Logistic Regression

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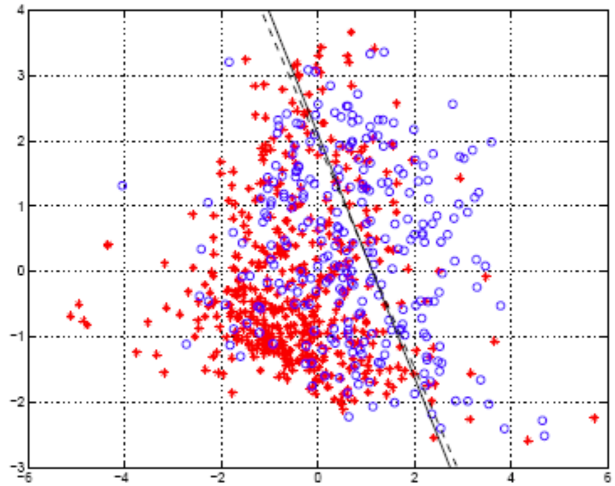
Classification Based on Probability

- Instead of just predicting the class, give the probability of the instance being that class
  - i.e., learn $p(y \mid \boldsymbol{x})$

- Comparison to perceptron:
  - Perceptron doesn't produce probability estimate



Logistic Regression

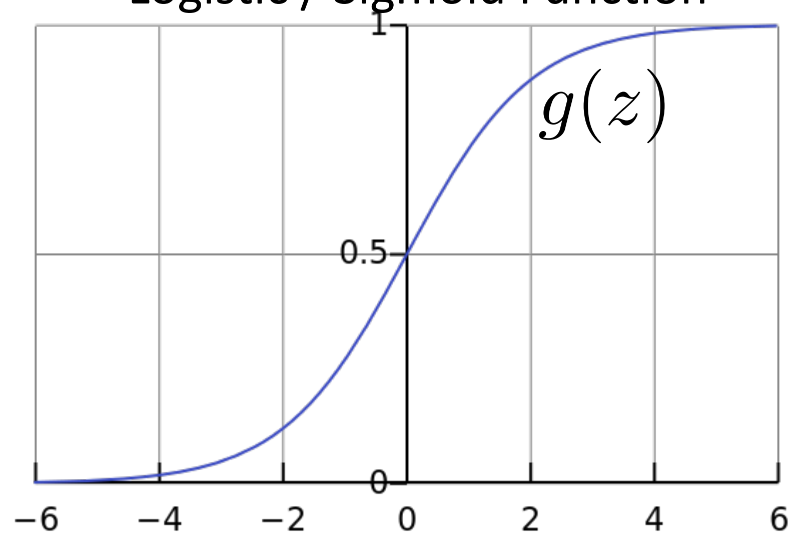
- Takes a probabilistic approach to learning discriminative functions (i.e., a classifier)
- $h_{\boldsymbol{\theta}}(\boldsymbol{x})$ should give $p(y = 1 \mid \boldsymbol{x}; \boldsymbol{\theta})$
  - Want $0 \leq h_{\boldsymbol{\theta}}(\boldsymbol{x}) \leq 1$
- Logistic regression model:

$$h_{\boldsymbol{\theta}}(\boldsymbol{x}) = g\left(\boldsymbol{\theta}^{\mathsf{T}} \boldsymbol{x}\right)$$

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

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

Logistic / Sigmoid Function



Interpretation of Hypothesis Output

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

Example: Cancer diagnosis from tumor size

$$\boldsymbol{x} = \left[\begin{array}{c} x_0 \\ x_1 \end{array} \right] = \left[\begin{array}{c} 1 \\ \text{tumorSize} \end{array} \right]$$

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

→ Tell patient that 70% chance of tumor being malignant

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

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

Another Interpretation

- Equivalently, logistic regression assumes that

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

odds of y = 1

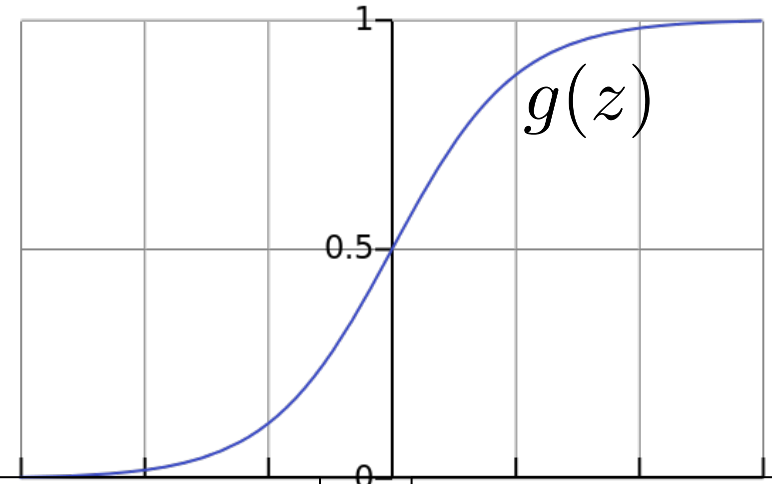
> **Side Note**: the odds in favor of an event is the quantity p / (1 − p), where p is the probability of the event
>
> E.g., If I toss a fair dice, what are the odds that I will have a 6?

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

Logistic Regression

$$h_{\boldsymbol{\theta}}(\boldsymbol{x}) = g\left(\boldsymbol{\theta}^{\mathsf{T}}\boldsymbol{x}\right)$$

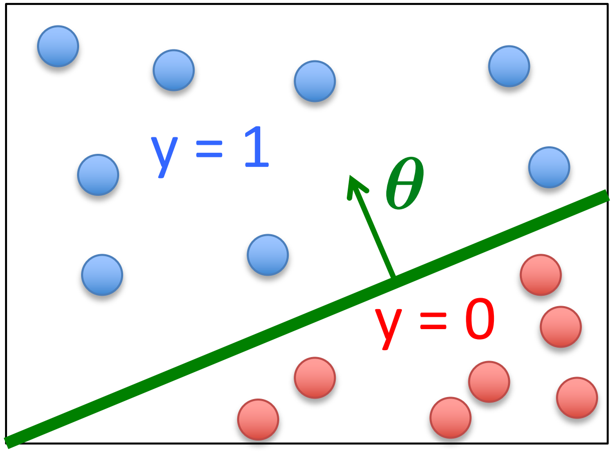
$$g(z) = \frac{1}{1+e^{-z}}$$



$\boldsymbol{\theta}^{\mathsf{T}}\boldsymbol{x}$ should be large <u>negative</u> values for negative instances

$\boldsymbol{\theta}^{\mathsf{T}}\boldsymbol{x}$ should be large <u>positive</u> values for positive instances

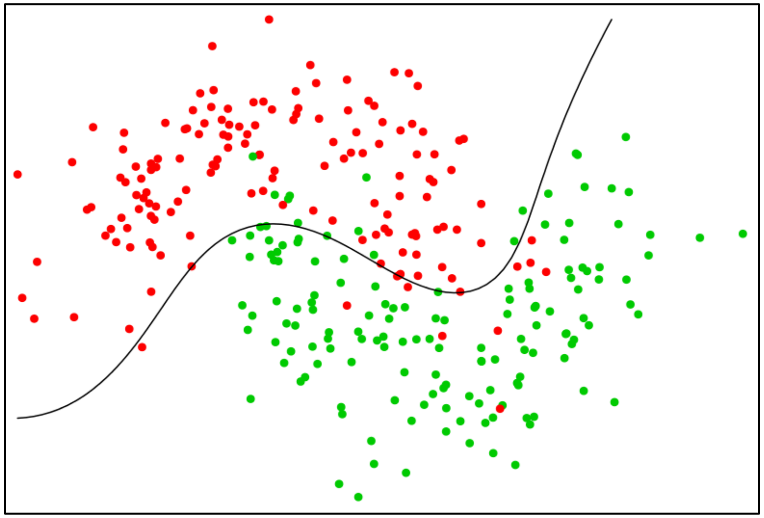
- Assume a threshold and...
  – Predict y = 1 if $h_{\boldsymbol{\theta}}(\boldsymbol{x}) \geq 0.5$
  – Predict y = 0 if $h_{\boldsymbol{\theta}}(\boldsymbol{x}) < 0.5$



Non-Linear Decision Boundary

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

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



Logistic Regression (continued)

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Last Time: Logistic Regression

- Given $\left\{ \left(\boldsymbol{x}^{(1)}, y^{(1)} \right), \left(\boldsymbol{x}^{(2)}, y^{(2)} \right), \ldots, \left(\boldsymbol{x}^{(n)}, y^{(n)} \right) \right\}$

  where $\boldsymbol{x}^{(i)} \in \mathbb{R}^d, \; y^{(i)} \in \{0, 1\}$

- Model: $h_{\boldsymbol{\theta}}(\boldsymbol{x}) = g\left(\boldsymbol{\theta}^\intercal \boldsymbol{x}\right)$

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

Logistic Regression Objective Function

- Shouldn't use squared loss as in linear regression:

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

  – Using the logistic regression model

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

  results in a non-convex optimization

Deriving the Cost Function via MLE

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

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

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

- Can take the log without changing the solution:

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

Deriving the Cost Function via MLE

- Expand as follows:

$$\boldsymbol{\theta}_{\mathrm{MLE}} = \arg\max_{\boldsymbol{\theta}} \sum_{i=1}^{n} \log p(y^{(i)} \mid \boldsymbol{x}^{(i)}; \boldsymbol{\theta})$$

$$= \arg\max_{\boldsymbol{\theta}} \sum_{i=1}^{n} \left[y^{(i)} \log p(y^{(i)}=1 \mid \boldsymbol{x}^{(i)}; \boldsymbol{\theta}) + \left(1 - y^{(i)}\right) \log \left(1 - p(y^{(i)}=1 \mid \boldsymbol{x}^{(i)}; \boldsymbol{\theta})\right) \right]$$

- Substitute in model, and take negative to yield

Logistic regression objective:

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

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

Intuition Behind the Objective

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

- Cost of a single instance:

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

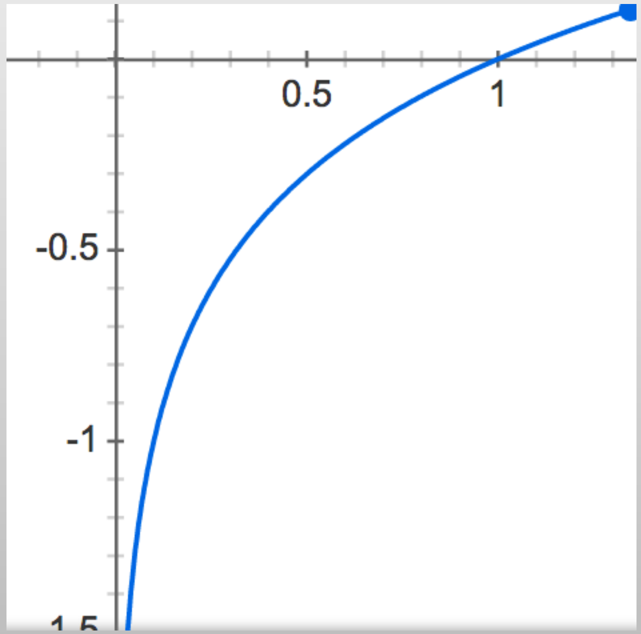
- Can re-write objective function as

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

Intuition Behind the Objective

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

Aside: Recall the plot of log(z)

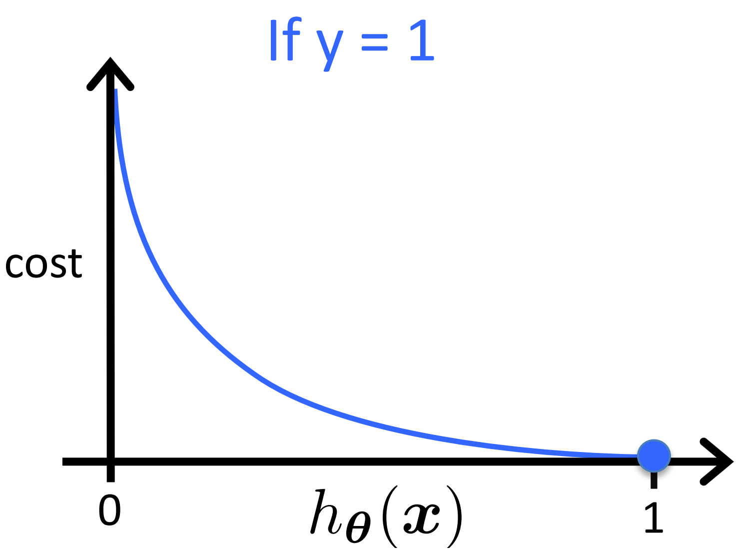


Intuition Behind the Objective

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

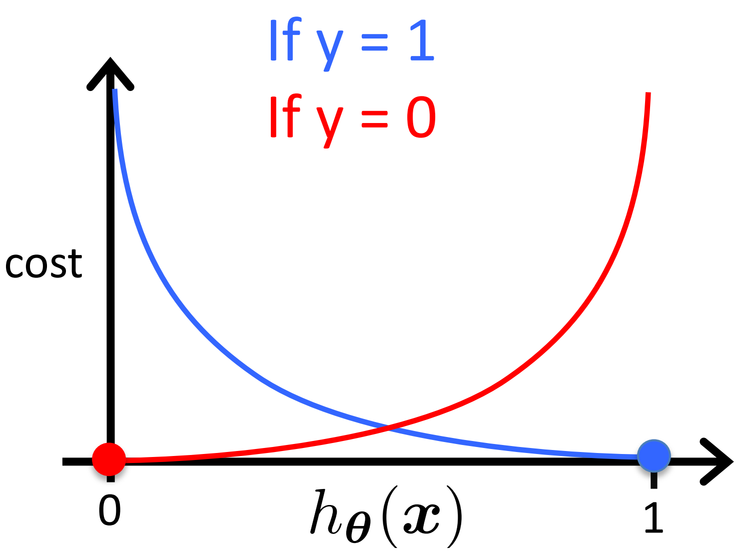
If y = 1

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



Intuition Behind the Objective

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



If y = 0

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

Based on example by Andrew Ng

Regularized Logistic Regression

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

- 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

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

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 ... d

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

Gradient Descent for Logistic Regression

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

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

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

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

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

Gradient Descent for Logistic Regression

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

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

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

This looks IDENTICAL to linear regression!!!

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

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