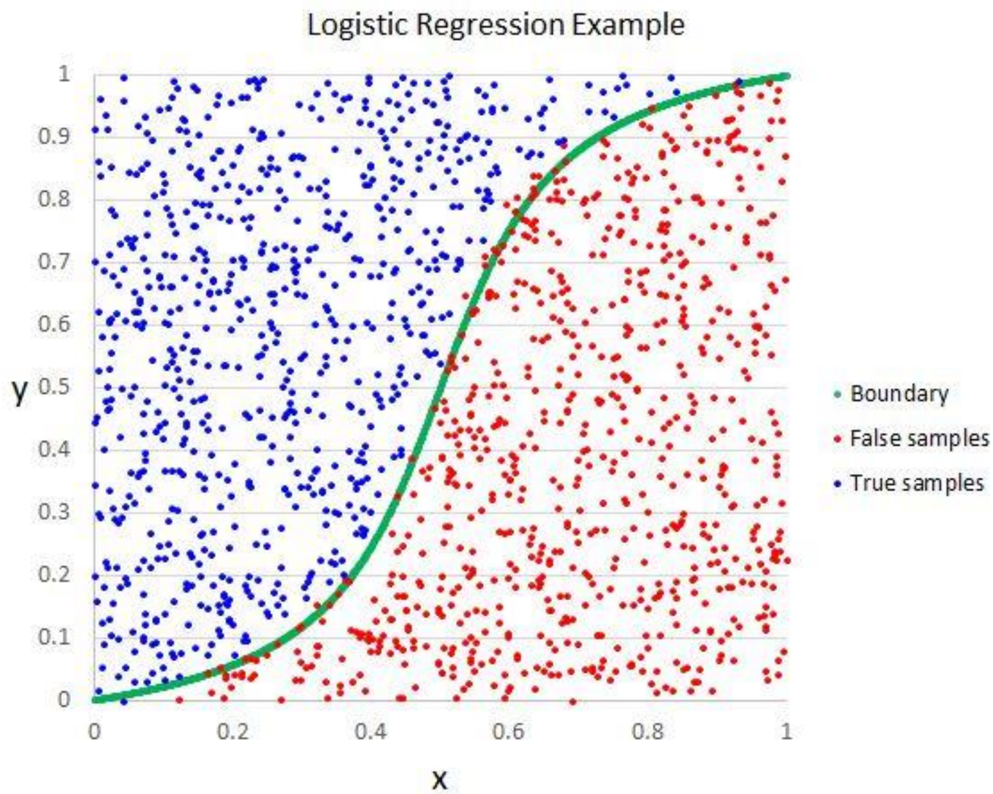
Logistic Regression (Logit)



Summary: Logistic regression is used in a classification problem. For example: determine whether a tumor is benign or malignant. The output of the classifier is a value 0 or 1 (for a binary classification problem). That means:

$$y \in \{0,1\}$$

$$0\text{: “negative class” (i.e. benign tumor)}$$

$$1\text{: “positive class” (i.e. malignant tumor)}$$

If $y \in \{0,1,2,\dots\}$, we call this a multi-class classification problem. In classification problem, the output should be either 0 or 1 (for binary classification problem). It should not output value $0 \le h(x) \le 1$.

1. Notation

- m: number of training examples
- n: number of features
- x: input variable
- y: output variable
- $x^{(i)}$: input features of i^{th} training example
- $x_j^{(i)}$: value of feature j in i^{th} training example
- $y^{(i)}$: output of i^{th} training example
- $(x^{(i)}, y^{(i)})$: i^{th} training example

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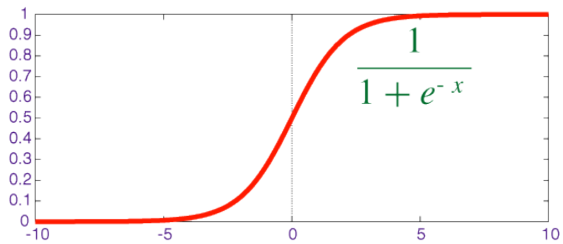
2. Hypothesis

$$h_\theta(x) = g(\theta^T x)$$

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

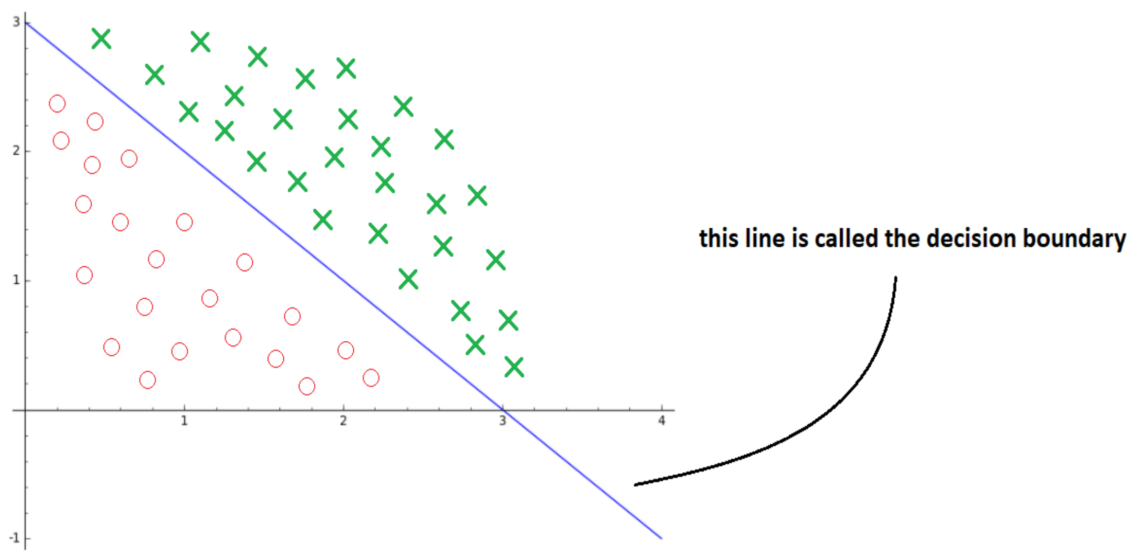
- The function $g(x)$ is called a sigmoid function.



- **Interpretation of the output of the hypothesis function:**
  - $h_\theta(x)$ is the estimated probability that $y = 1$ on input x
  - Example:
    - If $x = \begin{bmatrix} x_0 \\ x_1 \end{bmatrix} = \begin{bmatrix} 1 \\ tumorSize \end{bmatrix}$ $and\ h_\theta(x) = 0.7$
    - It tells the patient that there is a 70% chance the tumor is malignant
  - $h_\theta(x) = P(y = 1|x; \theta)$ → The probability that $y = 1$, given x, parameterized by θ.

3. Decision Boundary

- Consider this graph below:



- We have the decision boundary of the form $x_1 + x_2 = 3$ and the hypothesis $h_\theta = g(\theta_0 + \theta_1 x_1 + \theta_2 x_2)$. That means this graphs is predicting "$y = 1$" if $-3 + x_1 + x_2 \geq 0$

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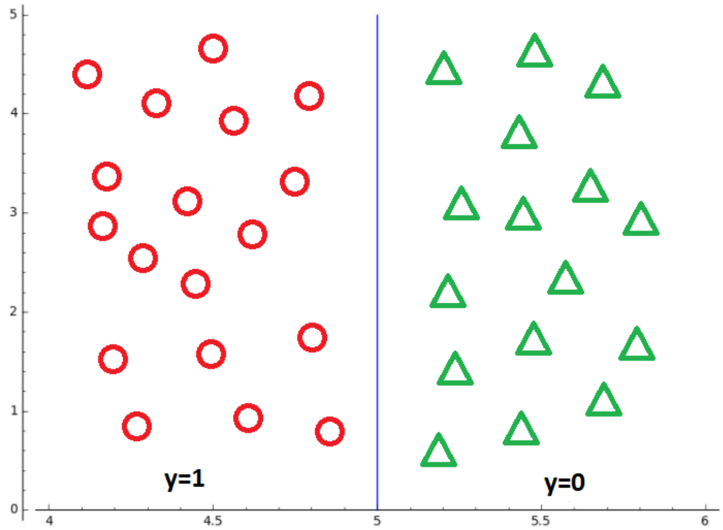
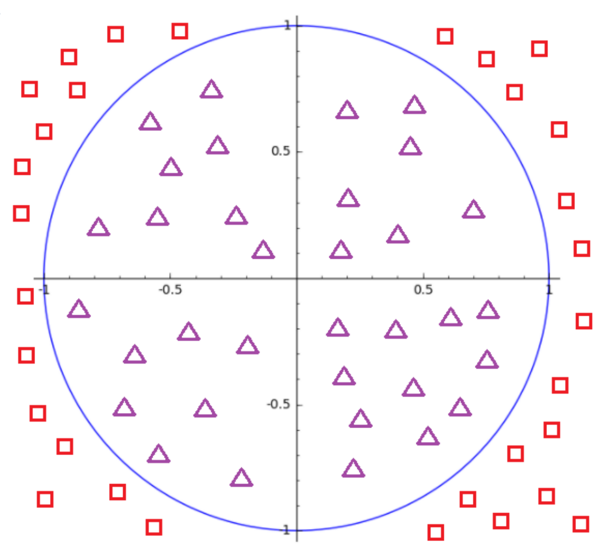
- Some other examples:



$$h_\theta(x) = g(5 - x_1)$$

$$\theta^T x = 5 - x_1$$

$$\rightarrow \begin{cases} x_1 \leq 5: \ y = 1 \\ x_1 > 5: \ y = 0 \end{cases}$$



$$h_\theta(x) = g(x_1^2 + x_2^2 - 1)$$

$$\theta^T x = x_1^2 + x_2^2 - 1$$

$$\rightarrow \begin{cases} x_1^2 + x_2^2 \geq 1: \ y = 1 \\ x_1^2 + x_2^2 < 1: \ y = 0 \end{cases}$$

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4. <u>Cost Function</u>

- Given a training set: $\{(x^{(1)}, y^{(1)}), (x^{(2)}, y^{(2)}), \ldots, (x^{(m)}, y^{(m)})\}$ with m examples and:

$$x \in \begin{bmatrix} x_0 \\ \vdots \\ x_n \end{bmatrix} \in \mathbb{R}^{n+1}, x_0 = 1$$

$$y \in \{0,1\}$$

$$h_\theta(x) = \frac{1}{1 + e^{\theta^T x}}$$

- Consider the cost function $J(\theta)$ in linear regression:

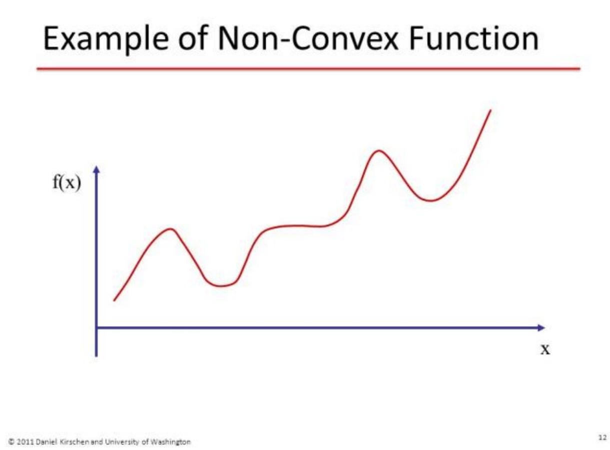
$$J(\theta) = \frac{1}{2m}\sum_{i=1}^{m}\left(h_\theta\left(x^{(i)}\right) - y^{(i)}\right)^2$$

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

$$= \frac{1}{m}\sum_{i=1}^{m} cost(h_\theta(x), y)$$

$$\rightarrow cost(h_\theta(x), y) = \frac{1}{2}(h_\theta(x) - y)^2$$

- If we apply the cost function from simple linear regression to logistic regression, it would result in a non-convex function.



- Therefore, we need to come up with a new cost function.

$$\mathrm{cost}(\mathrm{h}_\theta(x), y) = \begin{cases} -\log\left(h_\theta(x)\right) & if\ y = 1 \\ -\log\left(1 - h_\theta(x)\right) & if\ y = 0 \end{cases}$$

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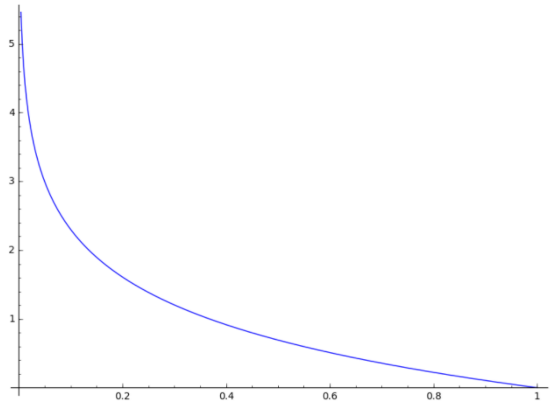
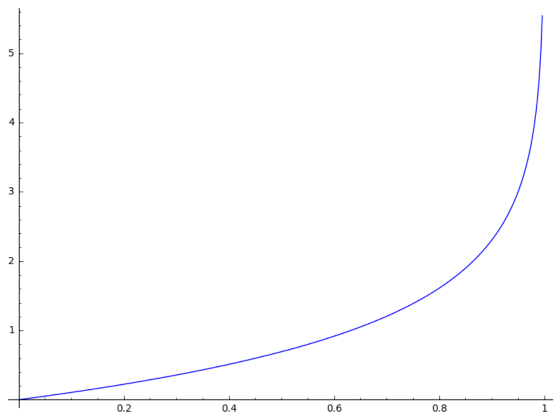


When $y = 1$:

- $if\ h_\theta(x) = 1, cost = 0$
- As $h_\theta(x) \to 0, cost \to \infty$



When $y = 0$:

- $if\ h_\theta(x) = 0, cost = 0$

As $h_\theta(x) \to 1, cost \to \infty$

- We can re-write the function above as following:

$$cost(h_\theta(x), y) = -y\log\big(h_\theta(x)\big) - (1-y)\log\big(1-h_\theta(x)\big)$$

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

- To fit parameters θ, we need to minimize $J(\theta)$
- To make a prediction on a new input x:

$$output\ h_\theta(x) = P(y=1|x;\theta) = \frac{1}{1+e^{-\theta^T x}}$$

5. Gradient Descent Algorithm

- We have:

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

$$\to \frac{\partial J}{\partial \theta_j} = \frac{1}{m}\sum_{i=1}^{m}\left(h_\theta\left(x^{(i)}\right) - y^{(i)}\right)x_j^{(i)} \qquad for\ j = 0 \ldots n$$

- We then have the gradient descent algorithm as follow:

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Repeat {

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

}

6. Vectorized Implementation

- A strategy to optimize gradient descent:

$$\theta := \theta - \frac{\alpha}{m}X^T\left(g(X\theta) - Y\right)$$

$$\theta \in \mathbb{R}^{n+1} \qquad Y \in \mathbb{R}^m$$

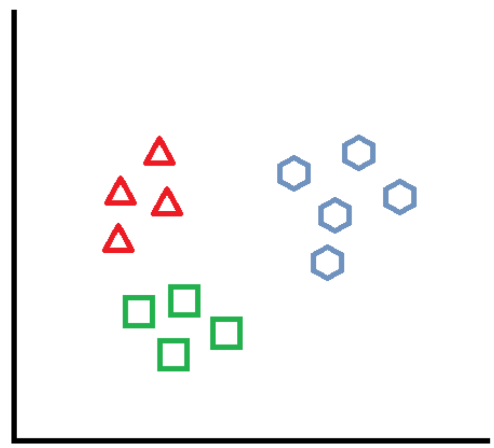
$$X \in M_{m\times(n+1)} \quad \rightarrow \quad X^T \in M_{(n+1)\times m}$$

7. Optimization Algorithm

- Some available optimization algorithms:
  - Gradient descent
  - Conjugate gradient
  - BFGS
  - L-BFGS
- Advantages of the last 3 algorithms:
  - No need to manually pick learning rate α. They automatically pick the best learning rate for each iteration
  - Often faster than gradient descent
- Disadvantages:
  - More complex

8. Multiclass Classification

- Examples:
  - Email foldering/tagging: work, friends, family, etc
  - Weather: sunny, cloudy, rain, snow



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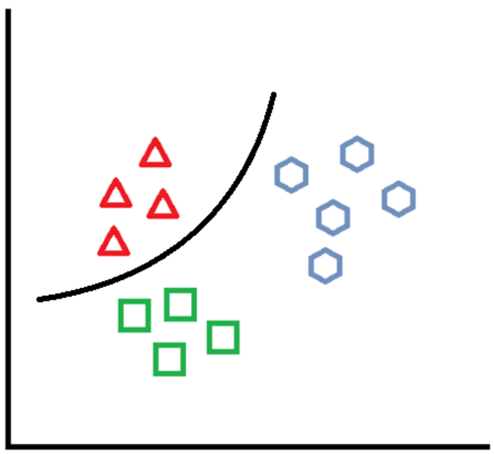
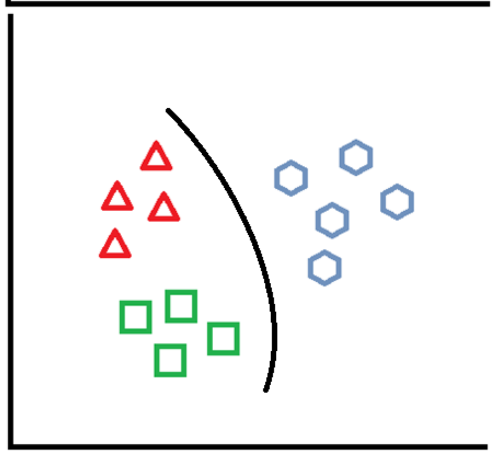
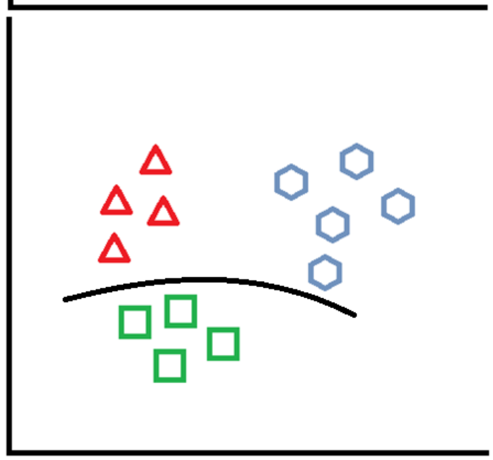
- One strategy to solve a multiclass classification problem is <u>One-vs-all (one-vs-rest) classification</u>. In the example above, we can set:
  - Class 1: triangle
  - Class 2: hexagon
  - Class 3: square
- Then break the problem above into 3 smaller binary classification problems



$$Classifier: h_\theta^{(1)}(x)$$
$$h_\theta^{(1)}(x) = P(y = 1|x, \theta)$$



$$Classifier: h_\theta^{(2)}(x)$$
$$h_\theta^{(2)}(x) = P(y = 2|x, \theta)$$



$$Classifier: h_\theta^{(3)}(x)$$
$$h_\theta^{(3)}(x) = P(y = 3|x, \theta)$$

- In one-vs-all classification, we train logistic regression classifiers $h_\theta^{(i)}$ for each class i to predict the probability that $y = i$

- On new input x, to make a prediction, pick the class i that maximizes the probability

$$\max_i h_\theta^{(i)}(x)$$

- For a logistic regression problem with n classes, using one-vs-all classification, we'll need to break it into n binary classification problems.

9. Problem of Overfitting

- Underfitting: poor performance on the training data, high bias, and poor performance on test data
- Overfitting: fit the training data very well but has a poor performance on the test set, which fail to generalize new examples. Overfitting has a high variance.
- There are 2 options to solve overfitting:
  - Reduce the number of features (manually or automatically)
  - Regularization
    - Keep all the features, but reduce the magnitude/values of the parameters θ
    - Work well when we have lots of features, each of which contributes a bit to the prediction of y

10. Regularization – Cost Function

- The ideas of regularization:
  - Penalize the parameters θ (make the values small)
  - → Get a "simpler" hypothesis
  - → Less prone to overfitting

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

$$\lambda: regularization\ parameter$$

- If λ is set too large, we'll have $\theta_1, \theta_2, \theta_n \approx 0$
  - → $h_\theta(x) \approx 0$
  - → We'll encounter underfitting problem
- Note:
  - We only penalize $\theta_1, \theta_2, \dots, \theta_n$ (Since θ_0 is set to be 1 by default)

11. Regularized Linear Regression

- Consider the regularized cost function $J(\theta)$ that we want to minimize

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

- Gradient descent for linear regression is written as follows:

Repeat until convergence {

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

$$\theta_j := \theta_j - \alpha \underbrace{\left\{\frac{1}{m}\sum_{i=1}^{m}\left[\left(h_\theta\left(x^{(i)}\right) - y^{(i)}\right)\left(x_j^{(i)}\right)\right] + \frac{\lambda}{m}\theta_j\right\}}_{\frac{\partial}{\partial\theta_j}\left(regularized\ J(\theta)\right)} \qquad for\ j := 1,2,\dots,n$$

}

- Consequently, we can re-write the gradient descent algorithm for regularized linear regression as follows:

Repeat until convergence {

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

$$\theta_j := \theta_j\left(1 - \alpha\frac{\lambda}{m}\right) - \alpha\frac{1}{m}\sum_{i=1}^{m}\left[\left(h_\theta\left(x^{(i)}\right) - y^{(i)}\right)\left(x_j^{(i)}\right)\right] \qquad for\ j := 1,2,\dots,n$$

}

- Notes:
  - $1 - \alpha\frac{\lambda}{m} < 1$ → which means this term will shrink θ_j
- Consider normal equation method for linear regression, applying regularization to this method, we'll have:

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

$Is\ a\ (n+1)\times(n+1)\ identity\ matrix\ with\ first\ value\ on\ diagonal\ line\ being\ 0$

- Regularization will take care of the non-invertibility issue in normal equation method, making the matrix become an invertible.

12. <u>Regularized Logistic Regression</u>

- Consider the cost function $J(\theta)$ for logistic regression in section 4 together with the regularized cost function $J(\theta)$ in section 10:

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

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

- We can come up with a regularized cost function for logistic regression as follows:

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

- The gradient descent algorithm for regularized logistic regression can be written as follows:

Repeat until convergence {

$$\theta_0 \coloneqq \theta_0 - \alpha\frac{1}{m}\left[\sum_{i=1}^{m}\left(h_\theta\left(x^{(i)}\right) - y^{(i)}\right)\left(x_0^{(i)}\right)\right]$$

$$\theta_j \coloneqq \theta_j\left(1 - \alpha\frac{\lambda}{m}\right) - \alpha\frac{1}{m}\sum_{i=1}^{m}\left[\left(h_\theta\left(x^{(i)}\right) - y^{(i)}\right)\left(x_j^{(i)}\right)\right] \qquad for\ j \coloneqq 1,2,\ldots,n$$

}

- Note: the algorithm looks identical to the gradient descent algorithm for regularized linear regression, however, the hypothesis h_θ for logistic regression is not the same.

13. <u>Mathematical Interpretation of The Partial Derivative of The Cost Function $J(\theta)$</u>

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

$$= -y\log\left(h_\theta(x)\right) + (y-1)\left(\log\left(1 - h_\theta(x)\right)\right)$$

$$= -y\log\left(h_\theta(x)\right) + y\left[\log\left(1 - h_\theta(x)\right)\right] - \log\left(1 - h_\theta(x)\right)$$

$$= y\left[\log\left(1 - h_\theta(x)\right) - \log\left(h_\theta(x)\right)\right] - \log\left(1 - h_\theta(x)\right)$$

$$= y\left[\log\left(\frac{e^{-\theta^T x}}{1 + e^{-\theta^T x}}\right) - \log\left(\frac{1}{1 + e^{-\theta^T x}}\right)\right] - \log\left(\frac{e^{-\theta^T x}}{1 + e^{-\theta^T x}}\right)$$

$$= y\left[\log\left(e^{-\theta^T x}\right) - \log\left(1 + e^{-\theta^T x}\right) + \log\left(1 + e^{-\theta^T x}\right)\right] - \log\left(e^{-\theta^T x}\right) + \log\left(1 + e^{-\theta^T x}\right)$$

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$$= y\log\left(e^{-\theta^T x}\right) - \log\left(e^{-\theta^T x}\right) + \log\left(1 + e^{-\theta^T x}\right)$$

$$= \log\left(e^{-\theta^T x}\right)(y - 1) + \log\left(1 + e^{-\theta^T x}\right)$$

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

$$= \frac{1}{m}\sum_{i=1}^{m}\left[\log\left(e^{-\theta^T x^{(i)}}\right)\left(y^{(i)} - 1\right) + \log\left(1 + e^{-\theta^T x^{(i)}}\right)\right]$$

$$\rightarrow \frac{\partial J}{\partial \theta_j} = \frac{1}{m}\sum_{i=1}^{m}\left[\frac{\left(e^{-\theta^T x^{(i)}}\right)\left(-x_j^{(i)}\right)}{e^{-\theta^T x^{(i)}}}\left(y^{(i)} - 1\right) + \frac{\left(e^{-\theta^T x^{(i)}}\right)\left(-x_j^{(i)}\right)}{1 + e^{-\theta^T x^{(i)}}}\right]$$

$$= \frac{1}{m}\sum_{i=1}^{m}\left[\left(-x_j^{(i)}\right)\left(y^{(i)} - 1\right) + \frac{\left(e^{-\theta^T x^{(i)}}\right)\left(-x_j^{(i)}\right)}{1 + e^{-\theta^T x^{(i)}}}\right]$$

$$= \frac{1}{m}\sum_{i=1}^{m}\left[\left(x_j^{(i)}\right)\left(1 - y^{(i)} - \frac{e^{-\theta^T x^{(i)}}}{1 + e^{-\theta^T x^{(i)}}}\right)\right]$$

$$= \frac{1}{m}\sum_{i=1}^{m}\left[\left(x_j^{(i)}\right)\left(\frac{1 + e^{-\theta^T x^{(i)}}}{1 + e^{-\theta^T x^{(i)}}} - \frac{e^{-\theta^T x^{(i)}}}{1 + e^{-\theta^T x^{(i)}}} - y^{(i)}\right)\right]$$

$$= \frac{1}{m}\sum_{i=1}^{m}\left[\left(x_j^{(i)}\right)\left(\frac{1}{1 + e^{-\theta^T x^{(i)}}} - y^{(i)}\right)\right]$$

$$= \frac{1}{m}\sum_{i=1}^{m}\left[\left(x_j^{(i)}\right)\left(h_\theta\left(x^{(i)}\right) - y^{(i)}\right)\right] \; for\ all\ j = 0 \ldots n$$