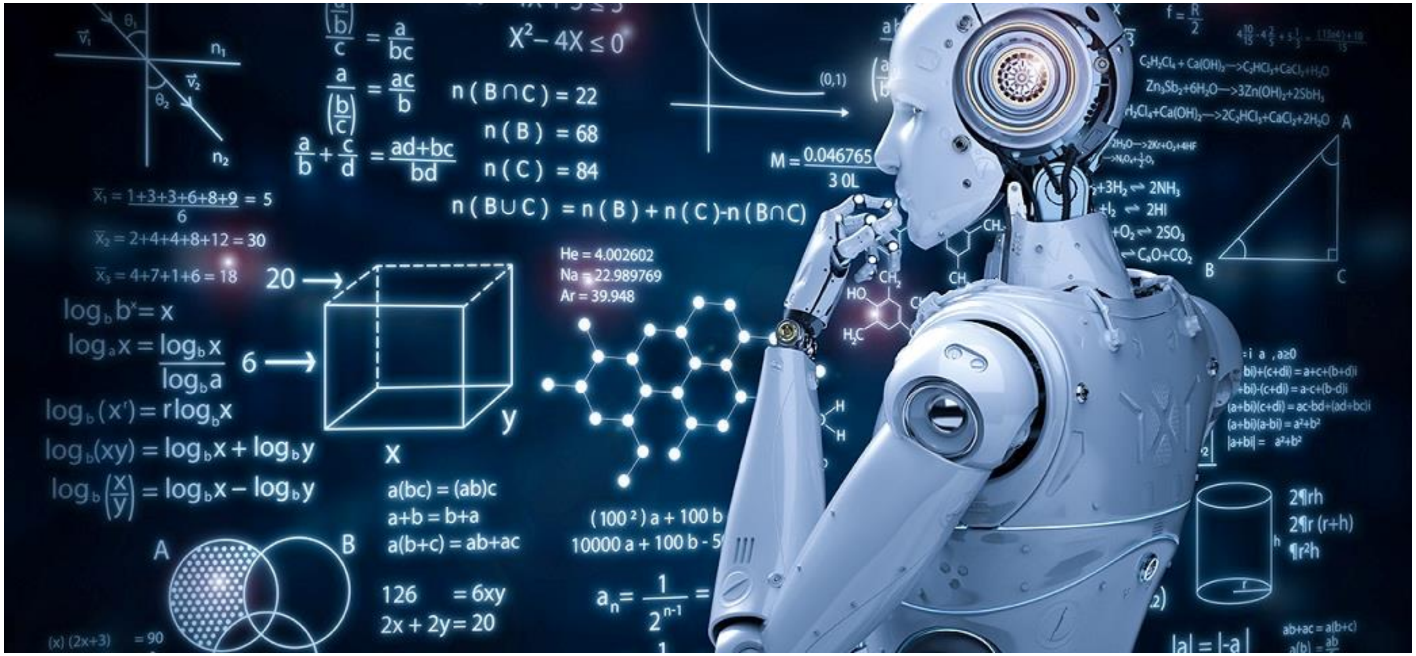
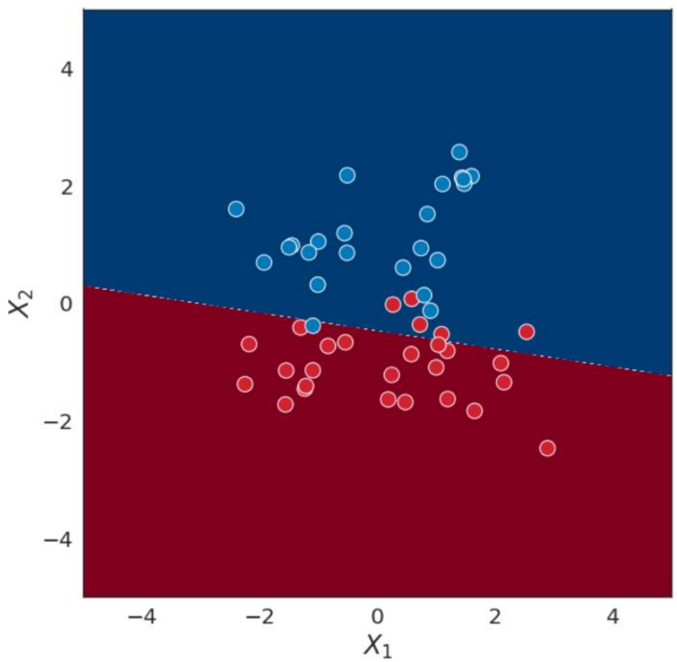


BBM406: Fundamentals of Machine Learning

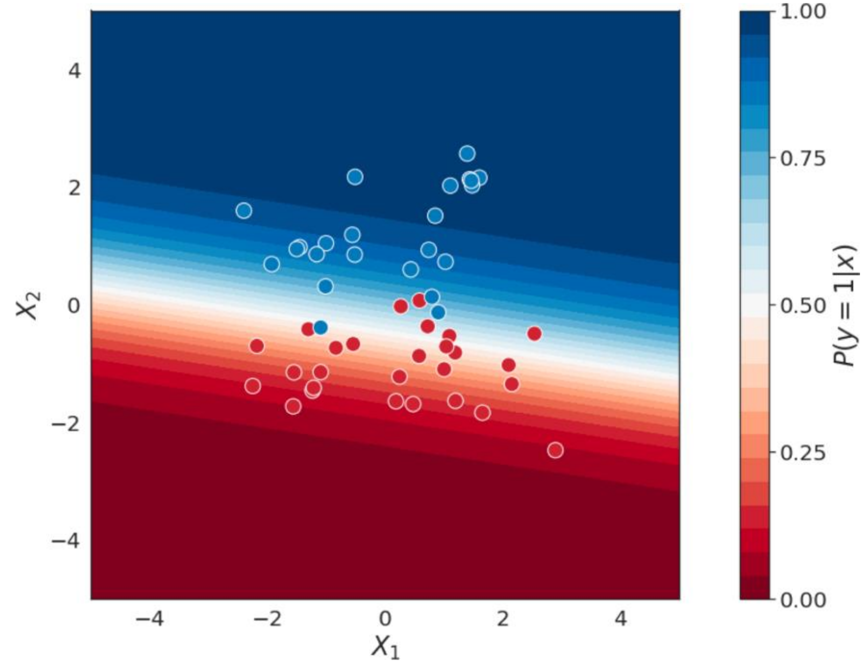
Logistic Regression

Types of Discriminative Methods

Class prediction



Probability prediction



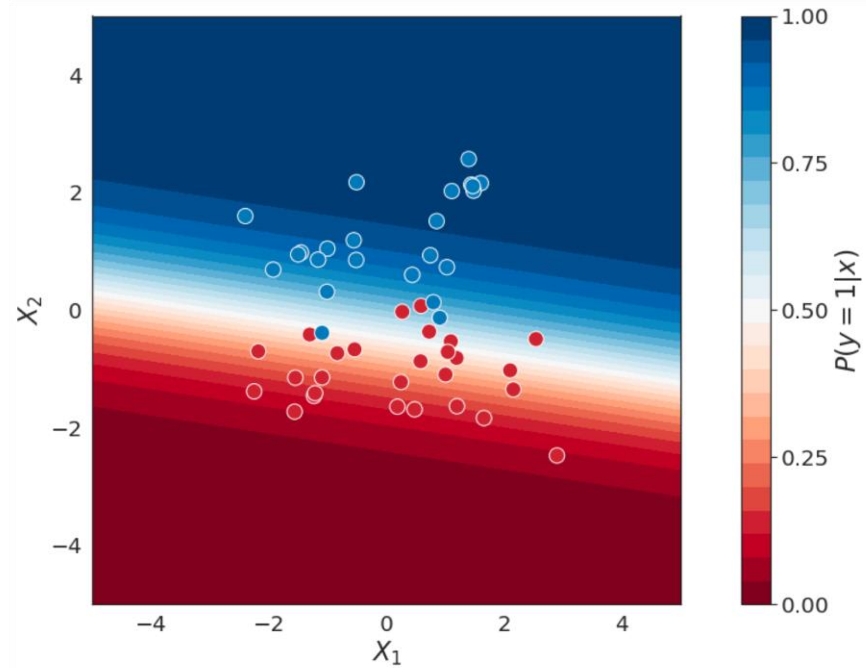
Classification Based on Probability

Class prediction

- Effective and useful
- Borderline cases are problematic

Key Idea: Instead of predicting only the class label, output the probability of the instance being within that class

  - o i.e., learn p(y |x)



Slides by Eric Eaton

Classification via Linear Regression ?

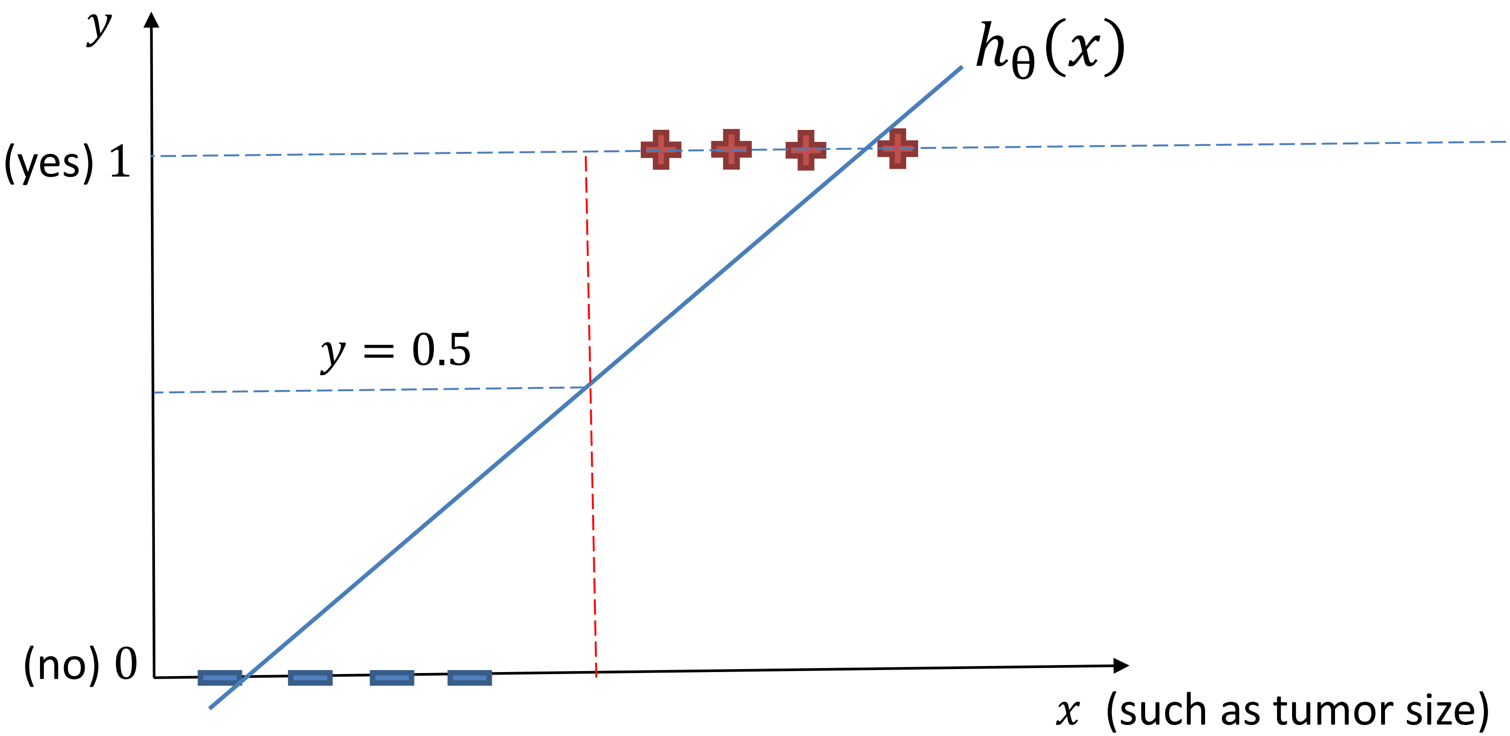
- Can we use linear regression for classification?
- Hypothesis function for linear regression is :

$$y = h_\theta(x) = \theta_0 + \theta_1 x_1 + \theta_2 x_2 + \cdots + \theta_d x_d = \theta^T x$$

$$\theta = \begin{bmatrix} \theta_0 \\ \theta_1 \\ \theta_2 \\ \dots \\ \theta_d \end{bmatrix} \qquad x = \begin{bmatrix} 1 \\ x_1 \\ x_2 \\ \dots \\ x_d \end{bmatrix} \qquad h_\theta(x) = \theta^T x$$

- $h_\theta(x)$ can take real values, so we can not use it for classification directly.

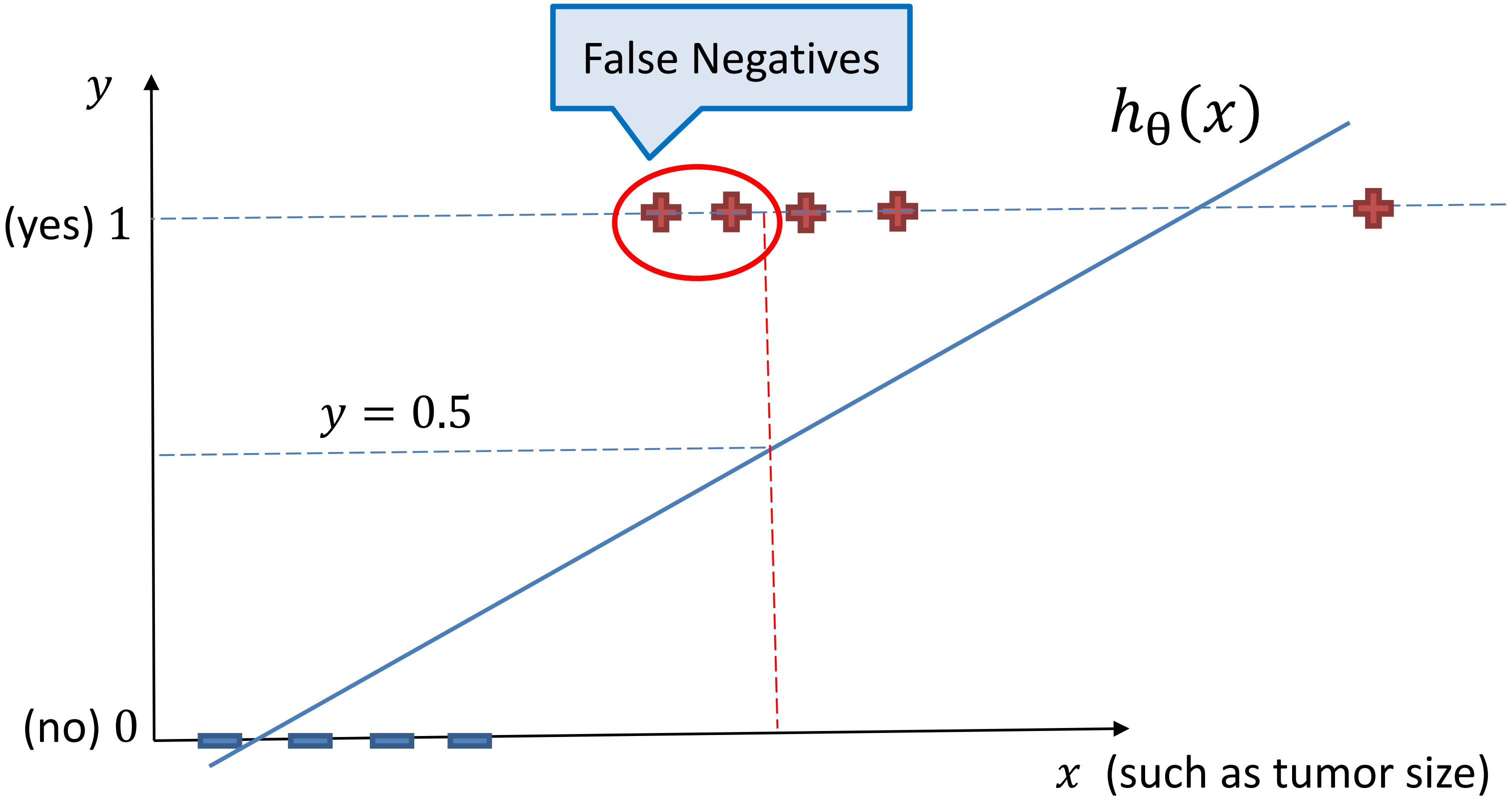
Linear Regression For Classification



- For this data, y=0.5 threshold looks good.
- However, if the new data arrives and $h_\theta(x)$ changes, is it still good?

Based on example by Andrew Ng

Linear Regression For Classification



- With the new data, $h_\theta(x)$ changed.
- And two positive instances are classified as negative

Based on example by Andrew Ng

Classification via Linear Regression ?

- We can apply thresholding but it is very dependent to data and sensitive to noise.
- Therefore, we need another approach for applying this for classification.

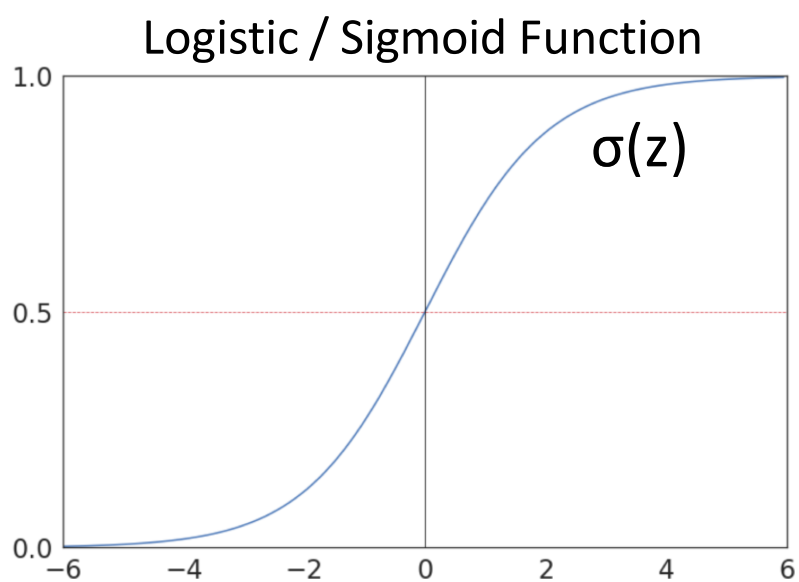
Logistic Regression

- Takes a probabilistic approach to learn discriminative functions
  - $h_\theta(x)$ should give us $p(y = 1|x; \theta)$
  - We want $0 \leq h_\theta(x) \leq 1$

Can't just use linear regression with a threshold

  - For this purpose we can use sigmoid (logistic) function:

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



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Logistic Regression

- By replacing our hypothesis in linear regression $h_\theta(x) = \theta^T x$ with logistic function, we obtain Logistic regression model :

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

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

$$\Rightarrow$$

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

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Interpretation of Hypothesis Output

$h_\theta(x)$ = estimated $p(y = 1|x; \theta)$

Example: Ocular tumor diagnosis from size

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

$$h_\theta(x) = 0.75$$

Tumor has a 75% chance of being malignant

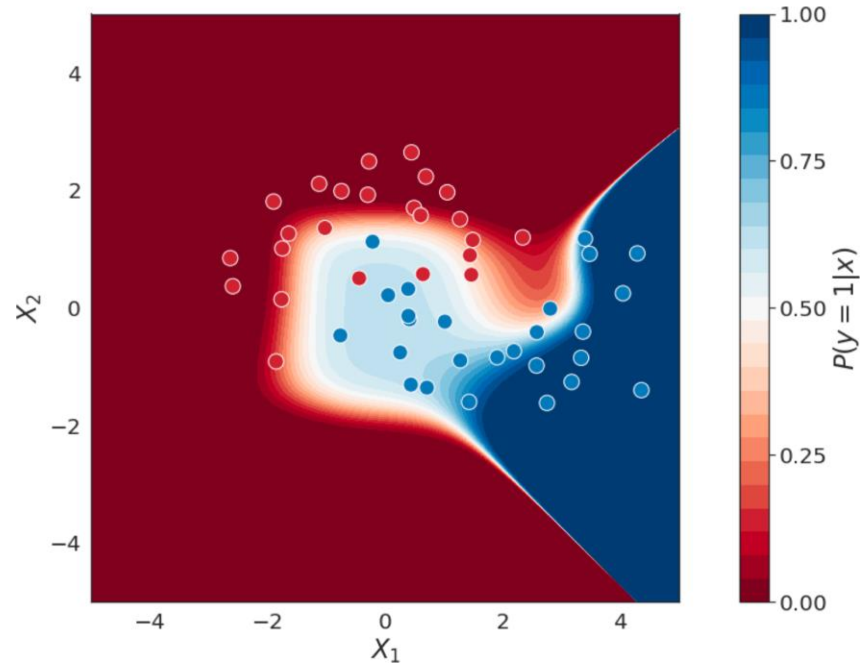
Note that: $p(y = 0|x; \theta) + p(y = 1|x; \theta) = 1$

Therefore, $p(y = 0|x; \theta) = 1 - p(y = 1|x; \theta)$

Non-Linear Decision Boundary

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

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



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Logistic Regression

- Given $\{(x^{(1)}, y^{(1)}), (x^{(2)}, y^{(2)}), \cdots, (x^{(n)}, y^{(n)})\}$

  Where $x^{(1)} \in R^d, y^{(i)} \in \{0,1\}$

- Model: $h_\theta(x) = \sigma(\theta^T x)$

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

$$\theta = \begin{bmatrix} \theta_0 \\ \theta_1 \\ \theta_2 \\ \dots \\ \theta_d \end{bmatrix} \qquad x = \begin{bmatrix} 1 \\ x_1 \\ x_2 \\ \dots \\ x_d \end{bmatrix}$$

Logistic Regression Objective Function

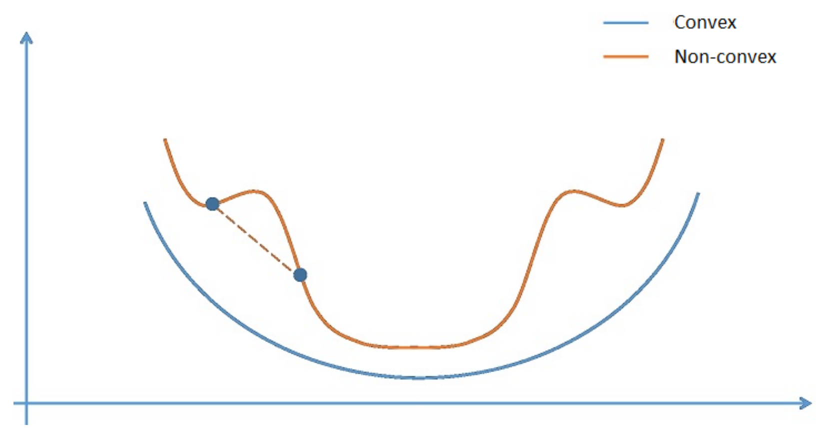
- Can't just use squared loss as in linear regression:

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

- Using the logistic regression model

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

results in a non-convex optimization



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Deriving the Cost Function via Maximum Likelihood Estimation

- Likelihood of data is given by:

$$l(\theta) = \prod_{i=1}^{n} P(y^{(i)} | x^{(i)}; \theta)$$

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

$$\theta_{MLE} = \underset{\theta}{\operatorname{argmax}}\, l(\theta) = \underset{\theta}{\operatorname{argmax}} \prod_{i=1}^{n} P(y^{(i)} | x^{(i)}; \theta)$$

- Can take the log without changing the solution:

$$\theta_{MLE} = \underset{\theta}{\operatorname{argmax}} \log \prod_{i=1}^{n} P(y^{(i)} | x^{(i)}; \theta) = \underset{\theta}{\operatorname{argmax}} \sum_{i=1}^{n} \log P(y^{(i)} | x^{(i)}; \theta)$$

Deriving the Cost Function via Maximum Likelihood Estimation

- Expand as follows:

$$\theta_{MLE} = \underset{\theta}{\operatorname{argmax}} \sum_{i=1}^{n} \log P(y^{(i)} | x^{(i)}; \theta)$$

$$= \underset{\theta}{\operatorname{argmax}} \sum_{i=1}^{n} y^{(i)} \log P\left(y^{(i)} = 1 \middle| x^{(i)}; \theta\right) + (1 - y^{(i)}) \log(1 - P\left(y^{(i)} = 1 \middle| x^{(i)}; \theta\right))$$

- Substitute in model and take negative to yield

Logistic regression objective: $\min_{\theta} J(\theta)$

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

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Intuition Behind the Objective

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

- Cost of a single instance:

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

- Can re-write objective function as

$$J(\theta) = -\sum_{i=1}^{n} cost(h_\theta\big(x^{(i)}\big), y^{(i)})$$

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

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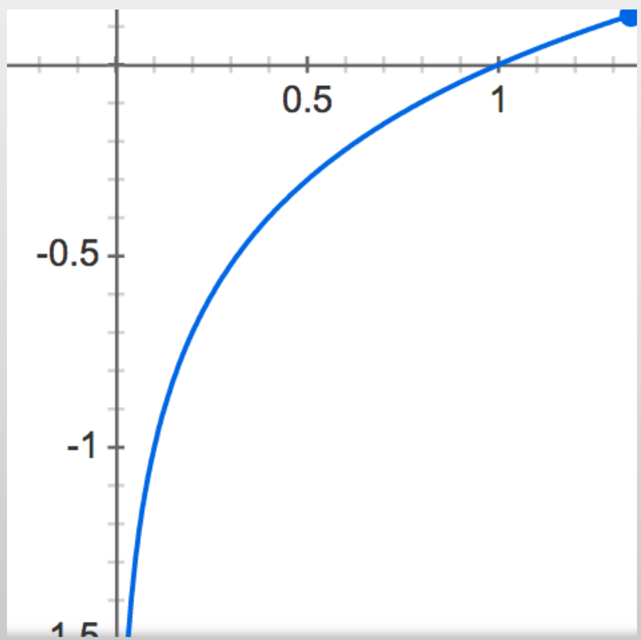
Intuition Behind the Objective

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

Aside: Recall the plot of $\log(z)$



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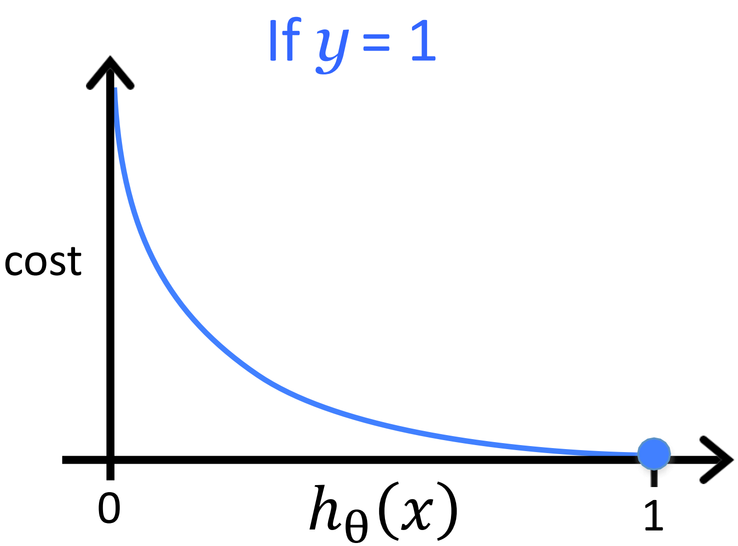
Intuition Behind the Objective

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

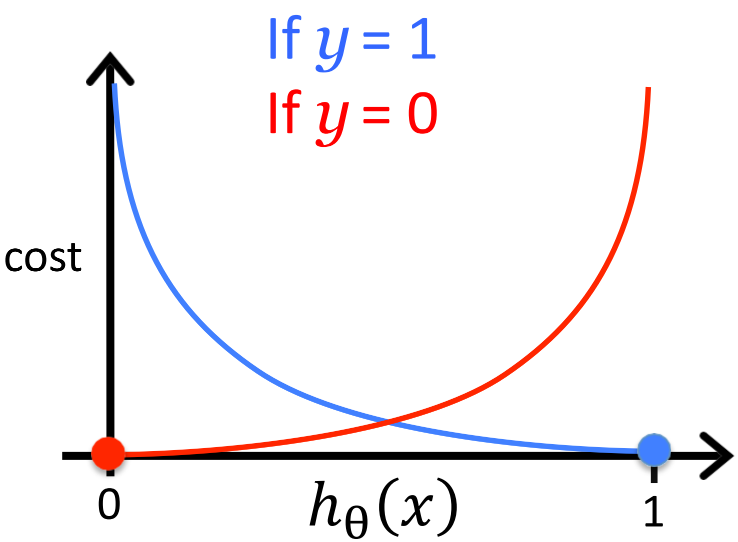


If $y = 1$

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

Intuition Behind the Objective

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



If $y = 0$

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

Based on example by Andrew Ng

Gradient Descent for Logistic Regression

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

Objective: $\min_\theta J(\theta)$

- Initialize θ
- Repeat until convergence

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

simultaneous update for j = 0 ... d

Use the natural logarithm (*ln = log*$_e$) to cancel with the *exp()* in $h_\theta(x)$

Gradient Descent for Logistic Regression

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

Objective: $\min_\theta J(\theta)$

- Initialize θ
- Repeat until convergence

simultaneous update for j = 0 ... d

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

This looks almost identical to linear regression, except 1/n term!

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

Gradient Descent for Logistic Regression

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

Objective: $\min_\theta J(\theta)$

- Initialize θ
- Repeat until convergence

simultaneous update for j = 0 ... d

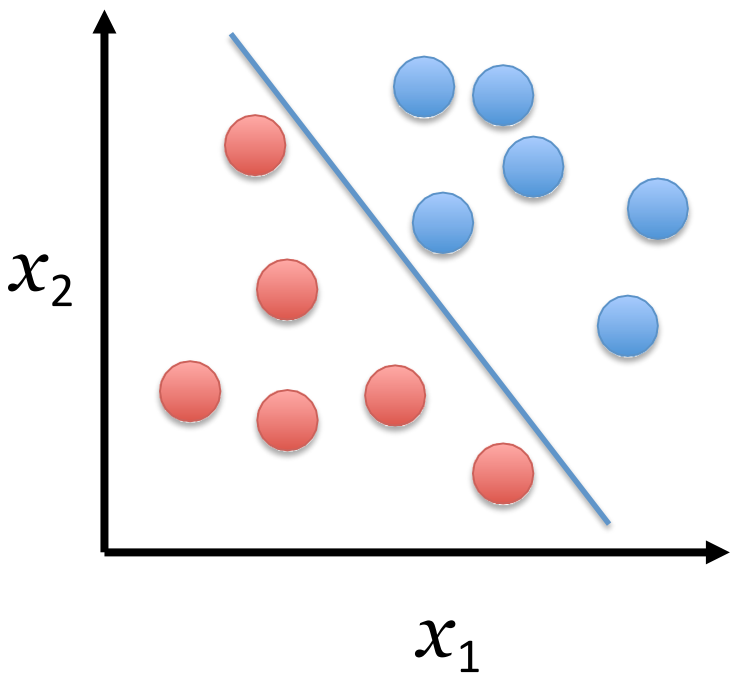
$$\theta_j \leftarrow \theta_j - \alpha \sum_{i=1}^{n}\left(h_\theta\left(x^{(i)}\right) - y^{(i)}\right) x_j^{(i)}$$

However, the form of the model is very different!

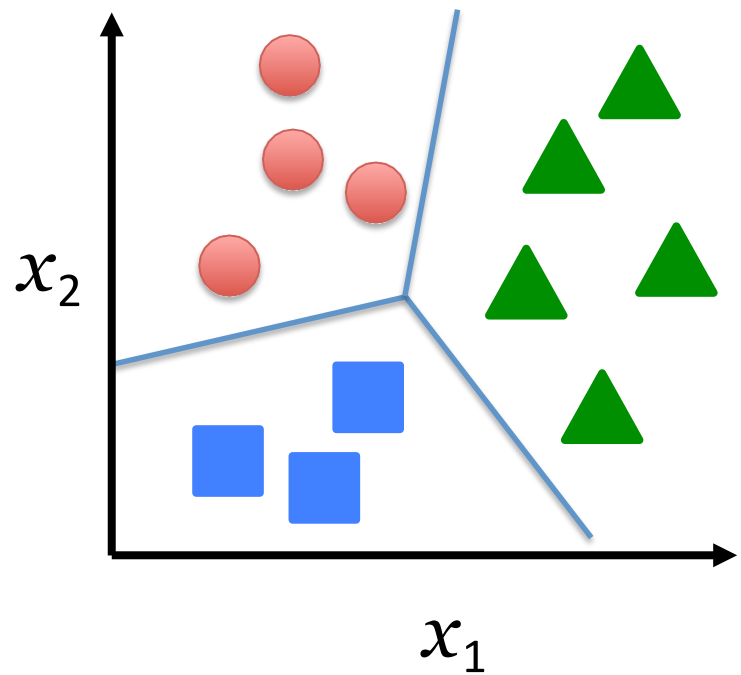
$$h_{\boldsymbol{\theta}}(\boldsymbol{x}) = \frac{1}{1+e^{-\boldsymbol{\theta}^\mathsf{T}\boldsymbol{x}}}$$

Multi-Class Classification

Binary classification:



Multi-class classification:

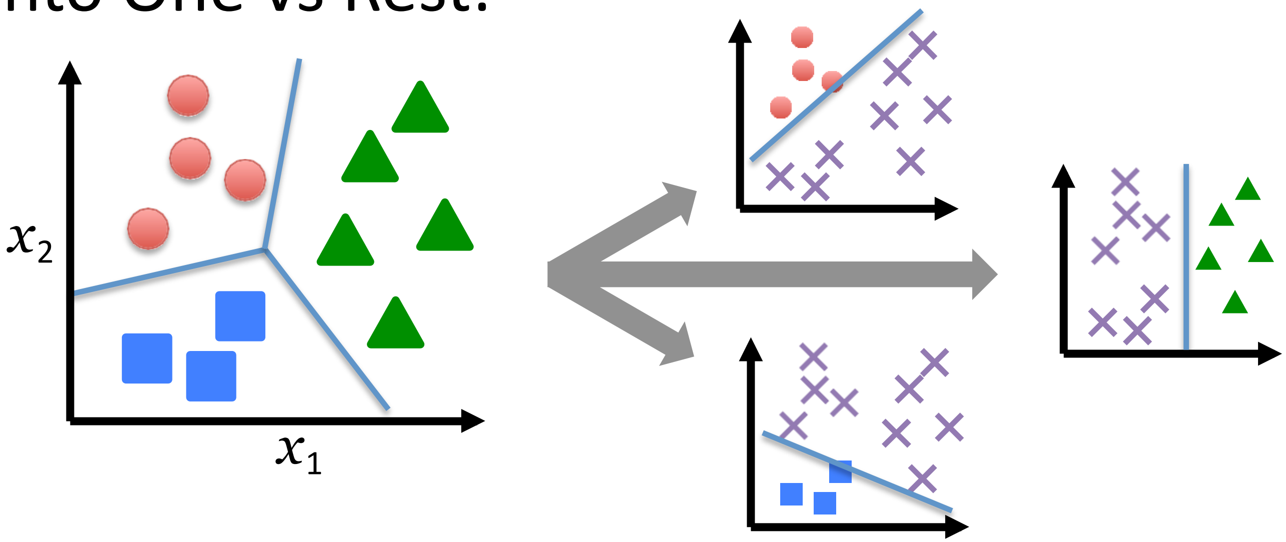


Disease diagnosis: healthy / cold / flu / pneumonia

Object classification: desk / chair / monitor / bookcase

Multi-Class Logistic Regression

Split into One vs Rest:



- Train a logistic regression classifier $h_\theta^{(i)}(x)$ for each class i to predict the probability that $y = i$

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Implementing Multi-Class Logistic Regression

- Use $h_\theta^{(c)}(x)$ as the model for class c
- Gradient descent simultaneously updates all parameters for all models
  - Same derivative as before

- On a new input x, predict class label by picking the class i that maximizes

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