



Logistic Regression

These slides were assembled by Eric Eaton, with grateful acknowledgement of the many others who made their course materials freely available online. Feel free to reuse or adapt these slides for your own academic purposes, provided that you include proper attribution. Please send comments and corrections to Eric.

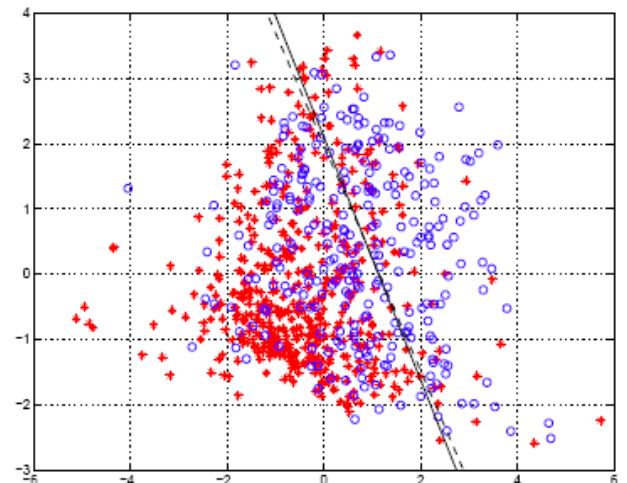
Classification Based on Probability

- Instead of just predicting the class, give the probability of the instance being that class
 - i.e., learn $p(y | \mathbf{x})$
- Comparison to perceptron:
 - Perceptron doesn't produce probability estimate

- Recall that:

$$0 \leq p(\text{event}) \leq 1$$

$$p(\text{event}) + p(\neg\text{event}) = 1$$



Logistic Regression

- Takes a probabilistic approach to learning discriminative functions (i.e., a classifier)

- $h_{\theta}(\mathbf{x})$ should give $p(y = 1 \mid \mathbf{x}; \theta)$

– Want $0 \leq h_{\theta}(\mathbf{x}) \leq 1$

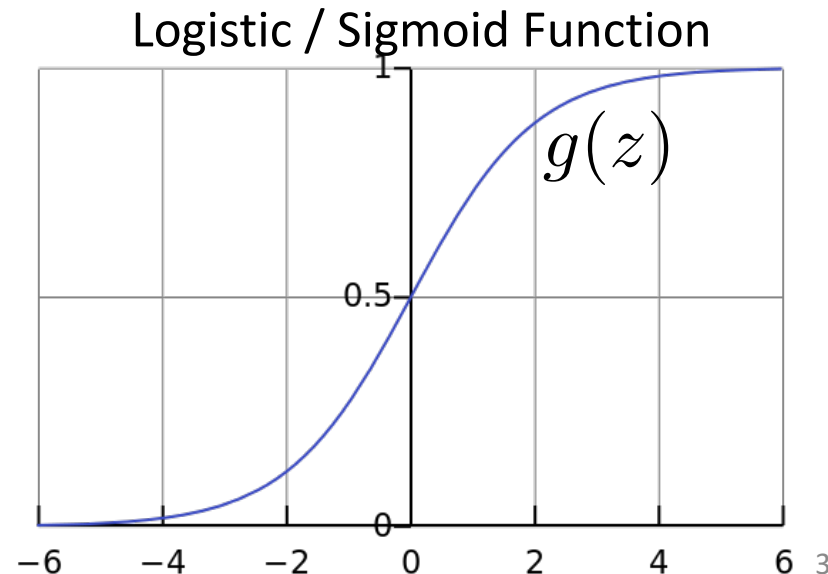
Can't just use linear regression with a threshold

- Logistic regression model:

$$h_{\theta}(\mathbf{x}) = g(\theta^{\top} \mathbf{x})$$

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

$$h_{\theta}(\mathbf{x}) = \frac{1}{1 + e^{-\theta^{\top} \mathbf{x}}}$$



Interpretation of Hypothesis Output

$$h_{\theta}(\mathbf{x}) = \text{estimated } p(y = 1 \mid \mathbf{x}; \theta)$$

Example: Cancer diagnosis from tumor size

$$\mathbf{x} = \begin{bmatrix} x_0 \\ x_1 \end{bmatrix} = \begin{bmatrix} 1 \\ \text{tumorSize} \end{bmatrix}$$

$$h_{\theta}(\mathbf{x}) = 0.7$$

→ Tell patient that 70% chance of tumor being malignant

Note that: $p(y = 0 \mid \mathbf{x}; \theta) + p(y = 1 \mid \mathbf{x}; \theta) = 1$

Therefore, $p(y = 0 \mid \mathbf{x}; \theta) = 1 - p(y = 1 \mid \mathbf{x}; \theta)$

Another Interpretation

- Equivalently, logistic regression assumes that

$$\log \frac{p(y = 1 \mid \mathbf{x}; \boldsymbol{\theta})}{p(y = 0 \mid \mathbf{x}; \boldsymbol{\theta})} = \theta_0 + \theta_1 x_1 + \dots + \theta_d x_d$$

odds of $y = 1$

Side Note: the odds in favor of an event is the quantity $p / (1 - p)$, where p is the probability of the event

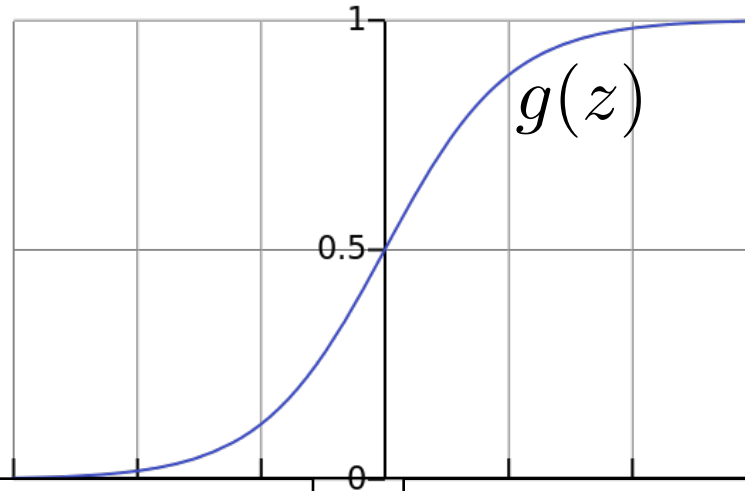
E.g., If I toss a fair dice, what are the odds that I will have a 6?

- In other words, logistic regression assumes that the log odds is a linear function of \mathbf{x}

Logistic Regression

$$h_{\theta}(\mathbf{x}) = g(\theta^{\top} \mathbf{x})$$

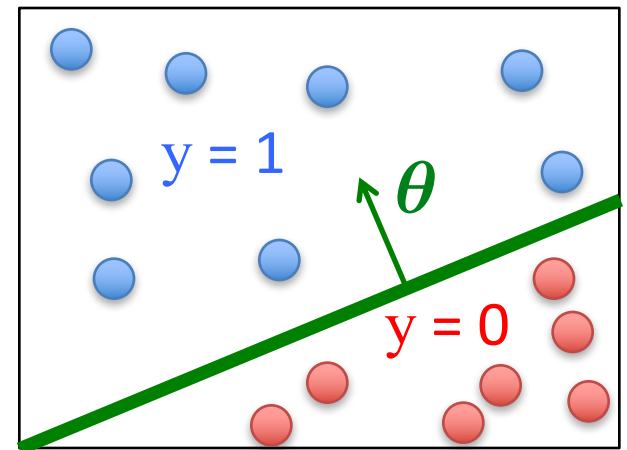
$$g(z) = \frac{1}{1 + e^{-z}}$$



$\theta^{\top} \mathbf{x}$ should be large negative values for negative instances

$\theta^{\top} \mathbf{x}$ should be large positive values for positive instances

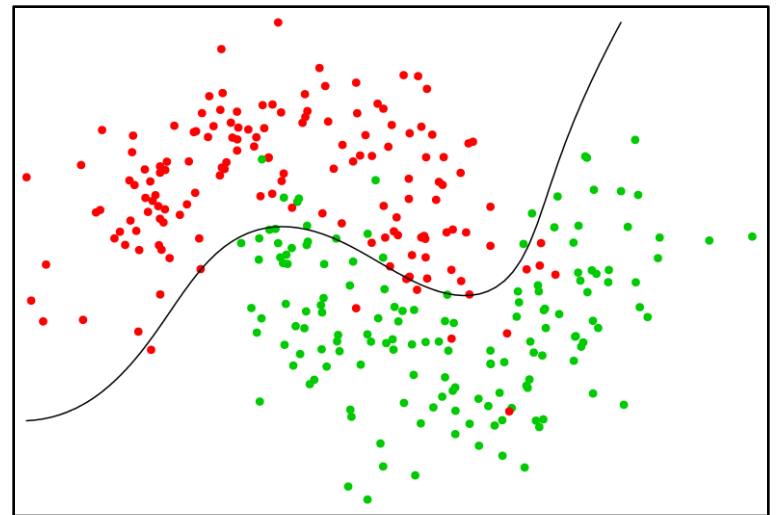
- Assume a threshold and...
 - Predict $y = 1$ if $h_{\theta}(\mathbf{x}) \geq 0.5$
 - Predict $y = 0$ if $h_{\theta}(\mathbf{x}) < 0.5$



Non-Linear Decision Boundary

- Can apply basis function expansion to features, same as with linear regression

$$\mathbf{x} = \begin{bmatrix} 1 \\ x_1 \\ x_2 \end{bmatrix} \rightarrow \begin{bmatrix} 1 \\ x_1 \\ x_2 \\ x_1 x_2 \\ x_1^2 \\ x_2^2 \\ x_1^2 x_2 \\ x_1 x_2^2 \\ \vdots \end{bmatrix}$$



Logistic Regression

- Given $\left\{ \left(\mathbf{x}^{(1)}, y^{(1)} \right), \left(\mathbf{x}^{(2)}, y^{(2)} \right), \dots, \left(\mathbf{x}^{(n)}, y^{(n)} \right) \right\}$
where $\mathbf{x}^{(i)} \in \mathbb{R}^d$, $y^{(i)} \in \{0, 1\}$

- Model: $h_{\boldsymbol{\theta}}(\mathbf{x}) = g(\boldsymbol{\theta}^T \mathbf{x})$

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

$$\boldsymbol{\theta} = \begin{bmatrix} \theta_0 \\ \theta_1 \\ \vdots \\ \theta_d \end{bmatrix} \quad \mathbf{x}^T = \begin{bmatrix} 1 & x_1 & \dots & x_d \end{bmatrix}$$

Logistic Regression Objective Function

- Can't just use squared loss as in linear regression:

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

- Using the logistic regression model

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

results in a non-convex optimization

Deriving the Cost Function via Maximum Likelihood Estimation

- Likelihood of data is given by: $l(\boldsymbol{\theta}) = \prod_{i=1}^n p(y^{(i)} \mid \mathbf{x}^{(i)}; \boldsymbol{\theta})$

- So, looking for the $\boldsymbol{\theta}$ that maximizes the likelihood

$$\boldsymbol{\theta}_{\text{MLE}} = \arg \max_{\boldsymbol{\theta}} l(\boldsymbol{\theta}) = \arg \max_{\boldsymbol{\theta}} \prod_{i=1}^n p(y^{(i)} \mid \mathbf{x}^{(i)}; \boldsymbol{\theta})$$

- Can take the log without changing the solution:

$$\begin{aligned} \boldsymbol{\theta}_{\text{MLE}} &= \arg \max_{\boldsymbol{\theta}} \log \prod_{i=1}^n p(y^{(i)} \mid \mathbf{x}^{(i)}; \boldsymbol{\theta}) \\ &= \arg \max_{\boldsymbol{\theta}} \sum_{i=1}^n \log p(y^{(i)} \mid \mathbf{x}^{(i)}; \boldsymbol{\theta}) \end{aligned}$$

Deriving the Cost Function via Maximum Likelihood Estimation

- Expand as follows:

$$\begin{aligned}\theta_{\text{MLE}} &= \arg \max_{\theta} \sum_{i=1}^n \log p(y^{(i)} | \mathbf{x}^{(i)}; \theta) \\ &= \arg \max_{\theta} \sum_{i=1}^n \left[y^{(i)} \log p(y^{(i)} = 1 | \mathbf{x}^{(i)}; \theta) + (1 - y^{(i)}) \log (1 - p(y^{(i)} = 1 | \mathbf{x}^{(i)}; \theta)) \right]\end{aligned}$$

- Substitute in model, and take negative to yield

Logistic regression objective:

$$\min_{\theta} J(\theta)$$

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

Intuition Behind the Objective

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

- Cost of a single instance:

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

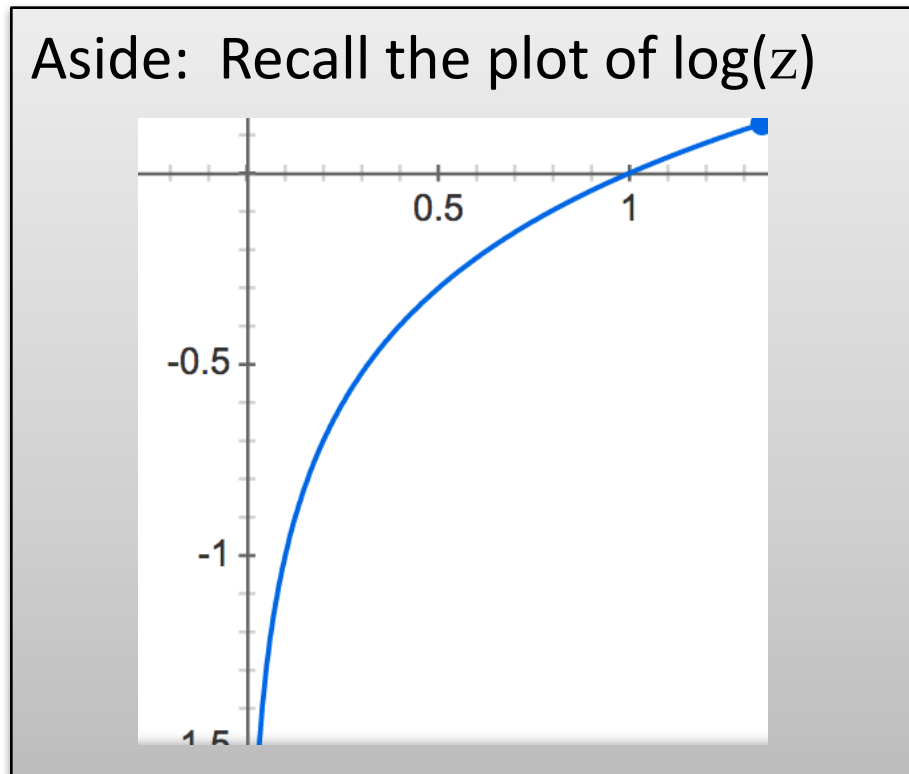
- Can re-write objective function as

$$J(\boldsymbol{\theta}) = \sum_{i=1}^n \text{cost}(h_{\boldsymbol{\theta}}(\mathbf{x}^{(i)}), y^{(i)})$$

Compare to linear regression: $J(\boldsymbol{\theta}) = \frac{1}{2n} \sum_{i=1}^n \left(h_{\boldsymbol{\theta}}(\mathbf{x}^{(i)}) - y^{(i)} \right)^2$

Intuition Behind the Objective

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



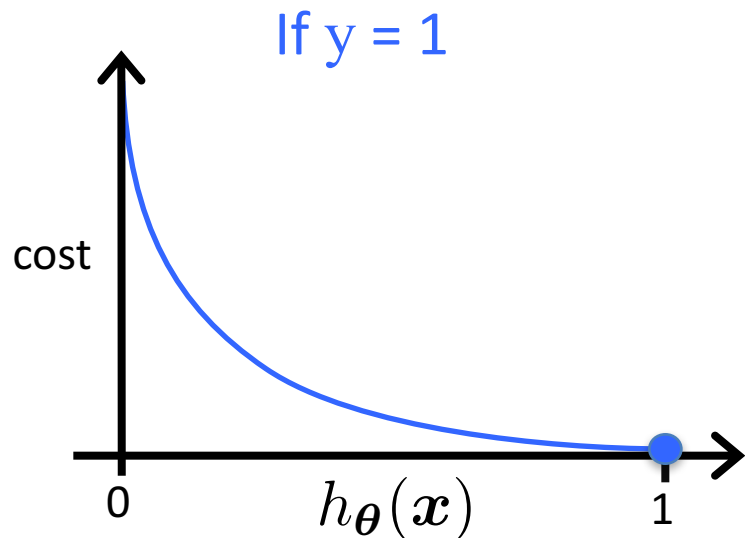
Intuition Behind the Objective

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

If $y = 1$

- Cost = 0 if prediction is correct
- As $h_{\theta}(\mathbf{x}) \rightarrow 0$, cost $\rightarrow \infty$
- Captures intuition that larger mistakes should get larger penalties

– e.g., predict $h_{\theta}(\mathbf{x}) = 0$, but $y = 1$

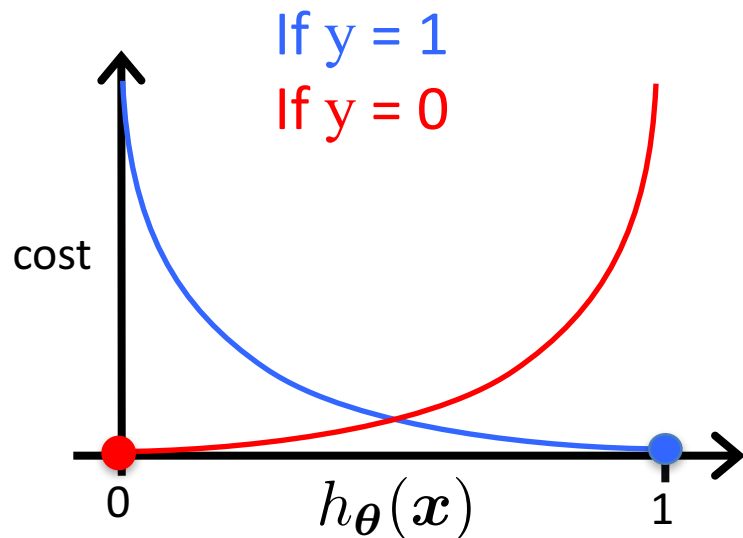


Intuition Behind the Objective

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

If $y = 0$

- Cost = 0 if prediction is correct
- As $(1 - h_{\theta}(\mathbf{x})) \rightarrow 0$, $\text{cost} \rightarrow \infty$
- Captures intuition that larger mistakes should get larger penalties



Regularized Logistic Regression

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

- We can regularize logistic regression exactly as before:

$$\begin{aligned} J_{\text{regularized}}(\boldsymbol{\theta}) &= J(\boldsymbol{\theta}) + \lambda \sum_{j=1}^d \theta_j^2 \\ &= J(\boldsymbol{\theta}) + \lambda \|\boldsymbol{\theta}_{[1:d]}\|_2^2 \end{aligned}$$

Gradient Descent for Logistic Regression

$$J_{\text{reg}}(\boldsymbol{\theta}) = - \sum_{i=1}^n \left[y^{(i)} \log h_{\boldsymbol{\theta}}(\mathbf{x}^{(i)}) + (1 - y^{(i)}) \log (1 - h_{\boldsymbol{\theta}}(\mathbf{x}^{(i)})) \right] + \lambda \|\boldsymbol{\theta}_{[1:d]}\|_2^2$$

Want $\min_{\boldsymbol{\theta}} J(\boldsymbol{\theta})$

- Initialize $\boldsymbol{\theta}$
- Repeat until convergence

$$\theta_j \leftarrow \theta_j - \alpha \frac{\partial}{\partial \theta_j} J(\boldsymbol{\theta})$$

simultaneous update
for $j = 0 \dots d$

Use the natural logarithm ($\ln = \log_e$) to cancel with the $\exp()$ in $h_{\boldsymbol{\theta}}(\mathbf{x})$

Gradient Descent for Logistic Regression

$$J_{\text{reg}}(\boldsymbol{\theta}) = - \sum_{i=1}^n \left[y^{(i)} \log h_{\boldsymbol{\theta}}(\mathbf{x}^{(i)}) + (1 - y^{(i)}) \log (1 - h_{\boldsymbol{\theta}}(\mathbf{x}^{(i)})) \right] + \lambda \|\boldsymbol{\theta}_{[1:d]}\|_2^2$$

Want $\min_{\boldsymbol{\theta}} J(\boldsymbol{\theta})$

- Initialize $\boldsymbol{\theta}$
- Repeat until convergence (simultaneous update for $j = 0 \dots d$)

$$\theta_0 \leftarrow \theta_0 - \alpha \sum_{i=1}^n \left(h_{\boldsymbol{\theta}}(\mathbf{x}^{(i)}) - y^{(i)} \right)$$

$$\theta_j \leftarrow \theta_j - \alpha \left[\sum_{i=1}^n \left(h_{\boldsymbol{\theta}}(\mathbf{x}^{(i)}) - y^{(i)} \right) x_j^{(i)} - \frac{\lambda}{n} \theta_j \right]$$

Gradient Descent for Logistic Regression

- Initialize θ
- Repeat until convergence (simultaneous update for $j = 0 \dots d$)

$$\theta_0 \leftarrow \theta_0 - \alpha \sum_{i=1}^n \left(h_{\theta} \left(\mathbf{x}^{(i)} \right) - y^{(i)} \right)$$

$$\theta_j \leftarrow \theta_j - \alpha \left[\sum_{i=1}^n \left(h_{\theta} \left(\mathbf{x}^{(i)} \right) - y^{(i)} \right) x_j^{(i)} - \frac{\lambda}{n} \theta_j \right]$$

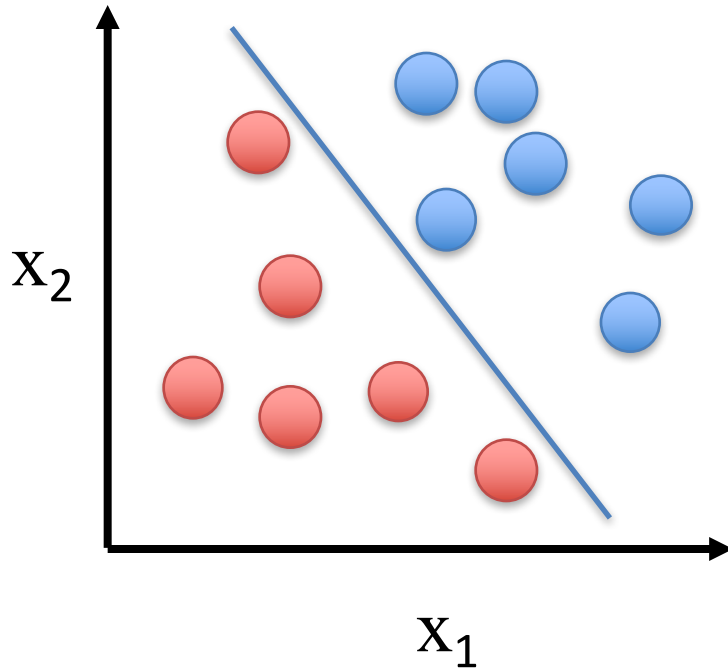
This looks IDENTICAL to linear regression!!!

- Ignoring the $1/n$ constant
- However, the form of the model is very different:

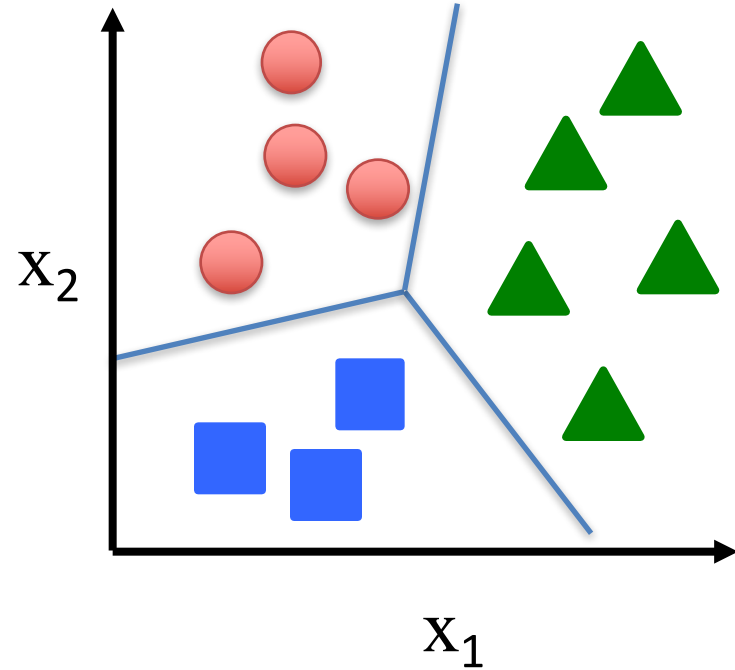
$$h_{\theta}(\mathbf{x}) = \frac{1}{1 + e^{-\theta^T \mathbf{x}}}$$

Multi-Class Classification

Binary classification:



Multi-class classification:



Disease diagnosis: healthy / cold / flu / pneumonia

Object classification: desk / chair / monitor / bookcase

Multi-Class Logistic Regression

- For 2 classes:

$$h_{\theta}(\mathbf{x}) = \frac{1}{1 + \exp(-\theta^T \mathbf{x})} = \frac{\exp(\theta^T \mathbf{x})}{\boxed{1} + \boxed{\exp(\theta^T \mathbf{x})}}$$

weight assigned to $y = 0$ weight assigned to $y = 1$

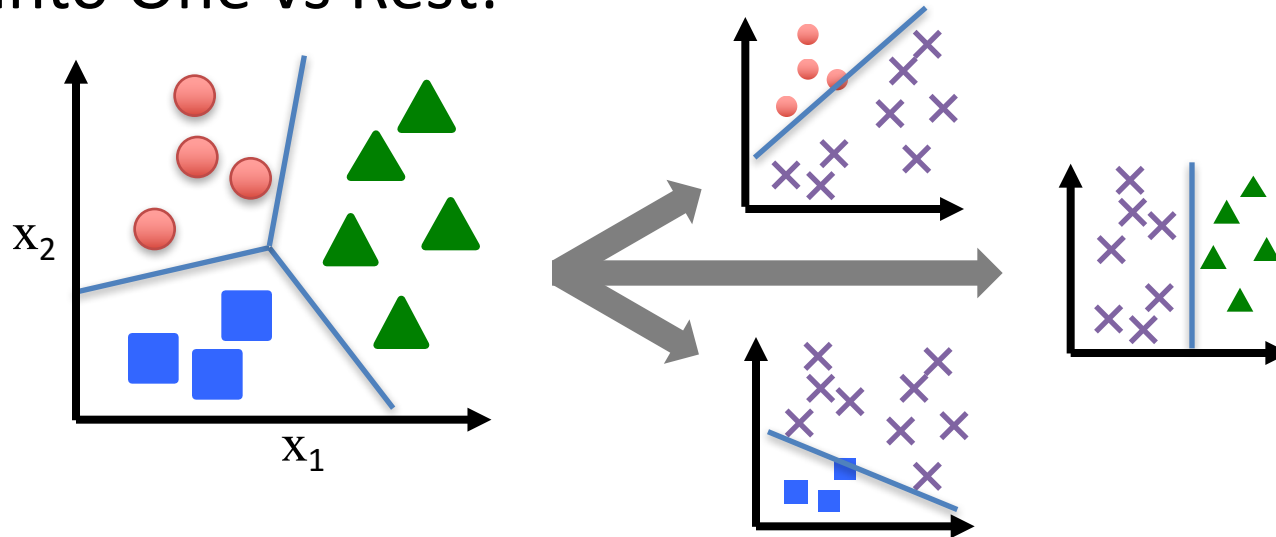
- For C classes $\{1, \dots, C\}$:

$$p(y = c \mid \mathbf{x}; \theta_1, \dots, \theta_C) = \frac{\exp(\theta_c^T \mathbf{x})}{\sum_{c=1}^C \exp(\theta_c^T \mathbf{x})}$$

– Called the **softmax** function

Multi-Class Logistic Regression

Split into One vs Rest:



- Train a logistic regression classifier for each class i to predict the probability that $y = i$ with

$$h_c(\mathbf{x}) = \frac{\exp(\boldsymbol{\theta}_c^T \mathbf{x})}{\sum_{c=1}^C \exp(\boldsymbol{\theta}_c^T \mathbf{x})}$$

Implementing Multi-Class Logistic Regression

- Use $h_c(\mathbf{x}) = \frac{\exp(\boldsymbol{\theta}_c^\top \mathbf{x})}{\sum_{c=1}^C \exp(\boldsymbol{\theta}_c^\top \mathbf{x})}$ as the model for class c
- Gradient descent simultaneously updates all parameters for all models
 - Same derivative as before, just with the above $h_c(\mathbf{x})$
- Predict class label as the most probable label

$$\max_c h_c(\mathbf{x})$$