Deep Learning Specialization

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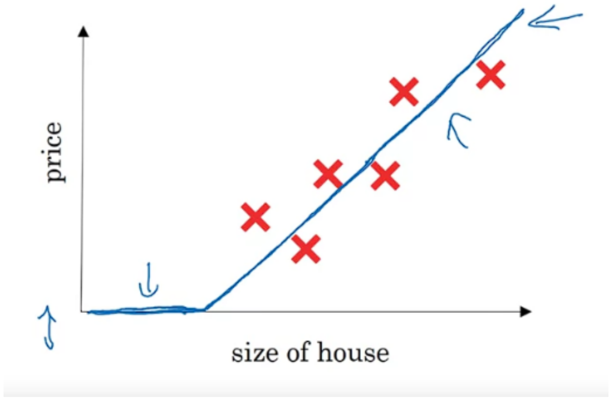
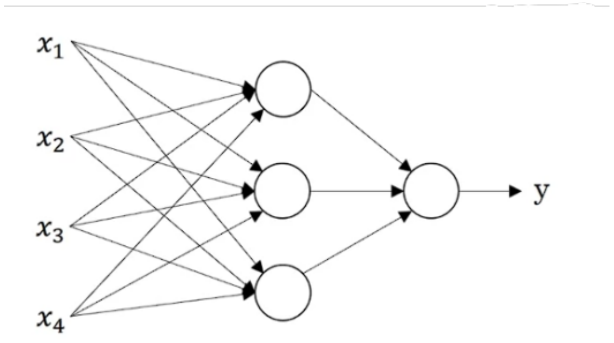
1 Neural Networks and Deep Learning

1.1 Introduction to Deep Learning

- Takes input x to a “neuron” and gives some output y



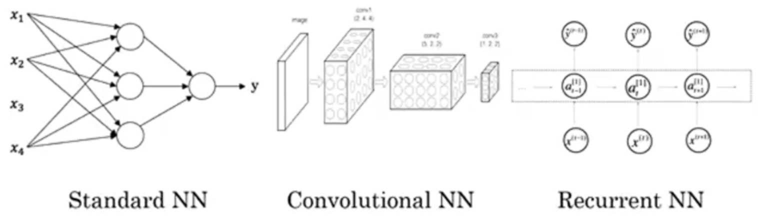
  - Simple neural network has a single input, neuron and output
  - x: size of the house
  - y: price of the house
  - Hypothesis (blue line) is a ReLU (Rectified Linear Unit)
- More complex neural networks can be formed by “stacking” neurons



- 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

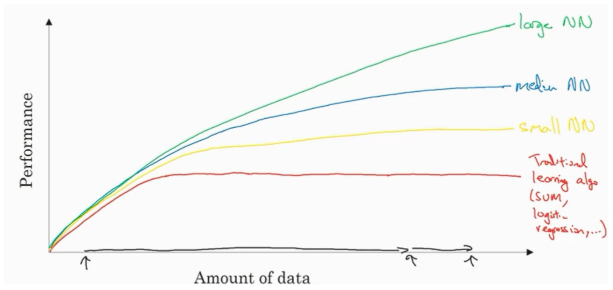
1.1.1 Supervised Learning

- 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 $(b * c * d, 1)$

```
X_flatten = X.reshape(X.shape[0], -1).T
```

Notation

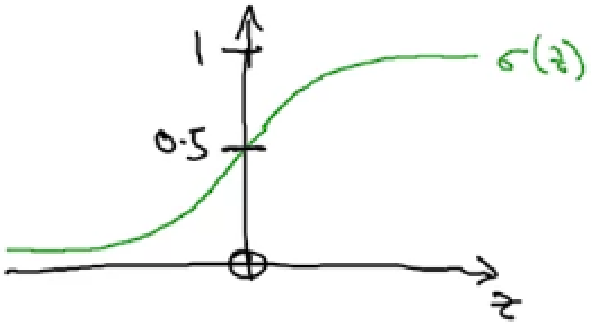
$$\{(x^{(1)}, y^{(1)}), (x^{(2)}, y^{(2)}), ..., (x^{(m)}, y^{(m)})\}$$

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

- $(x^{(i)}, y^{(i)})$: i^{th} training example
- $m = m_{train}$
- $m_{test} = \#$ of test examples
- $X = \begin{bmatrix} | & | & & | \\ x^{(1)} & x^{(2)} & ... & x^{(3)} \\ | & | & & | \end{bmatrix}$
  - $X \in \mathbb{R}^{n_x \times n}$
- $Y = \begin{bmatrix} y^{(1)} & y^{(2)} & ... & y^{(m)} \end{bmatrix}$
  - $Y \in \mathbb{R}^{1 \times m}$

Logistic Regression

- Given x, want $\hat{y} = P(y = 1|x)$
  - Since $\hat{y}$ is a probability, want $0 \leq \hat{y} \leq 1$
- 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
- 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 $\log(\hat{y})$ $\therefore$ want large $\hat{y}$
  - $\hat{y}$ has a max of 1 $\therefore$ want $\hat{y} = 1$
- If $y = 0$:
  - $\mathcal{L}(\hat{y}, y) = -log(1-\hat{y})$
  - Want large $\log(1-\hat{y})$ $\therefore$ want small $\hat{y}$
  - $\hat{y}$ has a min of 0 $\therefore$ want $\hat{y} = 0$
- Cost function:

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

  - Average loss function over all training examples

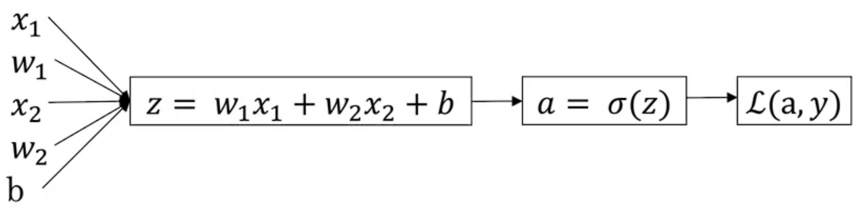
Gradient Descent

- 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

```
Repeat {
    w := w - $\alpha\frac{\partial J(w,b)}{\partial w}$
    b := b - $\alpha\frac{\partial J(w,b)}{\partial b}$
}
```

- Using the computation graph:

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



$$
\begin{aligned}
\frac{\partial \mathcal{L}(a,y)}{\partial z} &= \frac{\partial \mathcal{L}}{\partial a} \times \frac{\partial a}{\partial z} \\
&= (-\frac{y}{a} + \frac{1-y}{1-a}) \times a(1-a) \\
&= a - y
\end{aligned}
$$

$$
\begin{aligned}
\frac{\partial \mathcal{L}}{\partial w_1} &= x_1 \times \frac{\partial \mathcal{L}}{\partial z} \\
\frac{\partial \mathcal{L}}{\partial w_2} &= x_2 \times \frac{\partial \mathcal{L}}{\partial z} \\
\frac{\partial \mathcal{L}}{\partial b} &= \frac{\partial \mathcal{L}}{\partial z}
\end{aligned}
$$

- 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
        dw1 /= m
        dw2 /= m
        db /= m

        w1 := w1 - $\alpha$ dw1
        w2 := w2 - $\alpha$ dw2
        b := b - $\alpha$ db
```

- 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:

```
z = 0
for i in range(n_x):
    z += w[i] * x[i]
z += b
```

- 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

$$z^{(i)} = w^T x^{(i)} + b$$
$$a^{(i)} = \sigma(z^{(i)})$$
$$X = \begin{bmatrix} | & | & & | \\ x^{(1)} & x^{(2)} & \dots & x^{(m)} \\ | & | & & | \end{bmatrix}$$
$$w \in \mathbb{R}^{n_x} \quad X \in \mathbb{R}^{n_x \times m}$$

$$\begin{aligned} \begin{bmatrix} z^{(1)} & z^{(2)} & \dots & z^{(m)} \end{bmatrix} &= w^T X + \begin{bmatrix} b & b & \dots & b \end{bmatrix} \\ &= \begin{bmatrix} w^T x^{(1)} + b & w^T x^{(2)} + b & \dots & w^T x^{(m)} + b \end{bmatrix} \end{aligned}$$

- In Python:

```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`

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

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

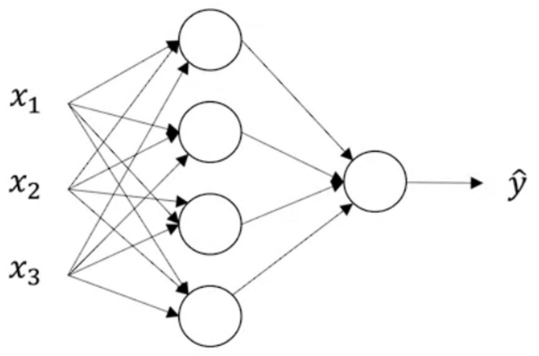
```python
Z = np.dot(w.T,X) + b
A = sigmoid(Z)
dz = A - Y
dw = 1/m * np.dot(X, dz.T)
db = 1/m * np.sum(dz)

# 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
- Each layer will have parameters w and b associated with them
- Each node in the NN will perform logistic regression with its inputs

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

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

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

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

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

$$\begin{aligned}
a^{[1]} &= \begin{bmatrix} a_1^{[1]} \\ a_2^{[1]} \\ a_3^{[1]} \\ a_4^{[1]} \end{bmatrix} \\
&= \sigma(z^{[1]})
\end{aligned}$$

$$z^{[2]} = W^{[2]} a^{[1]} + b^{[2]} \quad \rightarrow \quad a^{[2]} = \sigma(z^{[2]})$$

- 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)

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

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

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

$$\begin{aligned}
Z^{[1]} &= W^{[1]} X + b^{[1]} \\
A^{[1]} &= \sigma(Z^{[1]}) \\
Z^{[2]} &= W^{[2]} A^{[1]} + b^{[2]} \\
A^{[2]} &= \sigma(Z^{[2]})
\end{aligned}$$

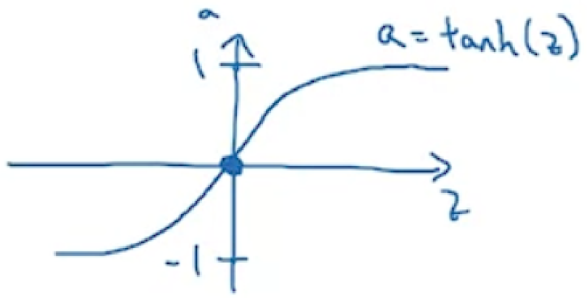
1.3.1 Activation Functions

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

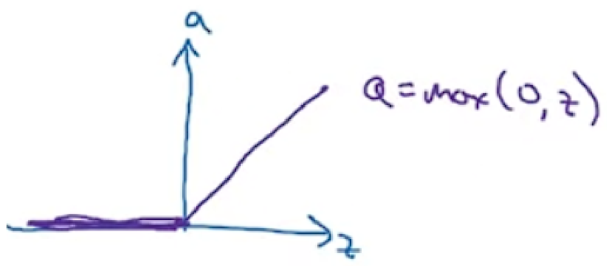
$$a_{sigmoid} = \frac{1}{1+e^{-z}}$$

- 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

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

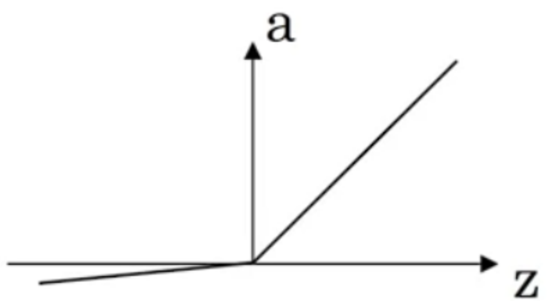


- For binary classification, the final output layer can use the sigmoid function
  - Want the value of $\hat{y}$ to be between 0 and 1
- For both the sigmoid and tanh functions, when z is large, the gradient is very small
  - Results in a slower gradient descent
- ReLU function has a gradient of 1 when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

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

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

  - tanh function

$$\begin{aligned}g(z) &= \tanh(z)\\ &= \frac{e^z - e^{-z}}{e^z + e^{-z}}\end{aligned}$$

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

- ReLU function

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

- Leaky ReLU function

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

1.3.2 Gradient Descent for Neural Networks

- 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:

$$\begin{aligned}Z^{[1]} &= W^{[1]}X + b^{[1]} \\ A^{[1]} &= g^{[1]}(Z^{[1]}) \\ Z^{[2]} &= W^{[2]}A^{[1]} + b^{[2]} \\ A^{[2]} &= g^{[2]}(Z^{[2]})\end{aligned}$$

- Backpropagation:

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

1.3.3 Random Initialization

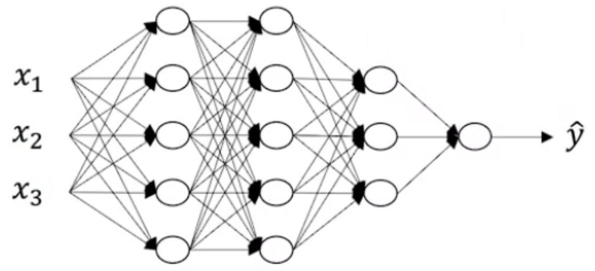
- Weights must be initialized randomly for a NN
  - Weights can be initialized to 0 for logistic regression
  - The bias terms b can be initialized
- If weights are initialized to 0, all neurons in a layer will compute the same hypothesis

```
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, $L = 4$
- $n^{[l]}$ = 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

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

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

- For a vectorized implementation

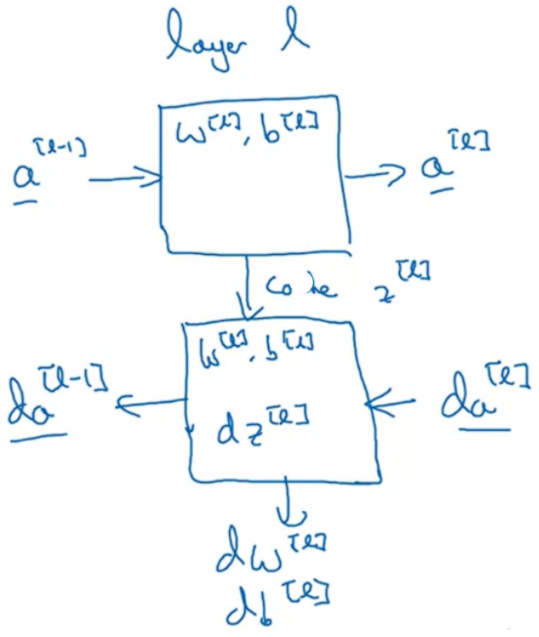
$$Z^{[l]} = W^{[l]}A^{[l-1]} + b^{[l]}$$

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

  - 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
  - $a^{[l]}, z^{[l]} : (n^{[l]}, 1)$
- 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
- 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
  - $dz^{[l]} = da^{[l]} * g^{[l]\prime}(z^{[l]})$
  - $dW^{[l]} = dz^{[l]} a^{[l-1]T}$

  - $db^{[l]} = dz^{[l]}$
  - $da^{[l-1]} = W^{[l]T} dz^{[l]}$
- For a vectorized implementation:
  - $dZ^{[l]} = dA^{[l]} * g^{[l]\prime}(Z^{[l]})$
  - $dW^{[l]} = \frac{1}{m} dZ^{[l]} A^{[l-1]T}$
  - $db^{[l]} = \frac{1}{m}$`np.sum`$(dZ^{[l]}$`, axis=1, keepdims=True`$)$
  - $dA^{[l-1]} = W^{[l]T} dZ^{[l]}$

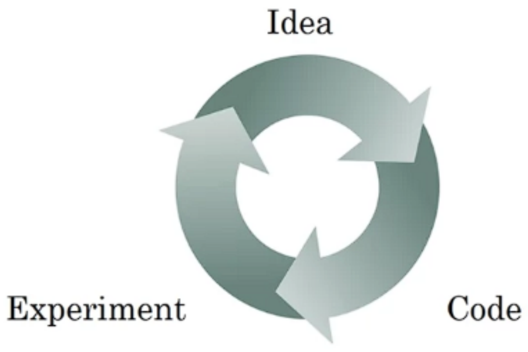
1.4.1 Parameters vs Hyperparameters

- 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
- 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:

$$J(w,b) = \frac{1}{m}\sum_{i=1}^{m}\mathcal{L}(\hat{y}^{(i)}, y^{(i)}) + \frac{\lambda}{2m}||w||_2^2$$

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

  - 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:

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

$$||w^{[L]}||^2 = \sum_{i=1}^{n^{[l]}} \sum_{j=1}^{n^{[l-1]}} (w_{i,j}^{[l]})^2$$

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

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

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

  - 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
- 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:

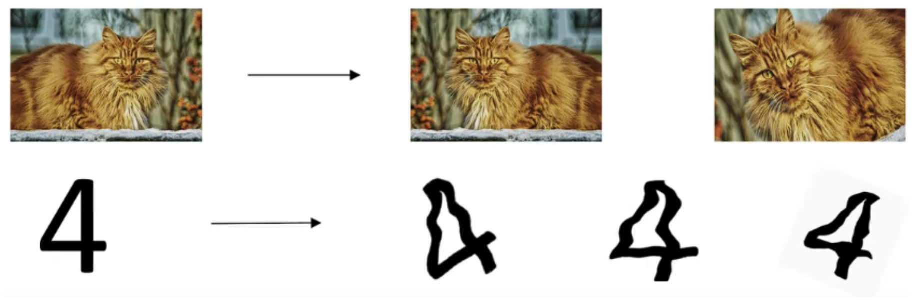
```
    d3 = np.random.rand(a3.shape[0], a3.shape[1]) < keep_prob
    a3 = np.multiply(a3, d3)
    a3 /= keep_prob
```

  - 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 1
- 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

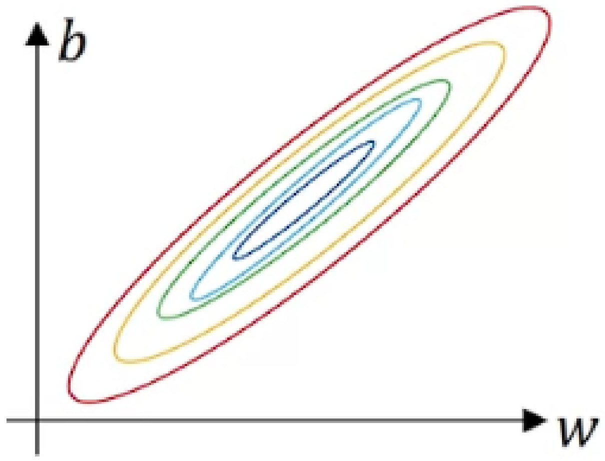


- Early stopping can be used to prevent overfitting from happening
  - If the NN is overfitting the data, the dev set error will initially decrease before increasing
  - Training of the NN can be stopped when the dev set error is lowest and the data has not been overfit
- Using early stopping links the 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

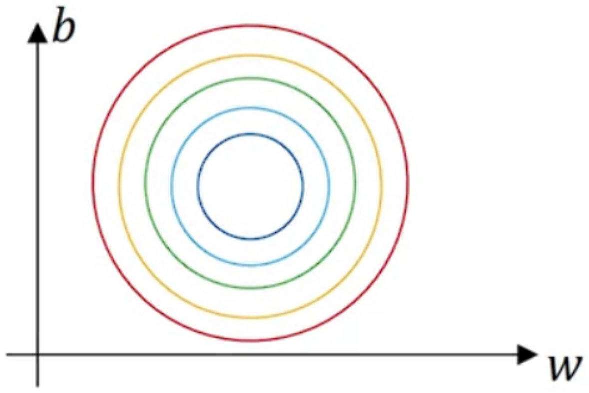
2.1.4 Setting up the Optimization Problem

- 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



- 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 $w_i x_i$

$$z = w_1x_1 + w_2x_2 + ... + w_nx_n$$

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

```
W^[l] = np.random.randn(shape) * np.sqrt(1/n^[l-1])
```

  - 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 $X^{\{t\}}$

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

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

    ...

    $A^{[l]} = g^{[l]}(Z^{[l]})$
  - 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 ($m \leq 2000$), 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 then 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 $\beta = 0.9$:

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

- 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
- 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

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

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

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

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

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

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

- Must choose many hyperparameters to run Adam optimization
  - α: needs to be tuned to the specific NN
  - β_1: 0.9 (default)
  - β_2: 0.999 (default)
  - $\epsilon : 10^{-8}$ (default)

Learning Rate Decay

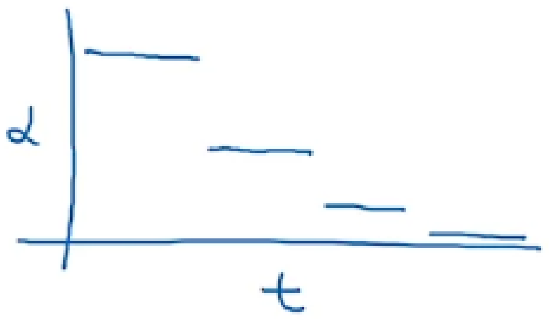
- For mini batch gradient descent, the algorithm will oscillate around the minimum point
- If the learning rate is reduced over time, then the oscillations will become smaller
  - During the initial steps of learning, algorithm can afford to take large steps
  - As the algorithm starts to converge, smaller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

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

  - Discrete staircase



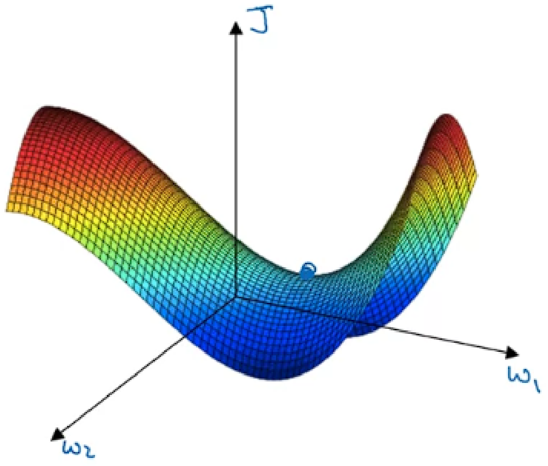
- Square root of epoch number

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

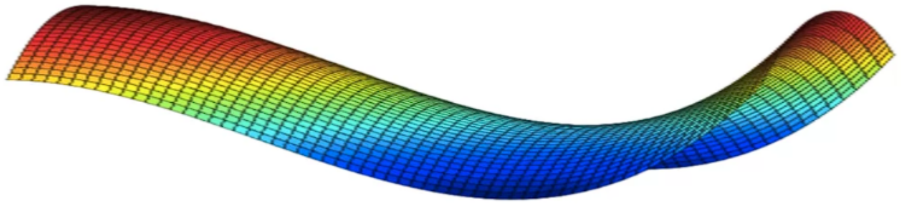
- Manual decay can be used for larger models that take a longer time to train

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