = b - \alpha V_{db}$$

- Taking the average of the gradients will slow down any unnecessary oscillations in the algorithm
 - Algorithm may oscillate at first but will start to take more direct steps to the minimum
- $\beta = 0.9$ is a common choice for most applications of momentum

RMSprop

- RMSprop takes the weighted average of the squares of the derivatives
- Derivatives will get divided by the RMS before the weights are updated

$$S_{dW} = \beta_2 S_{dW} + (1 - \beta) dW^2$$

$$S_{db} = \beta_2 S_{db} + (1 - \beta) db^2$$

$$W = W - \alpha \frac{dW}{\sqrt{S_{dw}}}$$

$$b = b - \alpha \frac{db}{\sqrt{S_{db}}}$$

- Updates in the direction of oscillation will be divided by a large number
 - Will allow the learning rate to be larger and therefore allows faster training
- \bullet In practice, very small value ϵ is added to the denominator for more numerical stability

Adam Optimization Algorithm

- Adam optimization shown to work well for a range of deep learning architectures
 - Merges Momentum and RMSprop to one algorithm
 - "Adam" stands for adaptive moment estimation
- On iteration t:
 - Compute dW, db using the current mini batch

$$V_{dw} = \beta_1 V_{dw} + (1 - \beta_1) dW, \quad V_{db} = \beta_1 V_{db} + (1 - \beta_1) db$$

$$S_{dw} = \beta_2 S_{dw} + (1 - \beta_2) dW^2, \quad S_{db} = \beta_2 s db + (1 - \beta_2) db^2$$

$$V_{dw}^C = \frac{V_{dw}}{1 - \beta_1^t}, \quad V_{db}^C = \frac{V_{db}}{1 - \beta_1^t}$$

$$S_{dw}^C = \frac{S_{dw}}{1 - \beta_2^t}, \quad S_{db}^C = \frac{S_{db}}{1 - \beta_2^t}$$

$$W := W - \alpha \frac{V_{dw}^C}{\sqrt{S_{dw}^C} + \epsilon}$$

$$b := b - \alpha \frac{V_{db}^C}{\sqrt{S_{db}^C} + \epsilon}$$

- Must choose many hyperparameters to run Adam optimization
 - $-\alpha$: needs to be tuned to the specific NN
 - $-\beta_1$: 0.9 (default)
 - β_2 : 0.999 (default)
 - $-\epsilon:10^{-8}$ (default)

Learning Rate Decay

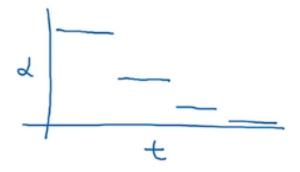
- For mini batch gradient descent, the algorithm will oscillate around the minimum point
- If the learning rate is reduced over time, then the oscillations will become smaller
 - $-\,$ During the initial steps of learning, algorithm can afford to take large steps
 - As the algorithm starts to converge, smaller steps are preferred

$$\alpha = \frac{1}{1 + \text{decay rate} \times \text{epoch num}} \alpha_0$$

- Other formulas can be used to decay the learning rate
 - Exponential decay

$$\alpha = 0.95^{\rm epoch\ num}\alpha_0$$

- Discrete staircase



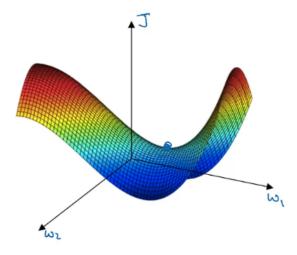
- Square root of epoch number

$$\alpha = \frac{k}{\sqrt{\text{epoch num}}} \alpha_0$$

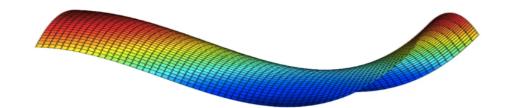
• Manual decay can be used for larger models that take a longer time to train

Local Optima

- Initial ideas believed that a cost function with many points of 0 gradient would have many local optima
 - When training a NN, most points with 0 gradient are saddle points



- For a point with 0 gradient, Each direction can either be a convex or concave function
 - For a local optima, must have a convex function in all directions
 - In a high dimensional space, chance of all directions being convex functions is very small
- Intuitions about lower dimensional spaces may not transfer to high dimensional spaces
- Plateaus are areas where the gradient is near to 0 for a large area



- Will take a very long time to move down off the plateau

- Learning will be slow but unlikely to get stuck in a local optima
- Optimization algorithms like Adam can help to speed up the training

2.3 Hyperparameter Tuning, Batch Normalization and Programming Frameworks

2.3.1 Hyperparameter Tuning

- Deep neural networks have many hyperparameters associated with the actual network and the training implementation
 - Numbers of layers and hidden units
 - Learning rate or method for learning rate decay
 - Hyperparameters for momentum or Adam optimization
 - Mini batch size
- Most important hyperparameter is the learning rate
 - Secondary importance can be given to momentum (β) , number of hidden units and the mini batch size
 - Number of layers and learning rate decay can be tuned last
 - Parameters for Adam optimization usually don't need to be tuned
- In practice, random values for the hyperparameters should be sampled and tested
 - If values are arranged in a grid, fewer distinct values can be tested
 - Choosing random values for the hyperparameters gives a higher chance of finding an optimum value for important hyperparameters
- Can use coarse to fine sampling scheme to find optimum values
 - Sample initial values and find which values work the best
 - "Zoom in" to the area and take more samples in the smaller region
- For some hyperparameters (number of layers / hidden units), can sample over a reasonable range
- Some hyperparameters may not have an even distribution (Learning rate between 0.0001 and 1)
 - Can use a log scale to ensure the numbers are better distributed

```
r = -4 * np.random.rand
learning_rate = 10 ** r
```

- Can look for a range $10^a...10^b$ and take a random sample $r \in [a, b]$
- For exponentially weighted averages, β will be around 0.9-0.999
 - Equivalent to averaging over the last 10 days or last 1000 days
 - Can sample values for 1β for $r \in [-3, -1]$
- For exponentially weighted averages, the sensitivity of the results is very high when β is close to 1
 - A change from 0.999 to 0.9995 will change the average from 1000 to 2000 examples
- Intuitions about the hyperparameters won't always transfer across applications
 - Ideas found in one application can still be applied to other applications
- Hyperparameters can become stale over time with changing data or hardware
 - Hyperparameters should be reevaluated every few months to ensure values are optimal
- Depending on resources, can babysit a single model or train models in parallel
 - For a single model, hyperparameters can be tweaked over time depending on training performance
 - If resources allow, can train the same model with many different hyperparameters and choose the best model

2.3.2 Batch Normalization

• Inputs to a NN can be normalized to speed up learning

$$X = \frac{X - \mu}{\sigma}$$

- Batch normalization normalizes the input values $Z^{[l]}$ to each layer
 - Can instead normalize the values $A^{[l]}$ after the activation function
- Given intermediate values $z^{(1)}, ..., z^{(m)}$:

$$\mu = \frac{1}{m} \sum_{i} z^{(i)}$$

$$\sigma^{2} = \frac{1}{m} \sum_{i} (z^{(i)} - \mu)^{2}$$

$$z_{norm}^{(i)} = \frac{z^{(i)} - \mu}{\sqrt{\sigma^{2} + \epsilon}}$$

$$\tilde{z}^{(i)} = \gamma z_{norm}^{(i)} + \beta$$

- γ and β are learnable parameters of the model
 - Allows the mean and variance of \tilde{z} to be set to any value

- If $\gamma = \sqrt{\sigma^2 + \epsilon}$, $\beta = \mu$, then $\tilde{z}^{(i)} = z^{(i)}$
- May not want mean 0 and standard deviation 1 for the activation function
- NN will have new parameters $\beta^{[1]}, \gamma^{[1]}, ..., \beta^{[L]}, \gamma^{[L]}$
 - Will be updated like normal parameters

$$\beta^{[l]} = \beta^{[l]} - \alpha d\beta^{[l]}$$

$$\gamma^{[l]} = \gamma^{[l]} - \alpha d\gamma^{[l]}$$

- Batch normalization is typically applied to mini batch gradient descent
 - Mean and variance will be calculated from the mini batch being used
- ullet When using batch normalization, normalization step removes the need for $b^{[l]}$ parameters
 - When subtracting the mean from the z values, the constant will get cancelled out
 - Mean of the \tilde{Z} values will be decided by the $\beta^{[l]}$ parameters
- Batch normalization will make weights deeper in a network more robust to changes earlier in the network
 - Data can have a covariate shift where the distribution changes after a generalization
 - Function mapping from X to Y can be the same but model may need to be retrained
 - Batch normalization will reduce the amount of movement of the distribution of the hidden values
- \bullet Even if there is a covariate shift in the data, batch norm will make the z values have the same mean and variance
 - The individual layers in the network will be more independent of each other
- Batch norm will also add a slight regularization effect
 - Each mini batch is scaled by the mean/variance of the specific mini batch
 - Normalizing with the mean/variance of the individual mini batch will add noise to the activations
 - Similar to dropout where the algorithm will not rely on any single hidden unit
 - Noise added to the z values is very small so dropout can be used as well
- If a larger mini batch size is used, noise is reduced and will have a smaller regularization effect.
- At test time, data will typically be processed one example at a time

- Cannot calculated the mean/variance of a single example
- Mean/variance can be estimated using exponentially weighted averages across the mini batches

2.3.3 Multi Class Classification

• Logistic regression can be generalized to apply to multiple classes

$$C = \text{number of classes}$$

- Output layer for the NN will have C units
 - Each unit will be the probability of each class
 - Sum of all numbers in the vector must be 1
- Softmax layer used in the output layer to output vector of probabilities
 - $-\ Z^{[L]}$ values are calculated as normal: $Z^{[L]}=W^{[L]}a^{[L-1]}+b^{[L]}$
 - Use the softmax activation function

$$t = e^{(Z^{[L]})}$$

$$a^{[L]} = \frac{t}{\sum_{i=1}^{C} t_i}$$

- Softmax activation function has a vector for its input and output
 - Other activation functions had a single value for input and output
- Largest input to softmax function will result in the largest output
 - "Hard max" function would return 1 for the largest input and 0 for the other inputs
- If C=2, softmax reduces to logistic regression
- Softmax classifier cannot be trained as a normal NN

$$\mathcal{L}(\hat{y}, y) = -\sum_{j=1}^{C} y_j \log \hat{y}_j$$

• Loss function will only be active for the ground truth class in the training set

$$J(W^{[1]}, b^{[1]}, \dots) = \frac{1}{m} \sum_{i=1}^{m} \mathcal{L}(\hat{y}^{(i)}, y^{(i)})$$

$$dz^{[L]} = \hat{y} - y$$

2.3.4 Deep Learning Frameworks

- For larger NNs, using a framework can save a lot of time
- Can look at the community behind the frameworks and the strengths
 - Ease of programming (development and deployment)
 - Running speed
 - Truly open (open source with good governance)
 - Application of NN

Tensorflow

• Assume a simple cost function:

$$J(w) = w^2 + 10w + 25$$

```
import numpy as np
import tensorflow as tf

w = tf.Variable(0, dtype=tf.float32)
optimizer = tf.keras.optimizers.Adam(0.1)

def train_step():
    with tf.GradientTape() as tape():
        cost = w ** 2 - 10 * w + 25
        trainable_variables = [w]
        grads = tape.gradient(cost, trainable_variables)
        optimizer.apply_gradients(zip(grads, trainable_variables))

for i in range(1000):
        train_step()
```

- No need to compute backpropagation steps with tensorflow
- More complex tensorflow program will have cost as a function of variables

```
w = tf.Variable(0, dtype=tf.float32)
x = np.array([1.0, -10.0, 25.0], dtype=np.float32)
optimizer = tf.keras.optmizers.Adam(0.1)
```

```
def training(x, w, optimizer):
    def cost_fn():
        return x[0] * w ** 2 + x[1] * w + x[2]

for i in range(1000):
        optimizer.minimize(cost_fn, [w])

return w
```

- Tensorflow will create a computation graph from the defined cost function
 - From the computation graph, tensorflow will compute the backpropagation steps

3 Structuring Machine Learning Projects

3.1 ML Strategy

3.1.1 Setting up a ML Project

- A machine learning project may have many ideas that can improve performance
 - Collect more data
 - Use a more diverse training set
 - Train the algorithm over a longer period of time
 - Use a different optimization algorithm (Adam instead of gradient descent)
 - Use a bigger/smaller network
 - Add dropout or L_2 regularization
 - Change the network architecture (activation functions or hidden units)
- Some methods may not be useful for the specific scenario
- ML strategy is changing with deep learning
 - Deep learning algorithms have different options when compared with previous generations
- Orthogonalization is where specific functions can be split up into different areas
- For a supervised learning system to perform well, system requires a chain of assumptions
 - Performance of algorithm on the training set must pass some threshold (\approx human-level performance)
 - Algorithm must be fit well to the dev set
 - Algorithm must be fit well to the test set
 - Algorithm must perform well in the real world
- Each step has specific "knobs" to tune to improve performance in the specific area
 - Training set: bigger network, Adam optimization
 - Dev set: regularization, bigger training set
 - Test set: bigger dev set
 - Real world: change dev set or cost function
- Early stopping can be used but is less orthogonalized
 - Worsens the performance on the training set

- Improves the performance on the dev set
- Single number evaluation metric can be used to test effectiveness of a model
- F1 score combines precision and recall into a single metric
 - Precision is the percentage of positively classified examples that are actually positive
 - Recall is the percentage of positive examples that are correctly classified
 - F1 score takes the harmonic mean of precision and recall

$$F_1 = \frac{2}{\frac{1}{P} + \frac{1}{R}}$$

- Having a well defined test set and single number evaluation metric will speed up iteration
- Scenario may have more than one type of metric that is relevant
 - Classification algorithm may value accuracy as well as running time
 - May not make sense to use a numerical function of some metrics
- Accuracy would be a optimizing metric and running time would be the satisficing metric
 - Goal can be to maximize accuracy subject to running time < 100ms
- For N different metrics:
 - 1 should be optimizing
 - -N-1 should be satisficing
- Dev set and test set should come from the same distribution
 - If different distributions are used, algorithm may perform on the dev set but not on the test set
 - Dev set and test set must have the same target
- Dev set should be used to evaluate the performance of different models
 - Setting up a dev set and an evaluation metric allows teams to iterate quickly

"Choose a dev set and test set to reflect data you expect to get in the future and consider important to do well on"

- Previous eras of machine learning had a 60%, 20%, 20%
- Modern eras of machine learning have much larger datasets
 - For 1000000 examples, can assign 1% each to dev and test set

- Larger amount of data in the training set will help algorithm

"Set your test set to be big enough to give high confidence in teh overall performance of your system"

- Some applications may only use a train and dev set
 - Specific scenario may not require high confidence in the overall performance of the algorithm
 - Must be careful to not overfit the dev set too much
- Evaluation metric may not give a full representation of the specific scenario
 - Cat classifier with very low error may allow some pornographic images through the algorithm
 - Algorithm with slightly higher error but no pornographic images would be preferred
- Evaluation metric should be changed if it doesn't correctly rank the algorithm's performance
 - Standard error function treats all images equally
 - Weight can be added to the error function to weight unwanted images higher
 - Requires labelling of unwanted images in dev and test set
- Task of changing evaluation metric is separate from changing cost function to achieve good performance
- Metric and/or dev/test set should be changed if performance on the application is not linked

3.1.2 Comparing to Human Level Performance

- With advances in deep learning, ML algorithms have much better performance
 - More feasible for algorithms to be competitive with human level performers
- Workflow of designing and building a ML system is more efficient when trying to learn something that humans can do
- For many ML projects, initial learning will be very fast as algorithm approaches human level performance
 - Rate of learning decreases after algorithm surpasses human level performance
 - Algorithm will approach Bayes optimal error
- Bayes optimal error is the best theoretical function for mapping from X to Y
 - For many tasks, human level performance is not very far from Bayes optimal error

- Once human level performance is surpassed, there may not be many areas to improve in
- If algorithm has lower than human level performance:
 - Get labelled data from humans
 - Gain insight from manual error analysis
 - Better analysis of bias/variance
- If human level performance is much lower than the training and dev set error, can focus on the bias of the algorithm
- If human level performance is close to the training error, can focus on the variance of the algorithm
- Human level performance can be used as an estimate for Bayes error
 - Difference between the Bayes error and training error is the avoidable bias
 - Difference between the training and dev set error can measure the variance
- For specialized tasks, different parties may have different errors for human classification
 - For medical image classification, a team of experienced doctors will have much lower error than an average human
 - Bayes error must be less than or equal to the lowest human error
 - Lowest human error can be used as estimate for Bayes error
- For publishing a paper or deploying a system, human error definition may be different
- When algorithm is very close to human level performance, can be hard to see if bias or variance should be trained
- With deep learning, algorithms in some areas can surpass human level performance
 - Online advertising
 - Product recommendations
 - Logistics
 - Loan approvals
- Above areas are not natural perception problems and come from structured data
 - Currently more challenging for computers to surpass humans in natural perception tasks
- ML has also surpassed humans in some natural perception tasks
 - Speech recognition
 - Some image recognition

- Medical tasks
- For supervised learning, must assume that the training set can be fit well (low avoidable bias)
 - The training set performance must also generalize well to the dev/test set (low variance)
- For high bias:
 - Train a bigger model
 - Train for longer or use a better optimization algorithm (momentum, RMSprop, Adam)
 - Change the NN architecture or find better hyperparameters
- For high variance:
 - Use more data
 - Use regularization $(L_2, dropout, data augmentation)$
 - Change the NN architecture or find better hyperparameters

3.1.3 Error Analysis

- Misclassified examples can be manually examined to look for any patterns
 - Finding patterns can give an upper bound of any increase in performance
- Different ideas for error analysis can be evaluated in parallel with a table
 - For each image, can fill in a checkbox for any patterns
 - Percentage of total for each pattern will give an idea of how to best improve performance
- Manual analysis may show new patterns in the errors
- Some errors may be incorrectly labelled examples in the dev/test set
 - Deep learning algorithms are quite robust to random errors in the training set
 - Algorithms are fairly susceptible to systematic errors in the training set
- Incorrectly labelled examples can be recorded in the error analysis table
 - Percentage of error caused by incorrect labels can be calculated to see if fixing labels is a worthwhile task
- Any processes should be applied to the dev and test set at the same time to ensure they come from the same distribution
 - Training set may end up coming from a different distribution than the dev/test set

- Can also look at examples that the algorithm got right to see if got any errors
- For a new ML system, priority should be to build initial system then iterate
 - Set up a dev/test set and evaluation metric
 - Build initial system quickly
 - Use bias/variance and error analysis to prioritize next steps
- Error analysis will give idea for next steps

3.1.4 Mismatched Training and Dev/Test Sets

- Deep learning algorithms perform best with a lot of training data
 - Many teams are putting as much data as possible into training sets
 - Extra data added to the training set will give a different distribution to the training set data
- Other sources of data may have more examples but can come from a slightly different distribution
- Data can be pooled together and randomly split into training, dev and test set
 - All data will come from the same distribution
 - Much of the dev set will come from the additional distribution of images rather than the original distribution
 - Algorithm will optimize to the wrong distribution of images
- Training set can be set to include all images from the additional distribution
 - Examples from the original distribution will be split between the dev and test set
 - Dev and test set will have the correct distribution of images
 - Training set will have a different distribution
- Estimate of bias and variance changes when training set has a different distribution to dev and test set
 - Comparatively high dev set error might mean dev set has more challenging images than training set
 - Data from the dev set will be new to the algorithm and will have a different distribution to the training data
- Portion of the training set can be set as the training-dev set
 - Should not be used for training but will have the same distribution as the training set
- For error analysis, can look at the training set, training-dev set and dev set

- Large difference between the training error and training-dev error indicates a variance problem
- Large difference between the training-dev error and dev error indicates a data mismatch problem
- Large difference between training error and human error indicates high bias problem
- Difference between the dev error and test error indicates degree of overfitting to the dev set
- For each distribution of data, can look at:
 - Human level error
 - Error on examples trained on
 - Error on examples not trained on
- For data mismatch:
 - Use manual data analysis to try understand the difference between training and dev sets
 - Can try to make the training set more similar to the dev set (collect more examples or use artificial data synthesis)
- For some applications, algorithm may overfit during artificial data synthesis
 - For speech recognition, same recording of noise may be added to many examples
 - As much as possible, should aim to get a large range of examples with data synthesis

3.1.5 Learning From Multiple Tasks

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