Machine Learning: Logistic Regression

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Classification

- Is a discrete categorization of an output variable, e.g. $y \in \{0, 1\}$
  - Can also have multiple classes, so some set $S \mid \text{len}(S) > 2$
- Linear regression -> threshold classifier output
  - E.g. if $h_\theta(x) \geq 0.5$ do $y = 1$ else $y = 0$
  - However is not effective when there are > 2 clusters -> DNU
- Classification - $y = 0$ or $y = 1$
  - $0 \leq h_\theta(x) \leq 1$
  - Binary classification
- bruh
  -

Hypothesis Representation

- Need $0 \leq h_\theta(x) \leq 1$
- $h\theta_0(x) = g(\theta^T x)$ where $g = \frac{1}{1+e^{-z}}$ is the sigmoid = logistical function and $z = \theta^T x$
  - $h_\theta(x) = \frac{1}{1+e^{-\theta^T x}}$
- Interpretation
  - $h_\theta(x)$ is estimated probability that $y = 1$ on input x
  - $h_\theta(x) = P(y = 1|x;\theta)$ is probability of $y = 1$ given x parameterized by θ
    * Due to total sum probability -> $P(y = 0|x;\theta) = 1 - P(y = 1|x;\theta)$

Decision Boundary

- Prediction boundary - If $h_\theta(x) \geq 0.5$ do $y = 1$ else $y = 0$
  - Thus $y = 0 \implies \theta^T x < 0$ and $y = 1 \implies \theta^T x \geq 0$
  - Graph the equation $\theta_0 + \theta_1 x_1 + ... + \theta_n x_n \geq 0$ (higher order planes of $\mathbb{R}^{n+1}$)
- Nonlinear decision boundaries
  - Have polynomial terms in features
  - Ex. $-1 + x_1^2 + x_2^2 \geq 0 \implies$ unit circle

Logistic cost function

$$\boxed{J(\theta) = \frac{1}{m} \sum_{i=1}^{m} \text{Cost}\left(h_\theta\left(x^{(i)}\right), y^{(i)}\right)}$$

- Setup/prime
  - Training set $S = \left\{\left(x^{(1)}, y^{(1)}\right), \left(x^{(2)}, y^{(2)}\right), \cdots, \left(x^{(m)}, y^{(m)}\right)\right\}$
    * m examples

    - A feature vector $x \in \begin{bmatrix} x_0 \\ x_1 \\ \vdots \\ x_n \end{bmatrix}$
    - $h_\theta(x) = \frac{1}{1+e^{-\theta^T x}}$
- $\text{Cost}\left(h_\theta\left(x\right), y\right) = \frac{1}{2}\left(h_\theta\left(x\right) - y\right)^2$
    - Is non-convex - many local extrema which may hinder gradient descent
- Cost function for logistic regression

$$\boxed{\text{Cost}\left(h_\theta(x), y\right) = \begin{cases} -\log\left(h_\theta(x)\right) \text{ if } y = 1 \\ -\log\left(1 - h_\theta(x)\right) \text{ if } y = 0 \end{cases}}$$

- Cost function behavior
    - Cost is 0 if $y = 1, h_\theta(x) = 1$
    - As $h_\theta(x) \to 0$, Cost $\to \infty$
    - If $h_\theta(x) = 0$ **but** $y = 1$, then learning algorithm penalized heavily

Simplified Cost Function

- Can rewrite cost function to be $\boxed{\text{Cost}(h_\theta(x), y) = -y\log(h_\theta(x)) - (1-y)\log(1-h_\theta(x))}$
    - Vectorized - $J(\theta) = \frac{1}{m} \cdot \left(-y^T\log(h) - (1-y)^T\log(1-h)\right)$ where $h = g(X\theta)$
- Gradient descent algorithm
    - Simultaneous update and iterate $\theta_j := \theta_j - \alpha\sum_{i=1}^{m}\left(h_\theta\left(x^{(i)}\right) - y^{(i)}\right)x_j^{(i)}$
    - Vectorized - $\theta := \theta - \frac{\alpha}{m}X^T(g(X\theta) - \vec{y})$

Advanced optimization

- Optimization algorithm -> minimize $J(\theta)$
    - Need to compute $J(\theta)$ and $\frac{\partial}{\partial\theta_j}J(\theta)$
- Algorithms
    - Gradient descent
    - Conjugate gradient
    - BFGS
    - L-BFGS
    - Do not need to manually pick α for last 3 -> but more complex
- Use `fminunc` in Octave

```
options = optimset('GradObj', 'on', 'MaxIter', 100);
initialTheta = zeros(2,1);
[optTheta, functionVal, exitFlag] = fminunc(@costFunction, initialTheta, options);
```

- Function for cost function
    - `function [jVal, gradient] = costFunction(theta)`
    - Must return $J(\theta)$ and gradient

Multiclass Classification with Logistic Regression

- One-vs-all classification
    - Combine remaining classes to 1 class and compare with another -> multiple binary classifications
    - Train a logistic regression classifier $h_\theta^{(i)}(x)$ for each class i to predict probability that $y = i$
    - Pick class that maximizes h -> $\max_i h_\theta^{(i)}(x)$

Overfitting

- Underfitting - high **bias**
  - Straight line fit - biased to linear trend
  - Too little features - n is small
- Overfitting - high **variance**
  - Space of possible hypothesis too large, can't find a good hypothesis
  - Too many features - n too large
    - Cannot generalize well to new examples
- Addressing overfitting
  - Reduce n - select necessary ones and model a selection algorithm
  - Regularization - keep features but reduce magnitude of values in θ
    - Works well with lots of features

Regularization cost function

- Small values for parameters θ_j for $j \in [0, n]$
  - Simpler hypothesis
  - Less prone to overfitting
- Modify cost function to shrink parameters

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

- Convention - only regularize $\theta_1, \ldots, \theta_n$ and ignore θ_0
- Regularization parameter λ controls tradeoff of small parameters and well-fitting
  - Therefore prevents overfitting
  - A large value highly reduces $\theta \to \vec{0}$ so $h_\theta(x) = \theta_0$ so a horizontal line is fitted
  - Important to choose

Regularized Linear Regression

- Gradient descent - separate terms in algorithm

```
Repeat
$\theta_0 := \theta_0 - \alpha\frac{1}{m}\sum_{i=1}^{m}\left(h_\theta\left(x^{(i)}\right) - y^{(i)}\right)x_0^{(i)}$
$\theta_j := \theta_j - \alpha\left[\left(\frac{1}{m}\sum_{i=1}^{m}\left(h_\theta\left(x^{(i)}\right) - y^{(i)}\right)x_j^{(i)}\right) + \frac{\lambda}{m}\theta_j\right]$
```

- Update rule can be expressed as $\theta_j := \theta_j\left(1 - \alpha\frac{\lambda}{m}\right) - \alpha\frac{1}{m}\sum_{i=1}^{m}\left(h_\theta\left(x^{(i)}\right) - y^{(i)}\right)x_j^{(i)}$
  - Term $1 - \alpha\frac{1}{m} < 1$ always so it reduces θ_j by some amount each update
  - Keeps 2nd term same as previously
- Normal equation

$$\theta = \left(X^TX + \lambda\begin{bmatrix} 0 & & & & \\ & 1 & & & \\ & & 1 & & \\ & & & \ddots & \\ & & & & 1 \end{bmatrix}\right)^{-1} X^Ty$$

- Matrix L near λ is $n + 1 \times n + 1$
  - Due to 0 as first element
- Given $\lambda > 0$

- If $m \leq n$ then $X^T X$ is noninvertible
  - Adding term λL makes $X^T X + \lambda L$ invertible

Regularized Logistic Regression

- Logistic growth prone to overfitting with many features (high n)
- Modify to use regularization
  - Add term $\frac{\lambda}{2m} \sum_{j=1}^{n} \theta_j^2$
- Treat θ_0 separately

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

- Advanced optimization method
  - Octave has 1-indexed vectors

```
function [jval, gradient] = costFunction(theta)
  jval = [code to get J(theta)]
  gradient(1) = [partial respect to theta_0]
  .
  .
  .
  gradient(n + 1) = [partial with respect to theta_n]
```