CSCE 633: Machine Learning

Lecture 12: Logistic Regression

Texas A&M University
Bobak Mortazavi

Goals

- Learn Logistic Regression!
- See how Gradient Descent helps Logistic Regression!
- Evaluate Measures of Performance with Cross-Validation

Important Questions

- Why do we need it? Classification vs. Regression
- Why not simply use Linear Regression?
- What are odds?
- How do we design Logistic Regression?
- How do we find optimal coefficients for Logistic Regression?

An example of questions that need classification

- A person arrives in the emergency room and has symptoms that present as 1 of 3 different conditions, which one is it?
- A bank must determine which transactions are fraudulent
- What is the likelihood someone will default on credit card payments?

- What are some other examples of classification problems?

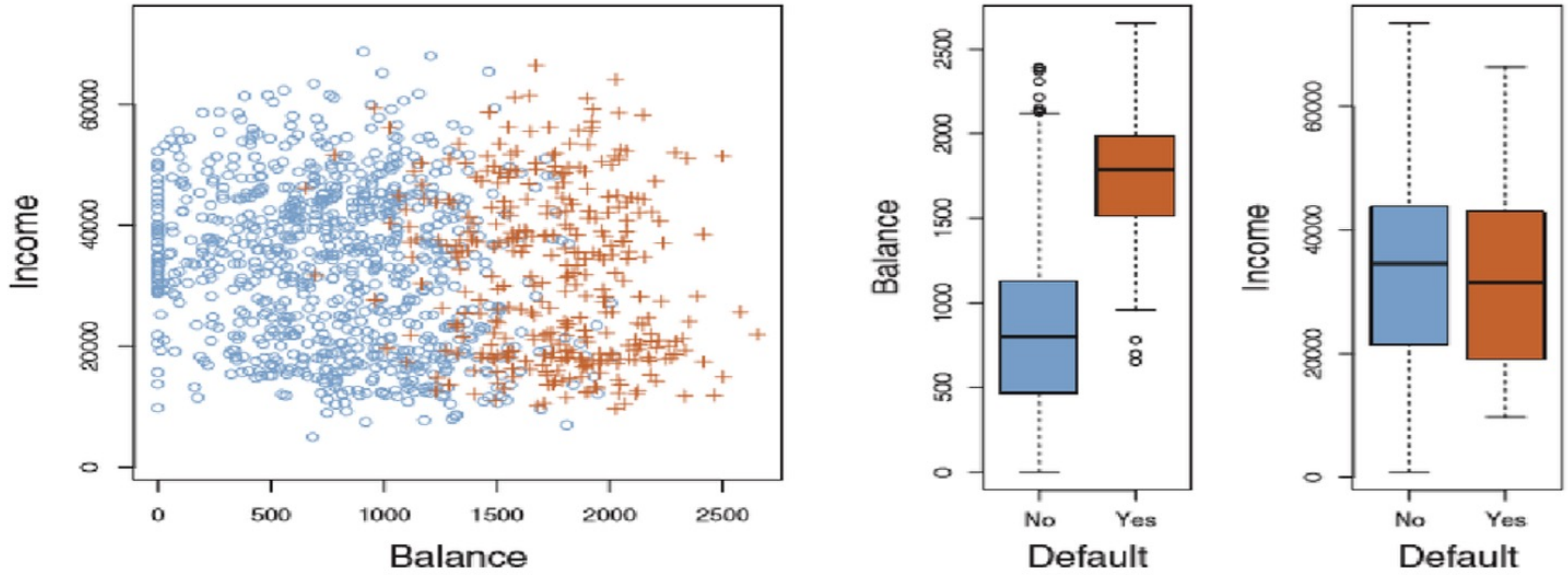
An example of questions that need classification

- A person arrives in the emergency room and has symptoms that present as 1 of 3 different conditions, which one is it?
- A bank must determine which transactions are fraudulent
- What is the likelihood someone will default on credit card payments?

- Still in the data scenario of $D = \{(x_i, y_i)\}_{i=1}^{n}$, but now $y \in \{0,1\}$

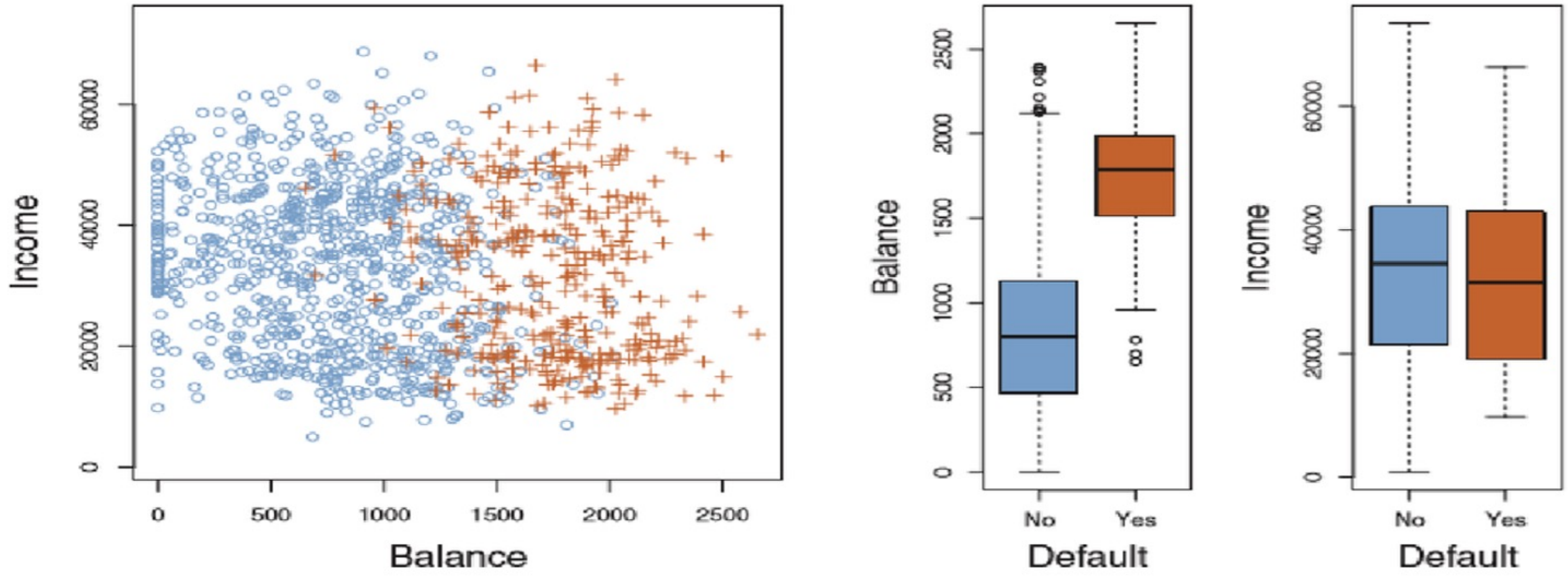
Credit Default Prediction

- Predict class A vs. class B
- Determine if two classes are separable



Credit Default Prediction

- Predict class A vs. class B
- Determine if two classes are separable
- Why not simply use linear regression and use values to determine classes?



Why not linear regression?

- Imagine someone comes into the emergency room, and presents with a likelihood of either heart attack, overdose, or treatment for broken bones - and you need a model to quickly determine which is highest/needs to be treated.

Why not linear regression?

- Imagine someone comes into the emergency room, and presents with a likelihood of either heart attack, overdose, or treatment for broken bones - and you need a model to quickly determine which is highest/needs to be treated.
- Encoding these outcomes presents a natural ordering (e.g. 1, 2, 3)

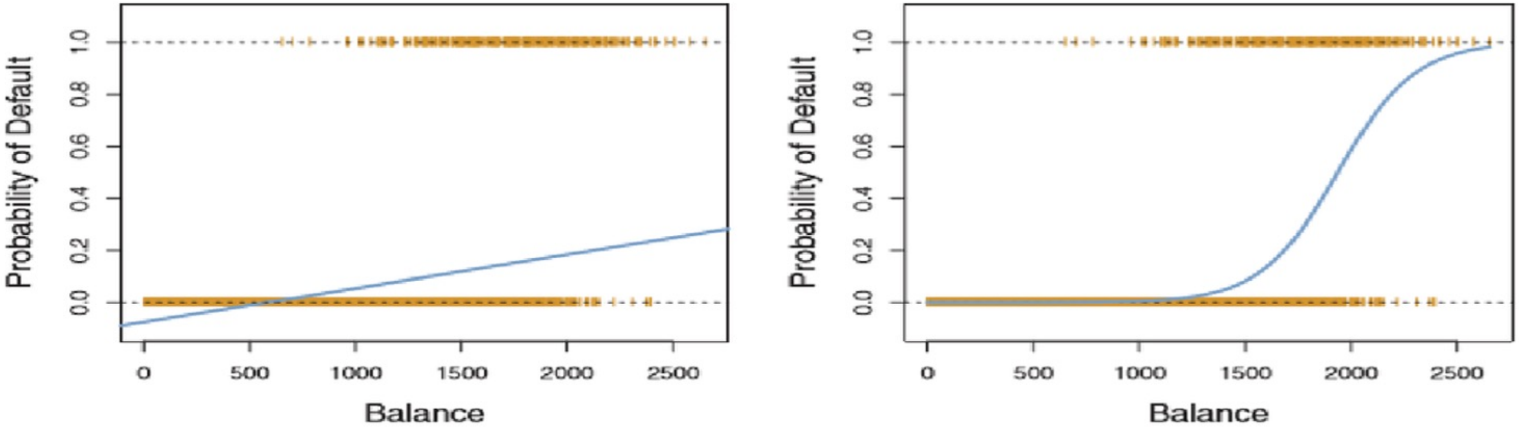
Why not linear regression?

- Imagine someone comes into the emergency room, and presents with a likelihood of either heart attack, overdose, or treatment for broken bones - and you need a model to quickly determine which is highest/needs to be treated.
- Encoding these outcomes presents a natural ordering (e.g. 1, 2, 3)
- But what is the right encoding to use here?

Why not linear regression?

- Imagine someone comes into the emergency room, and presents with a likelihood of either heart attack, overdose, or treatment for broken bones - and you need a model to quickly determine which is highest/needs to be treated.
- Encoding these outcomes presents a natural ordering (e.g. 1, 2, 3)
- But what is the right encoding to use here?
- When there are natural order to data it isn’t challenging – for example mild moderate or severe infection.
- In this case a linear regression can be calculated to model against 1, 2, and 3, where the gap between 1 and 2 and the gap between 2 and 3 would be considered the same.
- So perhaps a single binary 0 vs. 1 decision could use a linear regression?

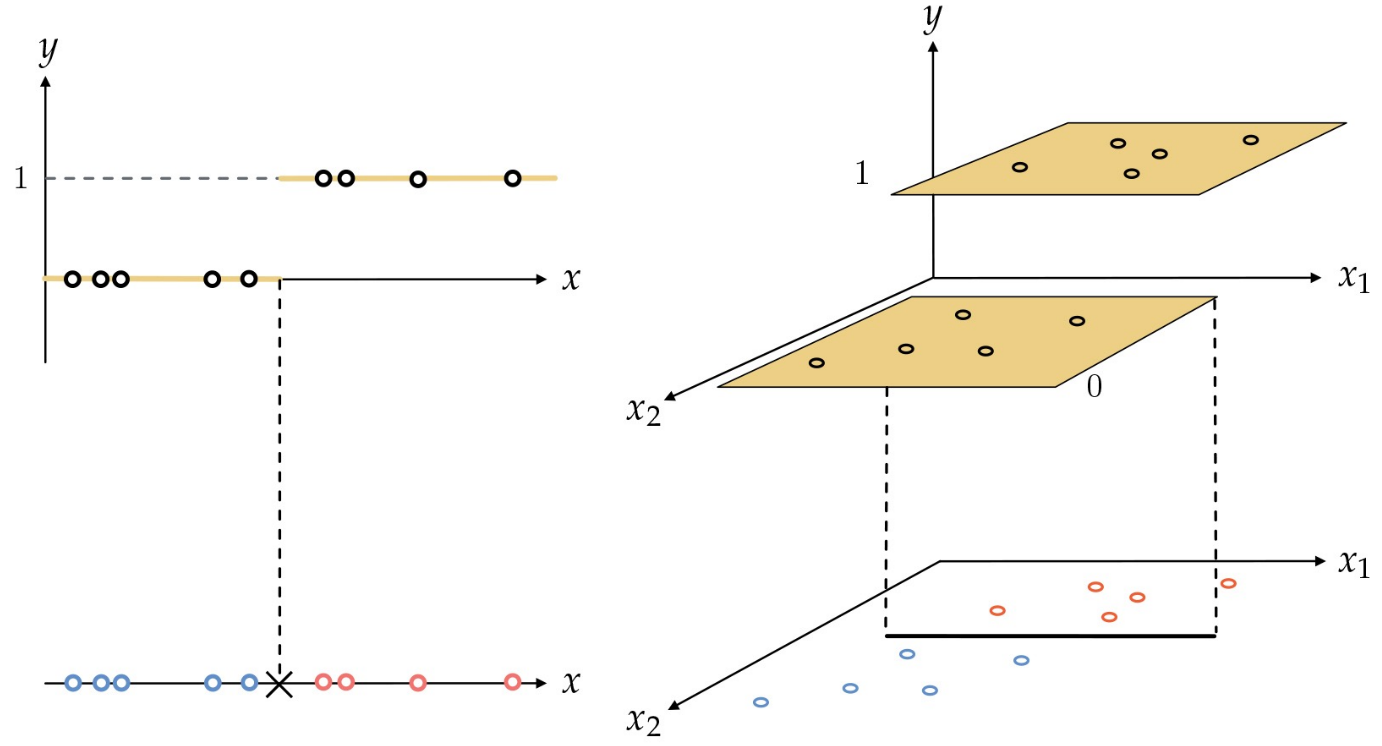
Linear vs. Logistic Regression



- Linear regression could pick a value such that $\hat{y} > \tau$ results in a class decision
- Hard to interpret. Look at the figure on the right – this is easy to predict as a probability p(default | balance)
- It would be nicest to predict the probability of y belonging to a class, then classifying if the probability is > 50%.

Decision Boundaries (Discriminative vs. Generative Models)

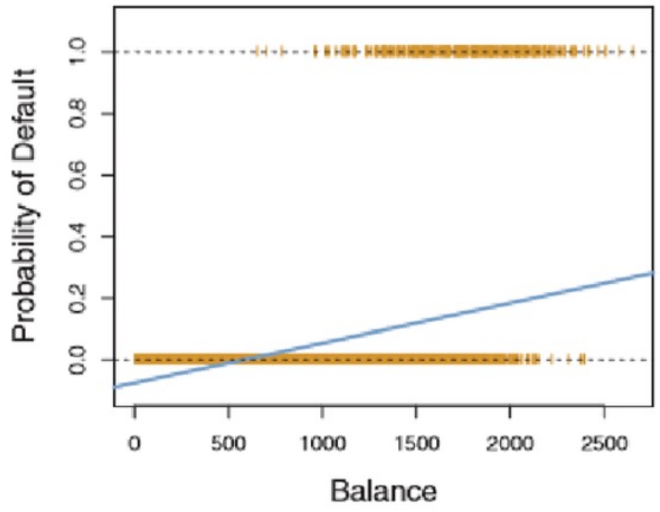
Classification – Step Functions



one-dimensional input:
decision boundary is a single point

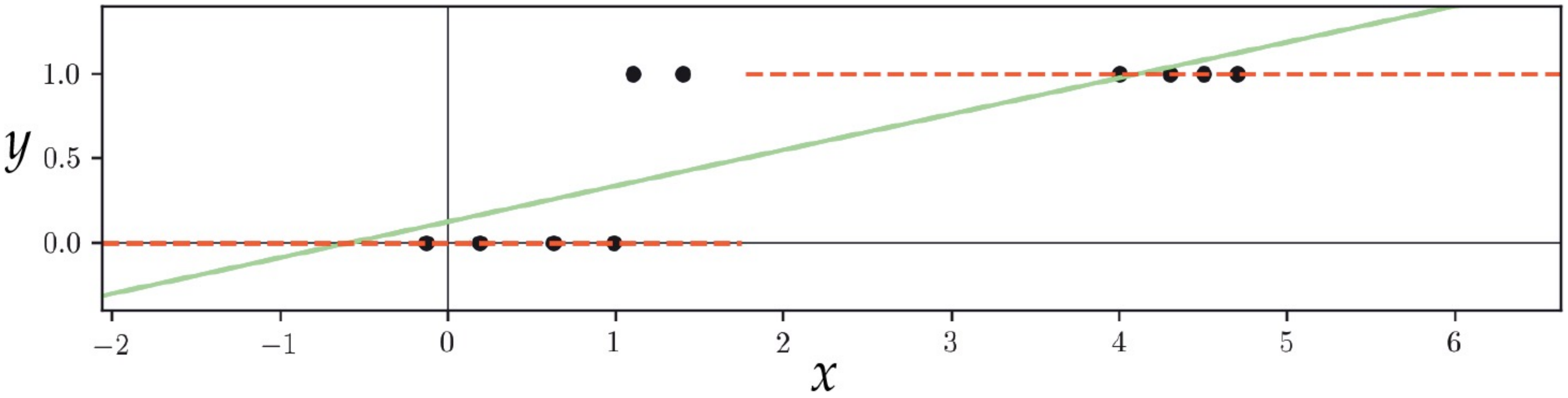
two-dimensional input:
decision boundary is a line

Linear Regression for Classification



If you set y > 0.5 as a decision rule – not clear it works
Hard to interpret – results are not contained in [0,1]

Step function from Linear Regression Boundary



Bernouli Distribution

- We can create a probability density function that represents a single experiment asking yes/no

$$Y \sim Bernoulli\ (\theta), Y \in \{0,1\}$$

$$p(y|\theta) = \ \theta^{I(y=1)}(1-\theta)^{I(y=0)} = \begin{cases} \theta\ , y = 1 \\ 1-\theta, y = 0 \end{cases}$$

- Can think of this as a coin toss experiment and the likelihood of heads vs. tails

Logistic Regression

- Parametric classification method (not regression), which is sometimes referred to as a "generalization" of linear regression because
  - We still compute a linear combination of feature inputs, $\boldsymbol{x}^{\boldsymbol{T}}\ \boldsymbol{w}$ (sometimes written $\boldsymbol{w}^{\boldsymbol{T}}\ \boldsymbol{x}$)
  - However, instead of estimating the continuous output variable, we pass this into a function

$$\mu(\boldsymbol{w}^{\boldsymbol{T}}\boldsymbol{x}) = \frac{1}{1 + e^{-(\boldsymbol{w}^{\boldsymbol{T}}\boldsymbol{x})}}$$

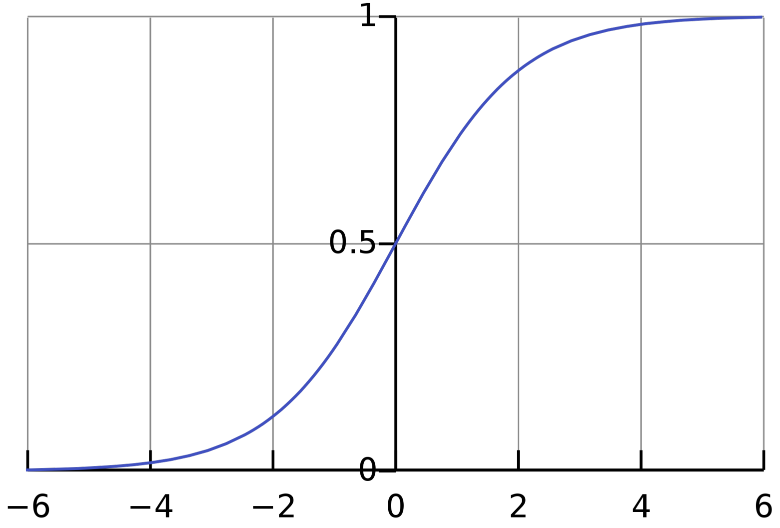
  - Where $0 \leq \mu(\boldsymbol{w}^{\boldsymbol{T}}\boldsymbol{x}) \leq 1$, and where the Gaussian noise of linear regression is replaced by the Bernoulli Distribution so that

$$p(y|\boldsymbol{x}, \boldsymbol{w}) = Ber(y|\mu(\boldsymbol{w}^{\boldsymbol{T}}\boldsymbol{x}))$$

  - Therefore, the output belongs to a class 1 (y = 1) with probability $\mu(\boldsymbol{w}^{\boldsymbol{T}}\boldsymbol{x})$, and class 0 (y = 0) with probability $1 - \mu(\boldsymbol{w}^{\boldsymbol{T}}\boldsymbol{x})$

Why use a Sigmoid Function?

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



- Has very nice properties for classification
  - Bounded between 0 and 1 <- thus interpretable as a probability
  - Monotonically increasing <- thus can be used for classification rules

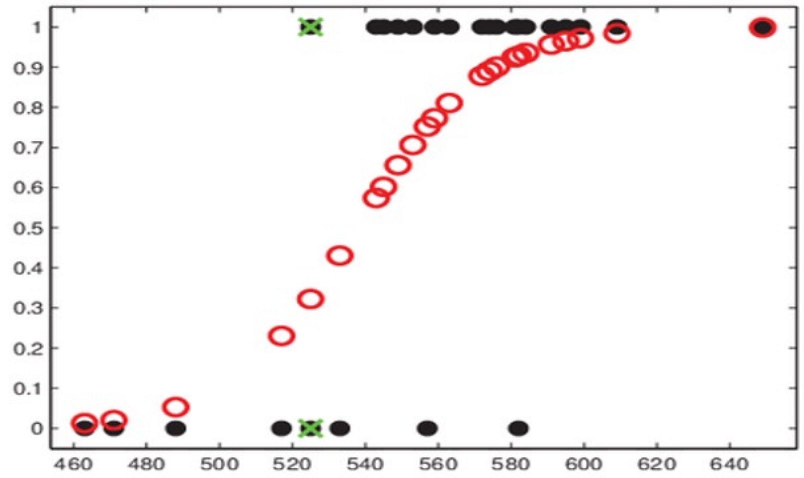
$\sigma(\boldsymbol{\eta}) > 0.5$, positive class (y = 1)

$\sigma(\boldsymbol{\eta}) \leq 0.5$, negative class (y = 0)

  - Nice computational properties for optimizing criterion function

Using logistic function for probability

- Classification task: Predict whether a student will pass a first year class or not
- Features: SAT Scores
- Data: set of SAT Scores and pass/fail labels
- Logistic Regression: Assigns each score to a pass probability (red circle), and assigns label with probability greater than 50%



Logistic Regression: Representation

- Setup classification problem for two classes
  - Input: $\boldsymbol{x} \in \mathbb{R}^{\boldsymbol{p}}$
  - Output: $y \in \{0, 1\}$
  - Training Data: $D = \{(x_1, y_1), \dots, (x_n, y_n)\}$
  - Model parameters: **w** (weights)
  - Model:

$$p(y\,|\boldsymbol{x}, \boldsymbol{w}) = \sigma\left(\boldsymbol{w}^{\boldsymbol{T}}\boldsymbol{x}\right), \sigma(\boldsymbol{\eta}) = \frac{1}{1+e^{-(\boldsymbol{\eta})}} = \frac{e^{\eta}}{1+e^{\eta}}$$

$$y = \begin{cases} 1, p(y\,|\boldsymbol{x}, \boldsymbol{w}) > 0.5 \\ 0, otherwise \end{cases}$$

Logistic Function

- Let's look at an example with a single variable x

$$p(y|x) = p(x) = \frac{e^{w_0 + w_1 x}}{1 + e^{w_0 + w_1 x}}$$

Logistic Function

- Let's look at an example with a single variable x

$$p(y|x) = p(x) = \frac{e^{\beta_0+\beta_1 x}}{1 + e^{\beta_0+\beta_1 x}}$$

- All values are between 0 and 1
- After some algebraic manipulation, we can re-write this as

$$\frac{p(x)}{1 - p(x)} = e^{\beta_0+\beta_1 x}$$

Logistic Function

- Let's look at an example with a single variable x

$$p(y|x) = p(x) = \frac{e^{\beta_0+\beta_1 x}}{1+e^{\beta_0+\beta_1 x}}$$

- All values are between 0 and 1
- After some algebraic manipulation, we can re-write this as

$$\frac{p(x)}{1-p(x)} = e^{\beta_0+\beta_1 x}$$

- These are called odds

Briefly: Odds

- Odds can be between 0 and infinity
- For example: 1 in 5 people will default. This is then with odds 1 out of 4

$p(x) = 0.2$ and then odds $\frac{0.2}{0.8} = \frac{1}{4}$

Briefly: Odds

- Odds can be between 0 and infinity
- For example: 1 in 5 people will default. This is then with odds 1 out of 4

$p(x) = 0.2$ and then odds $\frac{0.2}{0.8} = \frac{1}{4}$

- If we change this to 9 in 10 people

$p(x) = 0.9$ and then odds $\frac{0.9}{0.1} = \frac{9}{1}$ - the odds are 9 to 1

Logistic Function

- Let's look at an example with a single variable x

$$p(y|x) = p(x) = \frac{e^{w_0+w_1 x}}{1 + e^{w_0+w_1 x}}$$

- All values are between 0 and 1
- After some algebraic manipulation, we can re-write this as

$$\frac{p(x)}{1 - p(x)} = e^{w_0+w_1 x}$$

- These are called odds
- Then we can take the log of the odds (the log-odds or logit)

$$\log\left(\frac{p(x)}{1 - p(x)}\right) = w_0 + w_1 x$$

Multiple Logistic Regression

$$\log\left(\frac{p(x)}{1-p(x)}\right) = w_0 + w_1 x_1 + \cdots + w_p x_p$$

- $p(y|x,w) = Ber(y|\sigma(w^T x))$, with a linear decision boundary at p(x) > 0.5
- We can then calculate the negative of the log of the likelihood (negative log likelihood)

$$NLL(w) = -\sum_{i=1}^{n}\left(y_i \log\sigma(w^T x_i) + (1 - y_i)\log\left(1 - \sigma(w^T x_i)\right)\right)$$

Multiple Logistic Regression

$$\log\left(\frac{p(x)}{1-p(x)}\right) = w_0 + w_1x_1 + \cdots + w_px_p$$

- $p(y|x,w) = Ber(y|\sigma(w^Tx))$, with a linear decision boundary at p(x) > 0.5
- We can then calculate the negative of the log of the likelihood (negative log likelihood)

$$NLL(w) = -\sum_{i=1}^{n}\left(y_i \log\sigma(w^Tx_i) + (1 - y_i)\log\left(1 - \sigma(w^Tx_i)\right)\right)$$

- Now suppose we recast $\tilde{y} = \{-1, 1\}$, then

$$NLL(w) = -\sum_{i=1}^{n}\left(\log\left(1 + e^{-\tilde{y}_i w^T x_i}\right)\right)$$

- Which has no closed form solution

Logistic Regression: Evaluation

- Data likelihood (1 training sample)

$$p(y|x) = \begin{Bmatrix} \sigma(w^T x) & y = 1 \\ 1 - \sigma(w^T x) & otherwise \end{Bmatrix} = \sigma(w^T x)^y (1 - \sigma(w^T x))^{1-y}$$

- Data likelihood (all training samples)

$$L(D, w) = \prod_{i=1}^{n} p(y_i|x_i, w) = \prod_{i=1}^{n} \sigma(w^T x_i)^{y_i} (1 - \sigma(w^T x_i))^{1-y_i}$$

- Log Likelihood

$$l(D, w) = \sum_{i=1}^{n} \left(y_i \log \sigma(w^T x_i) + (1 - y_i) \log\left(1 - \sigma(w^T x_i)\right)\right)$$

- Negative Log Likelihood (the cross-entropy error)

$$nll(w) = -\sum_{i=1}^{n} \left(y_i \log \sigma(w^T x_i) + (1 - y_i) \log\left(1 - \sigma(w^T x_i)\right)\right)$$

Next Time

- Continued review of logistic regression
- Discuss why logistic regression has no closed form solution
- Discuss what makes optimizing logistic regression necessary
- Optimizing logistic regression to identify coefficients to variables