Coursera-Stanford-ML-Notes

Quentin Truong

20 June 2017 - ? July 2017

Contents

1 Week 1: Introduction

1.1 Overview

- Machine Learning: "A computer program is said to learn from experience E with respect to some class of tasks T and performance measure P, if its performance at tasks in T, as measured by P, improves with experience E."
- Supervised Learning: know what our correct output looks like
  - Regression: want continuous output
  - Classification: want discrete output
- Unsupervised Learning: little or no idea what our results should look like
  - Clustering: find groups according to similarity in various variables
  - Nonclustering: find structure in chaos

2 Week 2: Linear Regression with Multiple Variables

2.1 Overview

- Use linear regression for continuous output
- Choose gradient descent if many features (million+) because the inverse matrix required for the normal equation can become expensive to compute
- Normal equation will directly compute theta
- Normalize features if using gradient descent

2.2 Notation

$$
\begin{aligned}
m &= number\ of\ samples \\
n &= number\ of\ feature \\
x &= (n \times 1) \\
X &= (m \times n) \\
X_j &= (m \times 1) \\
\theta &= (n \times 1) \\
\theta_j &= (1 \times 1)
\end{aligned}
$$

2.3 Gradient Descent

$$
\begin{aligned}
\text{Hypothesis Function} \qquad & h_\theta(x) = \theta^\intercal \times x \\
\text{Vectorized Hypothesis Function} \qquad & h_\theta(X) = X \cdot \theta \\
\text{Linear Regression Cost Function} \qquad & J(\theta) = \frac{1}{2m} \sum (h_\theta(X) - y)^2 \\
\text{Derivative of Linear Regression CF wrt } \theta_j \qquad & \frac{\partial}{\partial \theta_j} J(\theta) = \frac{1}{m} \sum (h_\theta(X) - y) \ .* X_j \\
\text{Change in } \theta_j \qquad & \theta_j = \theta_j - \alpha \frac{\partial}{\partial \theta_j} \\
& \quad = \theta_j - \alpha \frac{1}{m} \sum (h_\theta(X) - y) \ .* X_j \\
\text{Vectorized Change in } \theta \qquad & \theta = \theta - \alpha \frac{1}{m} X^\intercal (X \cdot \theta - y)
\end{aligned}
$$

2.4 Normal Equation

$$
\theta = (X^\intercal \cdot X)^{-1} \cdot X^\intercal \cdot y
$$

3 Week 3: Logistic Regression

3.1 Overview

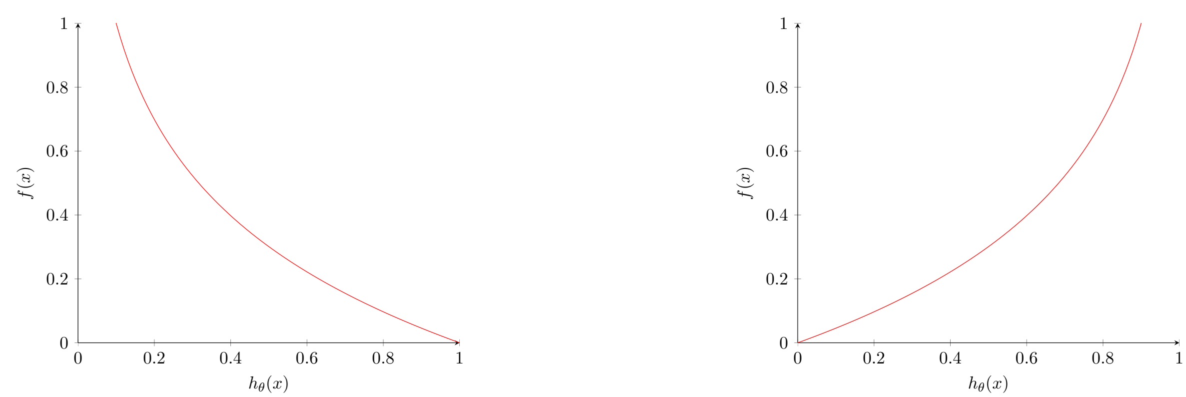
- Use logistic regression for discrete output (classification)
  - $h_\theta(x) = (y = 1|x; \theta)$; gives probability that the output is 1 given x
  - Sigmoid/Logistic function maps any real number to (0, 1)
  - Logarithm turns sum into product, allowing easier differentiation without altering search space
- For multi-class classification, use one-vs-all
  - Pick class i that maximizes $h_\theta^i(x)$
- Overfitting is when learned hypothesis fits training data well but fails to generalize; underfitting is when doesn't fit training data
- Address overfitting by reducing number of features, model selection, and regularization
  - Regularization results in simpler hypothesis and less overfitting
  - Extremely large λ will result in underfitting and gradient descent will fail to converge
  - Do not regularize λ_0
- Use other prewritten optimization algorithims (conjugate gradient, BFGS, L-BFGS) because they are faster

3.2 Logistic Regression Hypothesis Function

$$\begin{aligned} &\text{Sigmoid/Logistic Function} & g(z) &= \frac{1}{1+e^{-z}} \\ &\text{Hypothesis Function} & h_\theta(x) &= g(\theta^\intercal x) \\ & & &= \frac{1}{1+e^{-\theta^\intercal x}} \end{aligned}$$

3.3 Logistic Regression Cost Function

$$\begin{aligned} Cost(h_\theta(x), y) &= \begin{cases} -\log(h_\theta(x)) \text{ if y} = 1 \\ -\log(1-h_\theta(x)) \text{ if y} = 0 \end{cases} \\ &= -y\log(h_\theta(x)) - (1-y)\log(1-h_\theta(x)) \\ J(\theta) &= \frac{1}{m}\sum_{i=1}^{m}\text{Cost}(h_\theta(x^i), y^i) \\ J(\theta) &= \frac{-1}{m}\sum_{i=1}^{m}\left[y^i\log(h_\theta(x^i)) + (1-y^i)\log(1-h_\theta(x^i))\right] \end{aligned}$$



(a) if y=1

(b) if y=0

3.4 Proof of Logistic Regression Cost Function Derivative

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

Credit[1]

[1] https://math.stackexchange.com/questions/477207/derivative-of-cost-function-for-logistic-regression

3.5 Regularization

Regularizing Term	$\lambda \sum_{j=1}^{n} \theta_j^2$
Regularized Linear Regression CF	$J(\theta) = \frac{1}{2m} \sum_{i=1}^{m} (h_\theta(x^i) - y^i)^2 + \lambda \sum_{j=1}^{n} \theta_j^2$
Regularized Logistic Regression CF	$J(\theta) = \frac{-1}{m} \sum_{i=1}^{m} \left[y^i \log(h_\theta(x^i)) + (1 - y^i) \log(1 - h_\theta(x^i)) \right] + \frac{\lambda}{2m} \sum_{j=1}^{n} \theta_j^2$
Regularized GD (Lin/Log Regression)	$\begin{cases} \theta_0 = \theta_j - \alpha \left[\frac{1}{m} \sum_{i=1}^{m} (h_\theta(x^i) - y^i) x_0^i \right] \\ \theta_j = \theta_j - \alpha \left[\frac{1}{m} \sum_{i=1}^{m} (h_\theta(x^i) - y^i) x_j^i + \frac{\lambda}{m} \theta_j \right] \text{ (j=1,2,...,n)} \end{cases}$
Regularized Normal Equation	$\theta = (X^\intercal X + \lambda \begin{bmatrix} 0 & 0 & \cdots & 0 \\ 0 & 1 & \cdots & 0 \\ \vdots & \vdots & \ddots & \vdots \\ 0 & 0 & \cdots & 1 \end{bmatrix}_{n+1,n+1})^{-1} X^\intercal y$

4 Week 4: Artificial Neural Networks Representation

4.1 Overview

- Neural networks allow for non-linear classification in situations with many features
  - Necessary b/c 100 features at 3rd level polynomials generates 170k features, which quickly becomes intractable
  - "One learning algorithm" hypothesis; you can see with your tongue : brain learns using one algorithm, not thousands of different programs
  - Can have multiple hidden layers
  - Can have multiple outputs (one-vs-all for multi-class classification)
  - If network has s_j units in layer j and s_{j+1} units in layer $j+1$, then Θ^j will be of dimension $s_{j+1} \times s_j + 1$
    - The +1 comes from the addition in $\Theta^{(j)}$ of the bias node, x_0 and $\Theta_0^{(j)}$
- Forward Propogation is used to predict based on learned parameters
- Bias node gives each node a trainable constant value
  - Allows bias weight to shift the activation curve left/right
  - Other weights affect steepness
- Fun fact: For image recognition, particular order of pixels does not matter for ANN (but does for humans), you just need to keep the convention the same

4.2 Notation

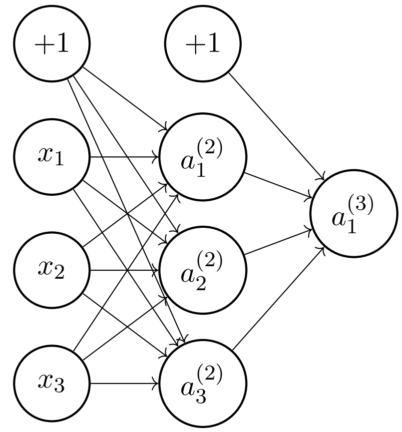
- $g(x)$: sigmoid function
- $\Theta^{(j)}$: matrix of weights controlling function mapping from layer j to layer j+1; each layer gets own Θ^j
- $\Theta_{j,0}, ..., \Theta_{j,n}$ weights corresponding to the inputs $a_0, ..., a_n$ going into z_j
- $w_{0,j}, ..., w_{n,j}$ weights corresponding to the inputs $a_0, ..., a_n$ going into z_j
- $z_k^{(j)}$: encompasses parameters inside of g function
- $a_i^{(j)}$: "activation" of unit i in layer j

4.3 Equations

$$\begin{aligned}
z_k^{(j)} &= \Theta_{k,0}^{(j-1)} x_0 + \Theta_{k,1}^{(j-1)} x_1 + ... + \Theta_{k,n}^{(j-1)} x_n \\
&= \Theta_{k,0}^{(j-1)} a_0^{(j-1)} + \Theta_{k,1}^{(j-1)} a_1^{(j-1)} + ... + \Theta_{k,n}^{(j-1)} a_n^{(j-1)} \\
z^{(j)} &= \Theta^{(j-1)} a^{(j-1)} \\
a^{(j)} &= g(z^{(j)})
\end{aligned}$$

4.4 Sample Three Layer System

$$\begin{bmatrix} x_0 \\ x_1 \\ x_2 \\ x_3 \end{bmatrix} \rightarrow \begin{bmatrix} a_1^{(2)} \\ a_2^{(2)} \\ a_3^{(2)} \end{bmatrix} \rightarrow h_\Theta(x)$$



$$\begin{aligned}
a_1^{(2)} &= g(\Theta_{1,0}^{(1)} x_0 + \Theta_{1,1}^{(1)} x_1 + \Theta_{1,2}^{(1)} x_2 + \Theta_{1,3}^{(1)} x_3) \\
a_2^{(2)} &= g(\Theta_{2,0}^{(1)} x_0 + \Theta_{2,1}^{(1)} x_1 + \Theta_{2,2}^{(1)} x_2 + \Theta_{2,3}^{(1)} x_3) \\
a_3^{(2)} &= g(\Theta_{3,0}^{(1)} x_0 + \Theta_{3,1}^{(1)} x_1 + \Theta_{3,2}^{(1)} x_2 + \Theta_{3,3}^{(1)} x_3) \\
h_\Theta(x) &= g(\Theta_{1,0}^{(2)} a_0^{(2)} + \Theta_{1,1}^{(2)} a_1^{(2)} + \Theta_{1,2}^{(2)} a_2^{(2)} + \Theta_{1,3}^{(2)} a_3^{(2)}) \\
&= g(z^3) \\
&= a_1^{(3)}
\end{aligned}$$

5 Week 5: Artificial Neural Network Learning

5.1 Notation

– L : total number of layers in the network
– s_l : number of units (not counting bias unit) in layer l
– K : number of output units/classes
– $h_\Theta(x)_k$: hypothesis that results in the kth output
– δ_k : Error signal

5.2 Cost Function

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

Picking training example	$\sum_{i=1}^{m}$
Picking output node	$\sum_{k=1}^{K}$
Picking layer	$\sum_{l=1}^{L-1}$
Picking node	$\sum_{i=1}^{s_l}$
Picking Θ	$\sum_{j=1}^{s_{l+1}}$

5.3 Backpropagation Algorithm

1. Set $a(1) := x(t)$
2. Perform forward propagation to compute $a(l)$ for $l = 2, 3, , L$
3. Using $y^{(t)}$, compute $\delta^L = a^{(L)} - y^{(t)}$
4. Compute $\delta^{(L-1)}, \delta^{(L-2)}, \ldots, \delta^{(2)}$ using $\delta^{(l)} = ((\Theta^{(l)})^T\delta^{(l+1)})\ .*\ a^{(l)}\ .*\ (1-a^{(l)})$
5. $\Delta_{i,j}^{(l)} := \Delta_{i,j}^{(l)} + a_j^{(l)}\delta_i^{(l+1)}$ or with vectorization $\Delta^{(l)} := \Delta^{(l)} + \delta^{(l+1)}(a^{(l)})^\intercal$
6. $\frac{\partial}{\partial\Theta_{ij}^{(l)}}J(\Theta) = D_{ij}^{(l)}$ where $\begin{cases} D_{i,j}^{(l)} := \frac{1}{m}\Delta_{i,j}^{(l)} \text{ (j = 0)} \\ D_{i,j}^{(l)} := \frac{1}{m}\left(\Delta_{i,j}^{(l)} + \lambda\Theta_{i,j}^{(l)}\right) \text{ (j} \neq \text{0)} \end{cases}$

5.4 Backpropagation Derivation - Base Case

$$\frac{\partial C}{\partial w_{ij}} = \frac{\partial C}{\partial z_j}\frac{\partial z_j}{\partial w_{ij}} \qquad \text{Cost } C \text{ varies wrt input accumulator } z_j,\ z_j \text{ varies wrt } w_{ij} \text{ (Chain Rule)}$$

$$\frac{\partial C}{\partial z_j} = \frac{\partial}{\partial z_j}(y_j - a_j)^2 \qquad \text{Cost defined as } (y_j - a_j)^2$$

$$= \frac{\partial}{\partial z_j}(y_j - g(z_j))^2$$

$$= -2(y_j - g(z_j))g'(z_j)$$

$$g'(z_j) = \frac{d}{dz_j}\frac{1}{1+e^{-z_j}} \qquad \text{Derivative of logistic function}$$

$$= \frac{1}{1+e^{-z_j}}\frac{e^{-z_j}}{1+e^{-z_j}}$$

$$= g(z_j)(1 - g(z_j))$$

$$\frac{\partial C}{\partial z_j} = -2(y_j - g(z_j))g(z_j)(1 - g(z_j))$$

$$= -2(y_j - a_j)a_j(1 - a_j)$$

$$\frac{\partial z_j}{\partial w_{ij}} = \frac{\partial}{\partial w_{ij}}\sum_q a_q w_{q,j} \qquad \text{Definition of } z_j \text{ as sum of previous node's inputs and their weights}$$

$$= a_i$$

$$\frac{\partial C}{\partial w_{ij}} = -2(y_j - a_j)a_j(1 - a_j)(a_i)$$

$$= -\Delta_j a_i$$

5.5 Backpropagation Derivation - Recursive Case

$$\frac{\partial C}{\partial w_{i,j}} = \sum_k \left(\frac{\partial C}{\partial z_k}\frac{\partial z_k}{\partial a_j}\frac{\partial a_j}{\partial z_j}\frac{\partial z_j}{\partial w_{i,j}}\right) \qquad C \text{ depends on } z_k,\ z_k \text{ depends on } a_j,\ a_j \text{ depends on } z_j,\ z_j \text{ depends on } w_{i.j}$$

$$\frac{\partial C}{\partial z_k} = -\Delta_k$$

$$\frac{\partial z_k}{\partial a_j} = \frac{\partial}{\partial a_j}\sum_s a_s w_{s,k}$$

$$= w_{j,k}$$

$$\frac{\partial a_j}{\partial z_j} = \frac{\partial}{\partial z_j}g(z_j)$$

$$= g(z_j)(1 - g(z_j))$$

$$= a_j(1 - a_j)$$

$$\frac{\partial z_j}{\partial w_{i,j}} = \frac{\partial}{\partial w_{i,j}}\sum_q a_q w_{q,j}$$

$$= a_i$$

$$\frac{\partial C}{\partial w_{i,j}} = \sum_k (-\Delta_k w_{j,k} a_j (1 - a_j) a_i)$$

$$= \sum_k (-\Delta_k w_{j,k}) a_j (1 - a_j) a_i$$

$$= -\Delta_j a_i$$

Credit [2] [3] [4]

5.6 Backpropagation Intuition

δ_k is the error signal from the output

$$\delta_k = (a_k - t_k) g'_k(z_k)$$

so, error wrt output weights is

$$\frac{\partial E}{\partial w_{j,k}} = \delta_k a_j$$

similarly, error wrt internal weights is

$$\frac{\partial E}{\partial w_{i,j}} = \delta_j a_i$$

the error is determined by following layer's error, so it may also be understood as

$$\frac{\partial E}{\partial w_{i,j}} = g'_j(z_j) \sum_k (\delta_k w_{j,k}) a_i$$

5.7 Gradient Checking

- Gradient checking ensures that backpropagation is actually working
  - Turn off gradient checking once backpropagation is verified to work
- Approximate the derivative of cost function using slope
  - Pick $\epsilon = 10^{-4}$
  - Check all Θ_j

$$\frac{\partial}{\partial \Theta_j} J(\Theta) \approx \frac{J(\Theta_1, \ldots, \Theta_j + \epsilon, \ldots, \Theta_n) - J(\Theta_1, \ldots, \Theta_j - \epsilon, \ldots, \Theta_n)}{2\epsilon}$$

5.8 Random Initialization

- Need Symmetry Breaking
  - All hidden units would receive the same signal and the same updates
  - Results in finding only one feature, redundantly copied many times over
- Fixed by randomly initializing each $\Theta_{ij}^{(l)}$ to a value in $[-\epsilon, \epsilon]$
  - A good choice of ϵ init is $\epsilon = \frac{\sqrt{6}}{\sqrt{L_{in} + L_{out}}}$, where $L_{in} = s_l$ and $L_{out} = s_{l+1}$, the number of units in the layers adjacent to $\Theta^{(l)}$

[2] https://pdfs.semanticscholar.org/69c2/814c7f8ca16aa836fd32e3c4975f8208e63f.pdf
[3] https://stats.stackexchange.com/questions/94387/how-to-derive-errors-in-neural-network-with-the-backpropagation-algorithm
[4] https://theclevermachine.wordpress.com/2014/09/06/derivation-error-backpropagation-gradient-descent-for-neural-networks/

6 Week 6: Advice for Machine Learning

6.1 Overview

– Training set: 60%
– Cross validation set: 20%
– Test set: 20%
– Randomize your data and plot learning curves to determine high/low variance

6.2 Evauating Hypothesis

$$\text{Linear regression} \qquad J_{test}(\Theta) = \frac{1}{2m_{test}} \sum_{i=1}^{m_{test}} (h_\Theta(x^{(i)}_{test}) - y^{(i)}_{test})^2$$

$$\text{Classification} \qquad err(h_\Theta(x), y) = \begin{cases} 1 \text{ if } h_\Theta(x) \geq 0.5 \text{ and } y = 0 \\ 1 \text{ if } h_\Theta(x) < 0.5 \text{ and } y = 1 \\ 0 \text{ otherwise} \end{cases}$$

$$\text{Test Error} \qquad = \frac{1}{m_{test}} \sum_{i=1}^{m_{test}} err(h_\Theta(x^{(i)}_{test}), y^{(i)}_{test})$$

6.3 Bias, Variance, Learning Curves

– High variance is when overfitting data
  - Get more training examples, try a smaller set of features, increase lambda
– High bias is when underfitting data
  - Add features, add polynomial features, decrease lambda
– Small neural networks are more prone to underfitting and are cheaper
– Large neural networks are more prone to overfitting and are more expensive