30-Aug-2020: Welcome Video, and What is Machine Learning

- Machine learning: algorithms; supervised, unsupervised, reinforcement, recommender. In this course, also will learn best practices.

31-Aug-2020: Supervised Learning, and Unsupervised Learning

- Supervised learning: right answers are given
- Regression: predicts continuous variable output; Classification: predicts discrete values
- Classification can have $1, \ldots, N, \ldots, \infty$ attributes. E.g. benignness/malignancy based on age, or age and tumor size, etc.
- Unsupervised learning a.k.a. clustering: Right answers aren't given. For example, news that links to different sources for the same topic.
- Cocktail party algorithm: separates two voices in a conversation, with two microphone recordings. Singular value decomposition is key to this algorithm.
- When learning machine learning, use Octave

1-Sep-2020: Model Representation, and Cost Function

- Training set notation: m is number of training examples, x are input examples, and y are the output variables. Together, (x, y) form a training example. Also denoted $(x^{(i)}, y^{(i)})$.
- In a linear regression, $h_\theta(x) = \theta_0 + \theta_1 x \equiv h(x)$.
- Cost function is

$$J(\theta_0, \theta_1) = \frac{1}{2m} \sum_{i=1}^{m} \left(h_\theta(x^{(i)}) - y^{(i)} \right)^2$$

- Want to minimize J w.r.t. θ_0 and θ_1.

4-Sep-2020: Cost Function, Intuition I&II; Gradient Descent

- Intuition I; Let $\theta_0 = 0$, then $\min_{\theta_1} J(\theta_1)$ is what we want
- Ex: $h_\theta(x) = \theta_1 x$ and let $(x, y) = \{(1,1), (2,2), (3,3)\}$.

$$\begin{aligned} J(\theta_1) &= \frac{1}{2m} \sum_{i=1}^{m} \left(h_\theta(x^{(i)}) - y^{(i)} \right)^2 \\ &\rightarrow \text{ If } \theta_1 = 0,\ h_\theta(x) \equiv 0 \\ J(0) &= \frac{1}{2 \times 3} (1 + 4 + 9) \\ &= \frac{14}{6} \end{aligned}$$

- $J(\theta_1)$ is parabolic
- We want $\min_\theta J(\theta)$; here, $\theta_1 = 1$ satisfies this criterion
- Intuition II; Let θ_0, θ_1 be free in $J(\theta_0, \theta_1)$ and $h_\theta(x)$.
- $J(\theta_0, \theta_1)$ is a paraboloid
- Gradient Descent; Use gradient descent to find (θ_0, θ_1) that minimizes $J(\theta_0, \theta_1)$.
- Differing starting guesses can give different local minima.
- Gradient descent algorithm:

$$\theta_j := \theta_j - \alpha \frac{\partial}{\partial \theta_j} J(\theta_0, \theta_1) \quad \text{for } j = 1, 2$$

- Simultaneously update θ_0, θ_1, α is called the learning rate.
- Ex: $\theta_0 = 1, \theta_2 = 2$ and $\theta_j := \theta_j + \sqrt{\theta_0 \theta_1}$.

$$\begin{aligned} \theta_0 &:= \theta_0 + \sqrt{\theta_0 \theta_1} \\ &= 1 + \sqrt{1 \times 2} \\ &= 1 + \sqrt{2} \\ \theta_1 &= \theta_2 + \sqrt{\theta_0 \theta_1} \\ &= 2 + \sqrt{1 \times 2} \quad \text{note here that we used the old value of } \theta_0 \\ &= 2 + \sqrt{2} \end{aligned}$$

5-Sep-2020: Gradient Descent Intuition, Gradient Descent for Linear Regression

- Gradient Descent Intuition: For simplicity, assume $\theta_0 = 0$
- One variable: $\theta_1 := \theta_1 - \alpha \frac{d}{d\theta_1} J(\theta_1)$; Newton-Raphson
- If α is too small, convergence may be very slow. If too large, it may miss the minimum.
- If θ_1 is already at a local minimum, g.d. leaves θ_1 unchanged since the derivative is zero.
- Gradient Descent for Linear Regression: We need derivatives

$$\frac{\partial}{\partial \theta_0} J(\theta_0, \theta_1) = \frac{1}{m} \sum_{i=1}^{m} \left(\theta_0 + \theta_1 x^{(i)} - y^{(i)} \right)$$
$$\frac{\partial}{\partial \theta_1} J(\theta_0, \theta_1) = \frac{1}{m} \sum_{i=1}^{m} \left(\theta_0 + \theta_1 x^{(i)} - y^{(i)} \right) \times x^{(i)}$$

- So, gradient descent finds the new θ variables as

$$\theta_0 := \theta_0 - \alpha \frac{1}{m} \sum_{i=1}^{m} \left(\theta_0 + \theta_1 x^{(i)} - y^{(i)} \right)$$
$$\theta_1 := \theta_1 - \alpha \frac{1}{m} \sum_{i=1}^{m} \left(\theta_0 + \theta_1 x^{(i)} - y^{(i)} \right) \times x^{(i)}$$

- This is called "batch gradient descent"; batch implies looking at all the training examples. This is represented by the $\sum_{i=1}^{m}$.
- Quiz Linear Regression with One Variable: 2) $m = \Delta y / \Delta x = (1 - 0.5)/(2 - 1) = 0.5 \implies y = 0.5x + b$; y-intercept is clearly zero since (0,0) is a data point.
- 3) $h_\theta(x)$; $\theta_0 = -1$, $\theta_1 = 2$; $h_\theta(6) = -1 + 2 \times 6 = 11$

9-Sep-2020: Linear Algebra Review

- Matrices and Vectors: Nothing new; in this course, index from 1.
- Addition and Scalar Multiplication: Nothing new
- Matrix Vector Multiplication: Nothing new;
- Ex: Let house sizes be $\{2104, 1416, 1534, 852.\}$. Let the hypothesis be $h_\theta(x) = -40 + 0.25x$.

$$\begin{bmatrix} 1 & 2104 \\ 1 & 1416 \\ 1 & 1534 \\ 2 & 852 \end{bmatrix} \begin{bmatrix} -40 \\ 0.25 \end{bmatrix} = \begin{bmatrix} -40 \times 1 + 0.25 \times 2104 \\ -40 \times 1 + 0.25 \times 1416 \\ -40 \times 1 + 0.25 \times 1534 \\ -40 \times 1 + 0.25 \times 852 \end{bmatrix} = \begin{bmatrix} h_\theta(2104) \\ h_\theta(1416) \\ h_\theta(1534) \\ h_\theta(852) \end{bmatrix}$$

  This essentially says data matrix $\times$ parameters = prediction
- Best to do this with built-in linear algebra function in Octave/Python. You can do it manually in a for-loop, but it'll be really slow.
- Matrix Multiplication: Take the same example. Now we have three hypotheses:

$$h_\theta(x) = -40 + 0.25x$$
$$h_\theta(x) = 200 + 0.1x$$
$$h_\theta(x) = -150 + 0.4x$$

  In matrix form, this becomes

$$\begin{bmatrix} 1 & 2104 \\ 1 & 1416 \\ 1 & 1534 \\ 2 & 852 \end{bmatrix} \begin{bmatrix} -40 & 200 & -150 \\ 0.25 & 0.1 & 0.4 \end{bmatrix} = \begin{bmatrix} 486 & 410 & 692 \\ 314 & 342 & 416 \\ 344 & 353 & 464 \\ 173 & 285 & 191 \end{bmatrix}$$

- Matrix Multiplication Properties: Not commutative. $AB \neq BA$. But it's associative. $ABC = (AB)C = A(BC)$.
- Identity matrix is I such that $AI = IA = A$. $I = \begin{bmatrix} 1 & 0 \\ 0 & 1 \end{bmatrix}$ in 2D.

- Inverse of A is A^{-1} such that $AA^{-1} = A^{-1}A = I$.
- Transpose of A is A^T. If $B = A^T$, then $B_{ij} = A_{ji}$.
- Quiz: 4) $u = \begin{bmatrix} 3 \\ -5 \\ 4 \end{bmatrix}, v = \begin{bmatrix} 1 \\ 2 \\ 5 \end{bmatrix}$, then $u^T v = \begin{bmatrix} 3 & -5 & 4 \end{bmatrix} \begin{bmatrix} 1 \\ 2 \\ 5 \end{bmatrix} = -3 + (-10) + 20 = 13$.

10-Sep-2020: Multiple Features

- Introduce other features: e.g. house price not just a function of square footage; Now, house price vs. sq. footage, age, number of bedrooms, etc.
- n is the number of features, $x_j^{(i)}$ represents the value of the j^{th} feature for the i^{th} training example; $x^{(i)}$ is a vector of all the features.
- Hypothesis: $h_\theta(x) = \theta_0 + \theta_1 x_1 + \theta_2 x_2 + \cdots + \theta_n x_n$. Let $x_0^{(i)} = 1$. Then, we can write this in matrix form as

$$x = \begin{bmatrix} x_0 \\ x_1 \\ \vdots \\ x_n \end{bmatrix}, \quad \theta = \begin{bmatrix} \theta_0 \\ \theta_1 \\ \vdots \\ \theta_n \end{bmatrix} \implies h_\theta(x) = \theta^T x$$

11-Sep-2020: G.D. for Multiple Variables, G.D. in Practice I - Feature Scaling, G.D. in Practice II - Learning Rate, Features and Polynomial Regression, Normal Equation

- Gradient Descent for Multiple Variables: For $n \geq 1$, gradient descent is

$$\theta_j := \theta_j - \alpha \frac{1}{m} \sum_{i=1}^{m} \left(h_\theta(x^{(i)}) - y^{(i)} \right) x_j^{(i)} \quad \text{for } j = 0, \ldots, n.$$

- G.D. in Practice I - Feature Scaling: ensure features have similar scales. E.g.: Houses in the data set have 1-5 bedrooms, and are between 0-2000 sq. ft. Scale these features to the order of 1. So, divide bedrooms by 5 so it's 0-1, and divide square footage by 2000, so it's 0-2.
- Feature should be $-1 \leq x_i \leq 1$.
- Mean renormalization; Subtract off the mean, and then scale. E.g. $x_1 = (\text{sq. footage} - 1000)/2000$ and $x_2 = (\text{bedrooms} - 2)/5$. More formally,

$$x_i \to \frac{x_i - \mu_i}{s_i} \quad \text{(mean renormalization)},$$

  where x_i is the feature, μ_i is the mean value of the i^{th} feature, and s_i is the range, or standard deviation, of the i^{th} feature.
- G.D. in Practice II - Learning Rate: We can plot $J(\theta)$ as a function of iterations, N; it should be a decreasing function.
- If $J(\theta)$ vs N diverges, you need a smaller learning rate, α.
- If $J(\theta)$ vs N falls, rises, falls, rises, etc., then use a smaller α.
- Features and Polynomial Regression: In the housing example, hypothesis could be $h_\theta(x) = \theta_0 + \theta_1 \times \text{length} + \theta_2 \times \text{depth}$. Maybe you think the relevant figure is area = length$\times$depth$\equiv x$. The hypothesis is $h_\theta(x) = \theta_0 + \theta_1 \times x$.
- Polynomial regression; e.g.

$$\theta_0 + \theta_1 x + \theta_2 \ x^2 + \theta_3 x^3$$
$$\theta_0 + \theta_1 x_1 + \theta_2 x_2 + \theta_3 x_3$$

  where $x_1 = x = \text{area}$, $x_2 = x^2 = \text{area}^2$, $x_3 = x^3 = \text{area}^3$. In polynomial regression, feature scaling becomes very important.
- Don't just have to have integer powers: e.g. $h_\theta(x) = \theta_0 + \theta_1 x + \theta_2 x^{1/2}$
- Normal Equation: Instead of using gradient descent to find $\min_\theta J$, use normal equation to do it analytically.
- Intuition; in 1-D, if $J(\theta) = a\theta^2 + b\theta + c$, you can find $dJ/d\theta = 0$ to get the extremum. In N-D, set $\partial_{\theta_j} J = 0$ for $j = 1, \ldots, N$.

- Say you have m training examples, each with n features. Let

$$\begin{aligned} X_{ij} &= x_j^{(i)} \\ Y_i &= y^{(i)} \\ \theta &= \left(X^T X\right)^{-1} X^T Y \end{aligned}$$

- If the training examples are $\left(x^{(1)}, y^{(1)}\right), \ldots, \left(x^{(m)}, y^{(m)}\right)$, then

$$x^{(i)} = \begin{bmatrix} x_0^{(i)} \\ \vdots \\ x_n^{(i)} \end{bmatrix}, X = \begin{bmatrix} {\vec{x}^{(1)}}^T \\ \vdots \\ {\vec{x}^{(m)}}^T \end{bmatrix}, Y = \begin{bmatrix} y^{(1)} \\ \vdots \\ y^{(m)} \end{bmatrix}, \theta = \left(X^T X\right)^{-1} X^T Y,$$

  where $x_0^{(i)} = 1$.
- With normal equation method, features don't have to be scaled.
- Normal equation method is slow if n is very large; Computing $(X^T X)^{-1}$ is costly. Inverting an $N \times N$ matrix costs $O(N^3)$.

12-Sep-2020: Normal Equation and Non-Invertibility

- What if $X^T X$ is signular? Octave's `pinv` (pseudo-inverse) takes care of that
- Causes; redundancy: e.g. area in ft^2 and in m^2; too few equations: $m < n$, fewer training examples compared to features, i.e. too few equations, too many unknowns.
- Quiz: 1) Midterm exam average $\mu_1 = (89 + 72 + 94 - 69)/4 = 81$; range is $s_1 = 94 - 69 = 25$, thus $x_1^{(3)} \to (x^{(3)} - \mu_1)/s_1 = (94 - 81)/25 = 0.52$
- 3) $X = \begin{bmatrix} x_0^{(1)} & \ldots & x_3^{(1)} \\ & \vdots & \\ x_0^{(14)} & \ldots & x_3^{(14)} \end{bmatrix}$ is 14×4.

13-Sep-2020: Octave Quiz

- Quiz: 1) A is 3×2, B is 2×3. Thus, AB and A+B^T are valid
- 4) u, v are 7×1. Calculate $u \cdot v$. This can be done via $u^T v$. In Octave, this is `sum(v.*w)` and `v'*w`

17-Sep-2020: Classification, Hypothesis Representation, Decision Boundary, Cost Function, Simplified Cost Function and Gradient Descent

- Classification: $y \in \{0, 1\}$ (binary), $y \in \{0, 1, 2, \ldots, N\}$ (multiclass)
- Could fit a linear $h_\theta(x) = \theta^T x$ and classify using a threshold of 0.5. Not good, though. Too sensitive to outliers. Also, $h_\theta(x)$ can be negative.
- Hypothesis Representation:

$$\begin{aligned} h_\theta(x) &= g(\theta^T x); \\ g(z) &= \frac{1}{1 + e^{-z}} \quad \text{sigmoid or logistic function; Fermi-Dirac distribution;} \\ &\implies h_\theta(x) = \frac{1}{1 + \exp\left(-\theta^T x\right)}. \end{aligned}$$

- $h_\theta(x)$ represents the probability that $y = 1$ on an input x. E.g. $\begin{bmatrix} x_0 \\ x_1 \end{bmatrix} = \begin{bmatrix} 1 \\ \text{tumor size} \end{bmatrix}$. If $g(x) = 70\%$, then there is a 70% chance that the tumor is malignant.
- $h_\theta(x) = P\left(y = 1 \middle| x; \theta\right)$ means "the probability that $y = 1$ given x, parametrized by θ"
- Probabilities sum to 1. $P\left(y = 1 \middle| x; \theta\right) + P\left(y = 0 \middle| x; \theta\right) = 1$.
- Decision Boundary: Can say if $h_\theta(x) \geq 0.5 \implies y = 1$, $h_\theta(x) < 0.5 \implies y = 0$.
- $g(z) \geq 0.5 \implies z \geq 0$. So, $h_\theta(x) = g(\theta^T x) \geq 0.5 \implies \theta^T x \geq 0$. Converse is true for < 0.5.
- Decision Boundary; Say $g(\theta_0 + \theta_1 x_1 + \theta_2 x_2)$. WLOG, let $\theta_1 = \theta_2 = 1$. On an x_2-x_1 diagram, this parametrizes a straight line. $x_2 = -x_1 + \theta_0$. The decision boundary is the set of points (x_2, x_1) s.t. $h_\theta(x) = 0.5$.

- Example; $\theta_0 = 5, \theta_1 = -1, \theta_2 = 0 \implies h_\theta(x) = g(5 - x_1)$. Decision boundary is implied by $x_1 = 5$. Where is $h \geq 0.5$? $5 - x \geq 0 \implies x_1 \leq 5$. This region corresponds to $y = 1$.
- Non-Linear Decision Boundaries; $g(\theta_0 + \theta_1 x_2 + \theta_2 x_2 + \theta_3 x_1^2 + \theta_4 x_2^2)$.
- Cost Function: Training set $\{(x^{(1)}, y^{(1)}), \ldots, (x^{(m)}, y^{(m)})\}$, $x^{(i)} = \begin{bmatrix} x_0^{(i)} \\ \vdots \\ x_n^{(i)} \end{bmatrix}$. m training examples, each with n features. $x_0^{(i)} \equiv 1$.
- Recall, for linear regression, $J(\theta) = \frac{1}{m} \sum_{i=1}^{m} \frac{1}{2} \left(h_\theta(x^{(i)}) - y^{(i)} \right)^2$. Define

$$\text{cost}(h_\theta(x), y) = \frac{1}{2} \left(h_\theta(x) - y \right)^2, \quad \text{for linear regression only}$$

so $J(\theta) = \frac{1}{m} \sum_{i=1}^{m} \text{cost}(h_\theta(x^{(i)}, y^{(i)})$.
- For log. regression, $J(\theta)$ is not convex, i.e. it has many local minima. Need a new cost function.
- For log. regression, $\text{cost}(h_\theta(x), y) = \begin{cases} -\log(h_\theta(x)) & \text{if } y = 1 \\ -\log(1 - h_\theta(x)) & \text{if } y = 0 \end{cases}$
- If $y = 1$, and $h_\theta(x) = 1$, the cost=0. As $h_\theta(x) \to 0$, cost $\to \infty$. Converse is also true for $y = 0$.
- Simplified Cost Function For Gradient Descent: Write out cost function in one equation

$$\text{cost}(h_\theta(x), y) = -y \log(h_\theta(x)) - (1 - y) \log(1 - h_\theta(x))$$

Plug into J.

$$J(\theta) = \frac{1}{m} \sum_{i=1}^{m} \left(-y^{(i)} \log \left(h_\theta(x^{(i)}) \right) - (1 - y^{(i)}) \log \left(1 - h_\theta(x) \right) \right)$$

Comes from "max likelihood estimation." Then find θ via $\min_\theta J(\theta)$. USe θ to make predictions $h_\theta(x) = 1/(1 + \exp(\theta^T x))$.
- Use g.d.: $\theta_j := \theta_j - \alpha \partial_{\theta_j} J(\theta)$. Computing the derivatives, we have

$$\theta_j := \theta_j - \alpha \sum_{i=1}^{m} \left(h_\theta(x^{(i)}) - y^{(i)} \right) x_j^{(i)},$$

which is the same as for linear regression, though h has a different meaning.

2-Oct-2020 Advanced Optimization, Multiclass Classification One-Vs.-All, Problem of Overfitting, Cost Function (Regularization), Reg. Lin. Regr., Reg. Log. Regr.

- Advanced Optimization; nothing new
- Multiclass Classification: One-vs.-all; e.g. weather: sunny, rainy, snowy, etc. $h_\theta^{(i)}(x) = P\left(y = i | \, x; \theta \right)$ represents the boundary separating class i from the rest.
- Quiz; $h_\theta(x) = g(\theta_0 + \theta_1 x + \theta_2 x)$. Let $\theta_0 = 6$, $\theta_1 = -1$, $\theta_2 = 0$. The argument, z, of g is positive. $z = 0 \implies x = 6$, and $z \geq 0 \implies x \leq 6$. So, for $y = 1$, $x \leq 6$.
- Problem of Overfitting; Underfit means high bias, overfit means high variance. Overfitting fails to generalize to new examples. To fix overfitting you can (i) reduce the number of examples, (ii) regularize to reduce the magnitude of the θ_i.
- Cost Function (Regularization); Add terms to the cost function such as $1000\theta_3^2$. This will force θ_3 down.
- But what if we don't know what features we want to be small? Do

$$J(\theta) = \frac{1}{2m} \left[\sum_{i=1}^{m} \left(h_\theta(x^{(i)}) - y^{(i)} \right)^2 + \underbrace{\lambda \sum_{i=1}^{m} \theta_j^2}_{\text{Regularization term}} \right],$$

where we do not penalize θ_0. If λ is too large, it underfits.

- Regularized Linear Regression; G.D. for lin. regr.:

$$\begin{aligned}\theta_j &:= \theta_j - \alpha\left[\frac{1}{m}\sum_{i=1}^{m}\left(h_\theta(x^{(i)}) - y^{(i)}\right)x^{(i)} + \frac{\lambda}{m}\theta_j\right] \\ &:= \theta_j\left(1 - \alpha\frac{\lambda}{m}\right) - \alpha\frac{1}{m}\sum_{i=1}^{m}\left(h_\theta(x^{(i)}) - y^{(i)}\right)x^{(i)},\end{aligned}$$

  where $1 - \alpha\lambda/m < 1$ which reduces θ_j.
- Normal equation becomes

$$\theta = \left(x^T x + \lambda\begin{bmatrix}0 & & & \\ & 1 & & \\ & & \ddots & \\ & & & 1\end{bmatrix}\right)^{-1} x^T y,$$

  and as long as $\lambda > 0$, the matrix will not be singular.
- Regularized Log. Regression; Cost function is

$$J(\theta) = -\frac{1}{m}\sum_{i=1}^{m}\left[y^{(i)}\log h_\theta(x^{(i)}) + (1-y^{(i)})\log\left(1 - h_\theta(x^{(i)})\right)\right] + \frac{\lambda}{2m}\sum_{i=1}^{m}\theta_j^2$$

- G.D. becomes (same cosmetically as for lin. regr.)

$$\theta_j\left(1 - \alpha\frac{\lambda}{m}\right) - \alpha\frac{1}{m}\sum_{i=1}^{m}\left(h_\theta(x^{(i)}) - y^{(i)}\right)x^{(i)}.$$

- Use `fminunc` (unc means unconstrained). For this, you need to give derivatives.

$$\begin{aligned}\frac{\partial}{\partial\theta_0}J(\theta) &= \frac{1}{m}\sum_{i=1}^{m}\left(h_\theta(x^{(i)}) - y^{(i)}\right)x_0^{(i)} \\ \frac{\partial}{\partial\theta_j}J(\theta) &= \frac{1}{m}\sum_{i=1}^{m}\left(h_\theta(x^{(i)}) - y^{(i)}\right)x_j^{(i)} + \frac{\lambda}{m}\theta_j\end{aligned}$$

6-Oct-2020 Neural Networks: Non-Linear Hypothesis, Neurons and the Brain

- e.g. identifying a car. Come up with a classification problem. Take images of a car and select two pixels. Take their intensity, and form an ordered pair $(I(p_1), I(p_2))$. Do this for cars and non-cars. Cars and non-cars will lie in different regions.
- If images were 50x50 pixels, $n = 2500$. (2500 pixels per image). This would make 3×10^6 quadratic features. So, log regression with quadratic features doesn't work.

7-Oct-2020 Model Representation I and II, Examples and Intutitions I and II

- Model Representation I; A neuron is a logistic unit. Input is $\{x_1, \ldots, x_n\} \to h_\theta(x) = g(\theta^T x)$ where $g(z) = (1 + \exp(-z))^{-1}$. Sigmoid activation function.
- We call x_0 the bias unit, and in neural networks, θ are called the weights. We call the inputs the "input layer", the last layer of neurons the "output layer," and the rest "hidden layers."
- $a_i^{(j)}$ is the activation of unit i in the layer j. $\Theta^{(j)}$ is the matrix of weights controlling the function mapping from layer j to layer $j+1$.
- cf. p. 20 of lecture 08.pdf for a detailed picture.
- If a network has s_j units in layer j and s_{j+1} units in layer $j+1$, then $\Theta^{(j)}$ is of dimension $s_{j+1} \times (s_j + 1)$.
- Model Representation II; Define $z_1^{(2)} = \Theta_{10}^{(1)}x_0 + \Theta_{11}^{(1)}x_1 + \Theta_{12}^{(1)}x_2 + \Theta_{13}^{(1)}x_3$ such that $a_1^{(s)} = g(z_1^{(2)})$

  Then let $z^{(2)} = \begin{bmatrix}z_1^{(2)} \\ z_2^{(2)} \\ z_3^{(2)}\end{bmatrix}$, $x = \begin{bmatrix}x_0 \\ x_1 \\ x_2 \\ x_3\end{bmatrix}$. Then, $z^{(2)} = \Theta^{(1)}x$ and $a^{(2)} = g(z^{(2)})$. (These last two are vectors, and g is applied element-wise. Here $\Theta^{(1)}$ is 3×4)

- cf. p. 23 of lecture 08.pdf. We may also call the input layer $a^{(1)}$. To add a bias for $a^{(3)}$, define $a_0^{(2)} = 1$. Thus $a^{(2)} \in \mathcal{R}^4$.
- This is forward propagation. In the example, on p. 23, imagine hiding the input layer. Then we have $a_1^{(2)}$, $a_2^{(2)}$, $a_3^{(2)}$ feeding to $a^{(3)}$.

$$\begin{aligned} a^{(3)} &= g(\Theta_{10}^{(2)} x_0 + \Theta_{11}^{(2)} x_1 + \Theta_{12}^{(2)} x_2 + \Theta_{13}^{(2)} x_3 \\ &= g(\theta_0 x_0 + \theta_1 x_1 + \theta_2 x_2 + \theta_3 x_3) \quad \text{drop some super/subscripts} \\ &= g(\theta^T x) \rightarrow \text{ just like log. regression.} \end{aligned}$$

  The difference comes in that it's not the straight inputs passed to the log regression. It's the "learned" features of the first layer.
- An architecture refers to how the networks are connected.
- Examples and Intutions I; x_1 NOR x_2 = NOT(x_1 XOR x_2). XOR is True if x_1 OR x_2 is True.
- cf. p. 34 of lecture 08.pdf for a n.n. implementation of AND, OR, and (NOT x_1) AND (NOT x_2)
- For a NOT, use a large negative weight on the neurons other than the bias.
- cf. p. 40-42 re: multiclass classification.

8-Oct-2020 Cost Function and Back Propagation, Backpropagation Algorithm

- Cost Function and Back Propagation; L = # of layers, s_l is # of units in layer l, excluding bias.
- Binary classification: $s_L = 1$, $h_\theta(x) \in \mathcal{R}$, $K = 1$ (i.e. a real number). $y = \{0, 1\}$.
  Multiclass classification: $s_L = K$, $h_\theta(x) \in \mathcal{R}^K$, $K \geq 3$, $y \in \mathcal{R}^K$ e.g. $\begin{bmatrix}1\\0\\0\\0\end{bmatrix}, \begin{bmatrix}0\\1\\0\\0\end{bmatrix}$, etc.
- For a n.n., $h_\theta(x) \in \mathcal{R}^K$, $[h_\theta(x)]_i = i^{th}$ output. The cost function is

$$\begin{aligned} J(\Theta) = -\frac{1}{m}\left[\sum_{i=1}^{m}\sum_{k=1}^{K} y_k^{(i)} \log\left(h_\Theta(x^{(i)})\right)_k + (1 - y_k^{(i)}) \log\left(1 - \left(h_\Theta(x^{(i)})\right)_k\right)\right] \\ + \frac{\lambda}{2m}\sum_{l=1}^{L-1}\sum_{i=1}^{s_l}\sum_{j=1}^{s_l+1}\left(\Theta_{ji}^{(l)}\right)^2. \end{aligned}$$

- Backpropagation Algorithm; Wish to get $\min_\Theta J(\Theta)$. Need $J(\Theta)$ and $\frac{\partial}{\partial \Theta_{ij}^{(l)}} J(\Theta)$ for all i, j, l.
- Suppose we have just one training example (x, y). See p.6 of lecture 09.pdf for forward propagation.
- δ_j^l represents the error of the j^{th} unit in the l^{th} layer.
  For the output layer, (cf. p. 7), $\delta_j^{(4)} = a_j^{(4)} - y_j = [h_\theta(x)]_j - y_j$. Vectorize this to have $\delta^{(4)} = a^{(4)} - y$.
- Look at $\delta^{(3)}$.

$$\delta^{(3)} = \left(\Theta^{(3)}\right)^T \delta^{(4)} \underbrace{.*}_{\text{element-wise}} g'\left(z^{(3)}\right),$$

  where g' is the derivative of the activation function. It can be shown that $g'(z^{(3)}) = a^{(3)} .* \left(1 - a^{(3)}\right)$. There is no $\delta^{(1)}$ since we assume there is no error to the input.
- We call this backpropagation since we start at the output layer and get $\delta^{(4)}$, and use it to get $\delta^{(3)}$, etc.
- Without regularization, we have

$$\frac{\partial}{\partial \Theta_{ij}^{(l)}} J(\Theta) = a_j^{(l)} \delta_i^{(l+1)}$$

- Now say the training set is $\{(x^{(1)}, y^{(1)}), \ldots, (x^{(m)}, y^{(,)})\}$. Let $\Delta_{ij}^{(l)} = 0$ for all i, j, l. Pseudocode:
- For i=1 to m:
  - $a^{(1)} = x^{(i)}$
  - Do forwards prop to get $a^{(l)}$ for $l = 2, \ldots, L$
  - Use $y^{(i)}$ to get $\delta^{(L)} = a^{(L)} - y^{(i)}$
  - Use back propagation to get $\delta^{(L-1)}, \ldots, \delta^{(2)}$
  - $\Delta_{ij}^{(l)} := \Delta_{ij}^{(l)} + a_j^{(l)} \delta_i^{(l+1)} \rightarrow$ vectorize: $\Delta^{(l)} := \Delta^{(l)} + \delta^{(l+1)} (a^{(l)})^T$

  Then, calculate

- $D_{ij}^{(l)} := \frac{1}{m}\Delta_{ij}^{(l)} + \lambda\Theta_{ij}^{(l)}$ if $j \neq 0$
- $D_{ij}^{(l)} := \frac{1}{m}\Delta_{ij}^{(l)}$ if $j = 0$

$$\implies \frac{\partial}{\partial\Theta_{ij}^{(l)}} J(\Theta) = D_{ij}^{(l)}$$

8-Oct-2020: Backpropagation Intutition, Implementation Note, Gradient Checking

- Backpropagation Intuition; Quiz: Suppose $\Theta_{11}^{(2)} = \Theta_{21}^{(2)} = 0$. After back propagation, what can you say about $\delta_1^{(3)}$? We know that $\delta_1^{(3)} = \Theta_{11}^{(3)}\delta_1^{(4)}$. So, there is insufficient information to tell.
- Implementation Note; Unrolling Parameters. In Octave, say `v` is a matrix. Then `v(:)` makes it a vector.
- Gradient Checking; Use symmetric difference. In 1-D

$$\frac{d}{d\theta} J(\theta) = \frac{J(\theta+\epsilon) - J(\theta-\epsilon)}{2\epsilon}.$$

  In N-D,

$$\frac{\partial}{\partial\theta_j} J(\theta) = \frac{J(\theta_1, \ldots, \theta_j + \epsilon, \ldots, \theta_n) - J(\theta_1, \ldots, \theta_j - \epsilon, \ldots, \theta_n)}{2\epsilon}$$

- Use this to compare to derivs we get from back-propagation. Don't use it for training! It will be very slow.