Classification, KNN, Logistic Regression (intro)

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Previous session …

- What is Learning?
- Regression - OLS
- Overfitting and underfitting
- Feature Selection
- Model Selection

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This session…

- Parametric and non-parametric models
- KNN
- Classification
- Decision boundary
- Logistic Regression (Intro)

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The session uses content from

- Book: An Introduction to Statistical Learning. James, Gareth, Daniela Witten, Trevor Hastie, and Robert Tibshirani, 2013, ISBN: 978-1-461-47137-0.

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Parametric Models

- E.g. Linear Regression
- Parametric methods involve a two-step model-based approach:
  - First, we make an assumption about the functional form, or shape, of f. For example, one very simple assumption is that f is linear in X:

$$f(X) = \theta_0 + \theta_1 X_1 + \theta_2 X_2 + \cdots + \theta_p X_p$$

  - After the model is selected, we use a certain procedure to estimate the parameters $\theta_0, \theta_1, \ldots, \theta_p$. (In linear regression, we estimated these parameters such that a pre-defined loss function J is minimized)

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Parametric Models - Advantage

- Assuming a parametric form for f simplifies the problem. It is generally easier to estimate a bounded set of parameters, than it is to fit an entirely arbitrary function f.

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Parametric Models - Disadvantage

- *The potential disadvantage* of a parametric approach is that the model we choose will usually not match the true unknown form of f.
- If the chosen model is too far from the true f, then our estimate will be poor.

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Non-parametric Models

- Non-Parametric models are not characterized by a *bounded set* of parameters.
- Non-parametric methods *do not make explicit assumptions about the functional form of f.*
- Instead, they seek an estimate of f that gets as close to the data points as possible without being too rough or wiggly (let the data speak for themselves rather than forcing them to speak through a tiny vector of parameters).

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Non-parametric Models - Advantage

- These approaches have the potential to accurately fit a wider range of possible shapes for f
- Good when you have sufficient number of examples and you don't want to worry about selecting the right features (no prior knowledge).

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Non-parametric Models – disadvantage

- Main disadvantage: a very large number of observations (typically far more than is typically needed for a parametric aprpoach) is required in order to obtain an accurate estimate for *f*

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Parametric and non-parametric models

- **Parametric Models**
  - Advantages:
    - Easier to understand, fast to learn, require much less data
  - Limitations
    - Constrained by a specific form, cannot model complex functional forms, strong assumptions about the data (limited complexity), poor fit if the chosen model is too far from the true function .
  - Popular methods
    - Linear regression
    - Logistic Regression
- **Non-parametric Models**
  - Advantages
    - Flexible: can adapt to a large number of functional forms, no assumptions about the underlying function (fits data better), can result in high performance predictive models.
  - Limitations
    - Requires much more data, overfitting is more likely to occur, harder to explain, slower to learn
  - Popular methods
    - K-nearest neighbors.
    - Decision trees
    - Support vector machines

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Classification

- We tend to refer to problems with a quantitative response as regression problems, while those involving a qualitative response are often referred to as classification problems
- Classification problems occur often, examples:
  1. An emergency room service that classifies possible medical condition based on a set of symptoms.
  2. An online banking service that classifies if a transaction being is fraudulent based on some user data such as IP address and past transaction history.
  3. An email service that indicates if a received email is spam or not.
  4. Identify which DNA mutations that may cause a give disease and which of these mutations don't based on DNA sequence data for several patients with and without that disease.

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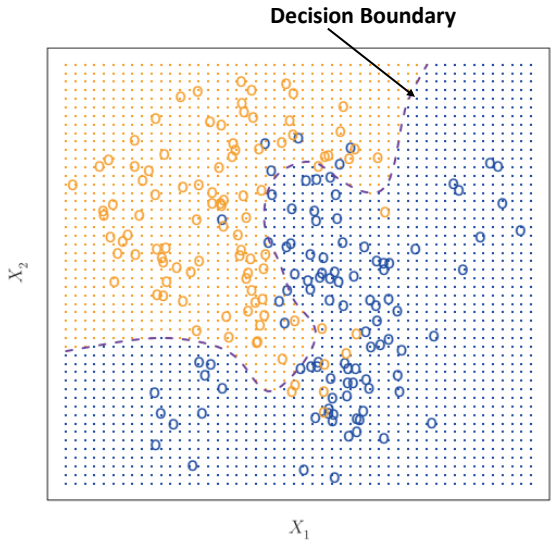
Classification



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KNN

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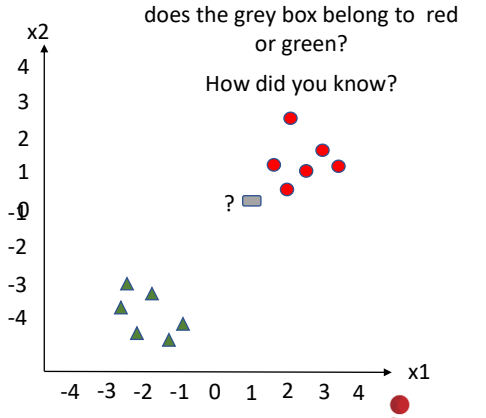
K- Nearest Neighbors (KNN) Classifier

- A Non-Parametric Model
- Key idea: the value of the output function is the known output of the nearest training instance.
- An example of *instance-based learning*: it constructs hypotheses directly from the training instances
- A *lazy learning* approach: it delays the use of training set until the system receives a query.



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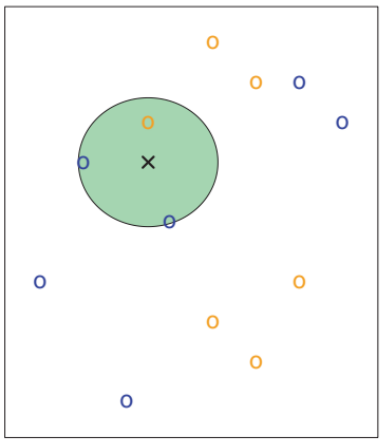
How does it work?

- Given a positive integer *K* and a test observation X_t, the KNN classifier first identifies the *K* points in the training data that are closest to X_t represented by $\mathcal{N}_0$.
- It then estimates the conditional probability for class *j* as the fraction of points in $\mathcal{N}_0$ whose response values equal *j*

$$\Pr(Y = j|X = X_t) = \frac{1}{K}\sum_{i\in\mathcal{N}_0} I(y_i = j)$$

$I(y_i = j)$is an *indicator variable* that equals 1 if $y_i = j$



The K-NN using K=3

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Algorithm

- Algorithm
  - For any given query x_q, find the closest k training instances
  - The output t_q is the class of the majority of k nearest instances

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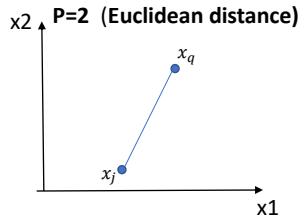
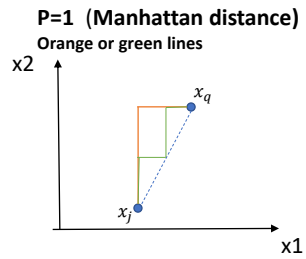
How we determine the neighbors? Distances

- Distance from a query point x_q to an example point x_j
- **Minkowski distance** $L^p(x_j, x_q) = (\sum_i (|x_{j,i} - x_q|^p)^{\frac{1}{p}}$
- Use p=2 (Euclidean distance) if the dimensions are measuring similar properties (e.g. width, height, and depth)
- Use p=1 (Manhattan distance) if the dimensions are dissimilar (e.g. age, weight, and gender)





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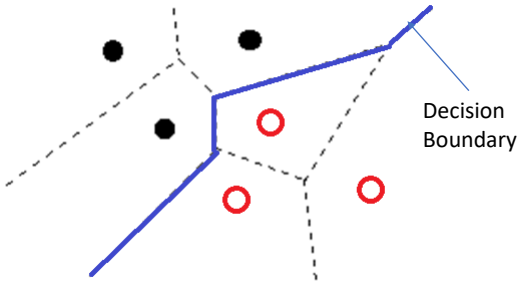
Nearest Neighbour

- The value of the output class is calculated
- All points within R1 are closer to P1 than any other point in the training set



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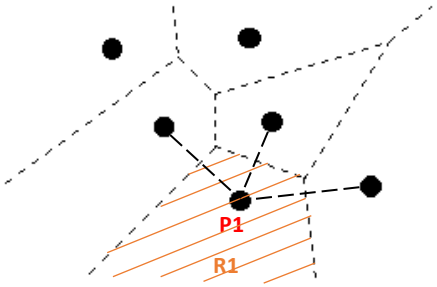

Voronoi diagram

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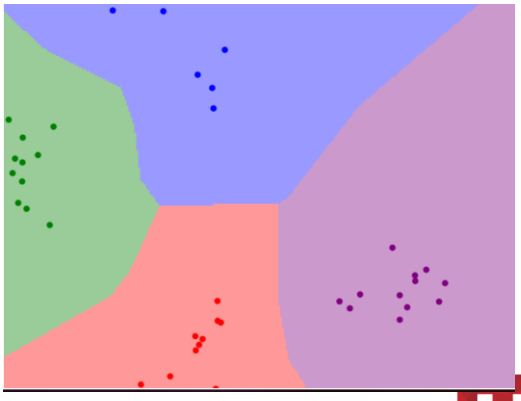
KNN

- The value of the output function is calculated by taking the plurality vote of the k nearest neighbors.
- To avoid ties, k is always chosen to be an odd number
- Can we use it for regression? How?

http://vision.stanford.edu/teaching/cs231n-demos/knn/



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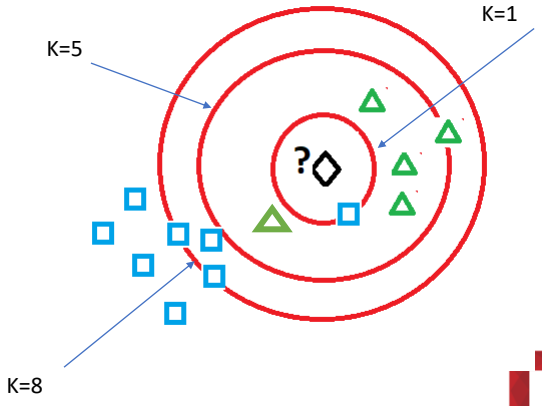
Choosing the right k

- Too small K means, more sensitive to noise (high variance, low bias).
- Too large K, you will have a less flexible may include instances from other classes (high bias, low variance)



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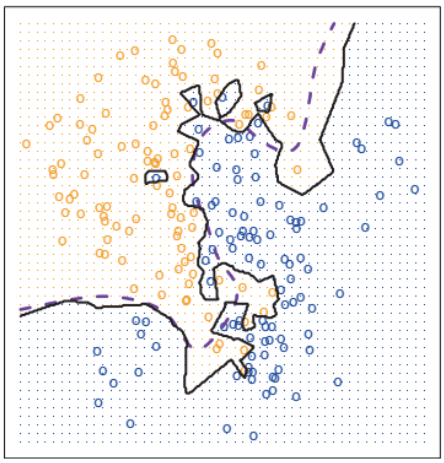
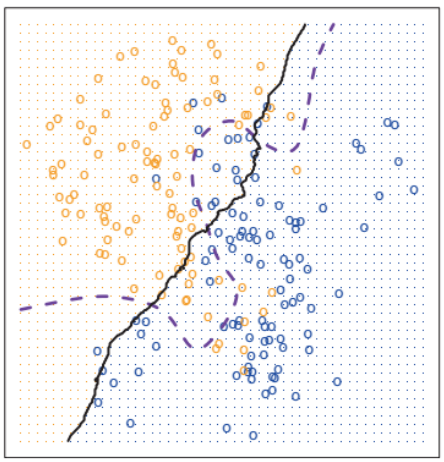
A comparison of the KNN decision boundaries

KNN: K=1



More sensitive to noise

KNN: K=100



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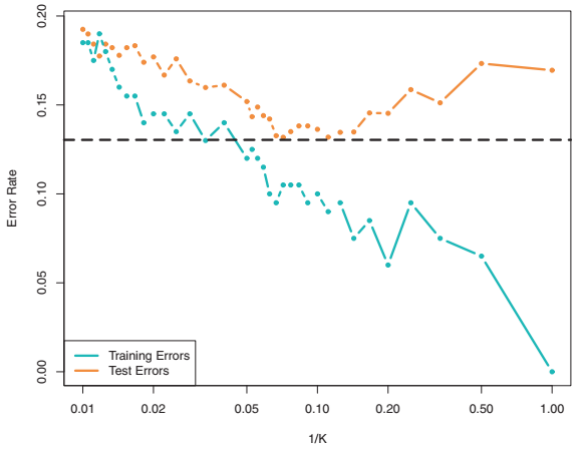
Test and training errors



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Considerations

- Nearest Neighbor Search:
  - To find the nearest neighbours we need to find the distance to all N training examples (brute force search) O(dN), d number of dimensions
  - To improve the efficiency and make the algorithm faster we can use data structures such as K-d trees (require pre-sorting) to speed up the search process (via space partitioning mechanism)- good for low-medium dimensions – can miss neighbours – complexity (O(dlogN))
  - Hashing techniques such as Locality sensitive hashing (**LSH**) can be used to approximate the nearest neighbor search in high dimensions.
- Other considerations to improve the result of KNN
  - Curse of dimensionality: required number of training sets increases with the dimension.
  - Consider reducing d by removing irrelevant and correlated dimensions.
  - Consider reducing N by removing redundant data (e.g. condensing)

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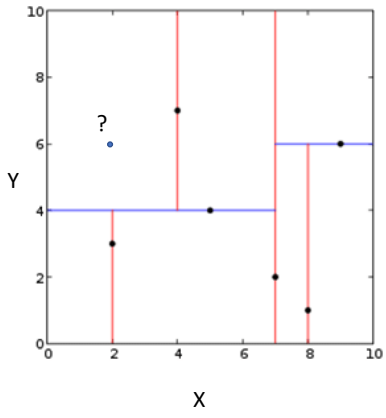
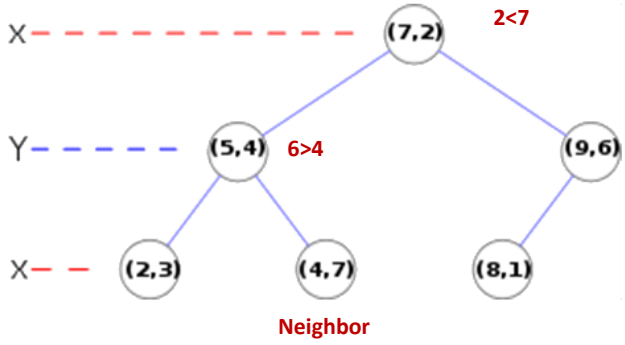
K-d trees



Find neighbor of
(6,2)



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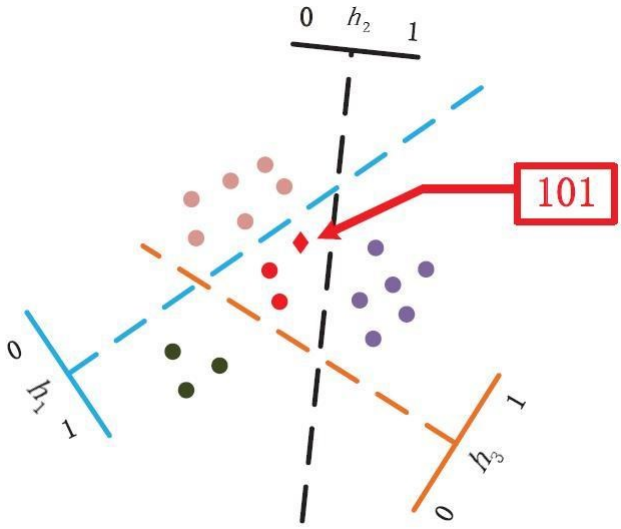
Locality Sensitive Hashing



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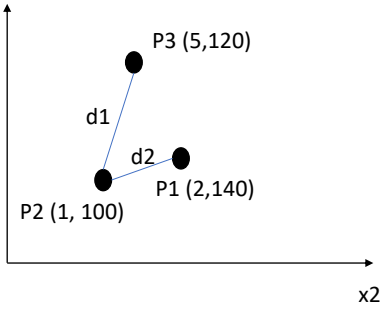
Why we need feature scaling?

- d1 = $sqrt\left((5-1)^2+(120-100)^2\right) = 20.39$
- d2 = $sqrt\left((2-1)^2+(140-100)^2\right) = 40.01$
- Which attribute determine the distance?
- If one attribute has a broad range of values, the distance will be governed by this attribute (will be more important in the classification)
- Objective functions in many algorithms will not work properly without feature scaling.



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Normalization

- Linearly scale the range (for example: scale the range in [0,1]

$$x_i' = \frac{x_i - \min(x)}{\max(x) - \min(x)}$$

- When the value of x_i' is the minimum value in the given dataset, the numerator will be 0, and hence x_i' is 0
- When the value of x_i' is the maximum value in the in the given dataset, the numerator is equal to the denominator and thus the value of x_i' is 1
- If the value of x_i' is between the minimum and the maximum value, then the value of x_i' is between 0 and 1
- Disadvantage: you end up with smaller standard deviations, which can suppress the effect of outliers

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Standardization

- Another scaling technique that scales the feature values so that the mean of the scaled attribute becomes zero and the standard deviation is 1.
- Scale each dimension to have zero-mean and unit-variance

$$x_i' = \frac{x_i - \bar{x}}{\sigma}$$

- where $\bar{x}$ is the mean of the feature vector and σ is the standard variation

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Logistic Regression (Intro)

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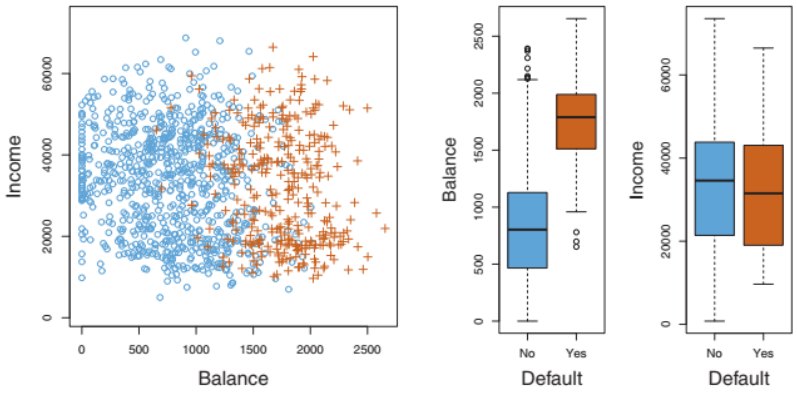
Classification Example

- The individuals who defaulted failed to make a payment on your credit card) on their credit card payments are shown in orange, and those who did not are shown in blue (how can we classify them).
- Individuals who defaulted tended to have higher credit card balances than those who did not.



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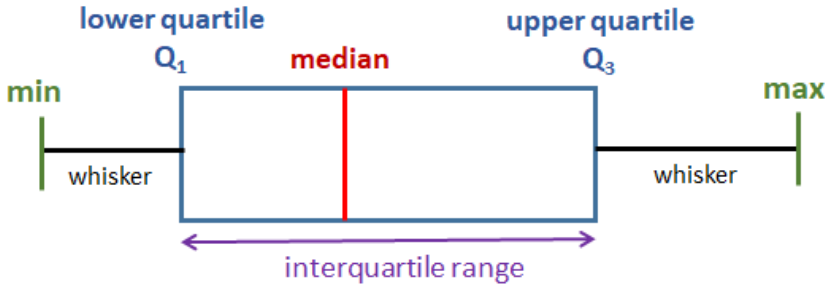
Box and Whisker Plot



https://www.onlinemathlearning.com/box-plot.html

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Can we use Linear Regression

- Assume you are classifying a credit card transaction and you choose
  - 1 for fraudulent transactions
  - 0 for non-fraudulent transaction
- Can we use linear regression such that it produces y =1 for fraudulent transactions and y=0 for non-fraudulent transaction? What is the problem with this approach?

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Problem if you try to use linear regression

- One problem is that if you choose a different code (e.g. 0 for fraudulent transactions and 1 for non-fraudulent transaction) will lead to a different model. How about if you use 50 for fraudulent and 150 for non-fraudulent?
- Unless the values of the output response has a natural ordering nature (such as mild, moderate and severe), how can we order different classes (e.g. different medical conditions)

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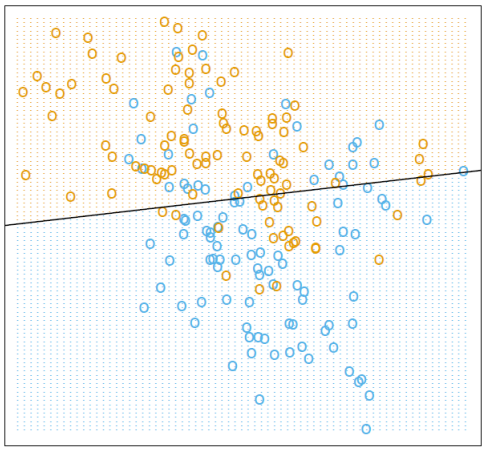
Linearly separable problems

- The classifier has a linear decision boundary that separate the space into two regions.
- $\hat{y} = \theta_0 + \theta_1 x_1 + \theta_2 x_2 + \cdots .$
- Output (o)=
$$\begin{cases} Class\ 1 & if\ \hat{y} \geq 0 \\ Class\ 2 & if\ \hat{y}\ otherwise \end{cases}$$
- o= $sign(\hat{y})$



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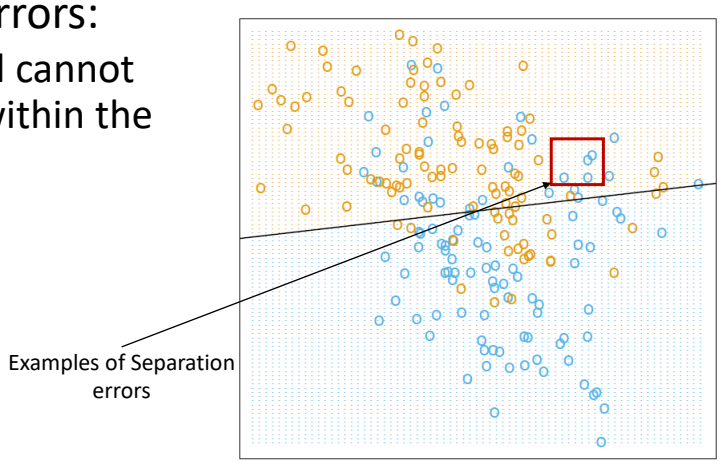
How about separation errors

- Causes for separation errors:
  - The model is simple and cannot capture the variations within the data
  - Noise in the data and mislabelling



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How Can We Estimate the Model Parameters?

- Zero-one loss.

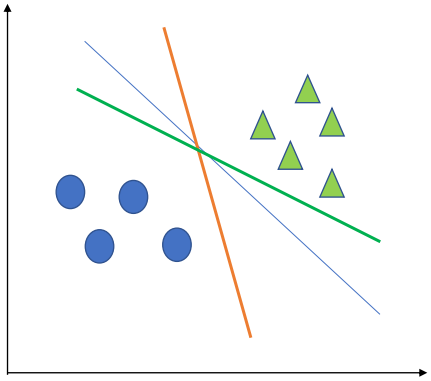
$$l_{0-1}(o,t) = \begin{cases} 1 \; if \; t \neq o \\ 0 \; if \; t = o \end{cases}$$

Is it easy to minimize this function? Why?

- Asymmetric Binary Loss (ABL)

$$l_{ABL}(o,t) = \begin{cases} \alpha \; if \; t = 1 \; and \; o = -1 \\ \beta \; if \; t = -1 \; and \; o = 1 \\ 0 \; if t = o \end{cases}$$

What is the problem with such functions?



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Logistic Regression

- Logistic regression models the *probability* that the output belongs to a particular category $\Pr(Y = k|X = x)$ using the logistic (sigmoid) function.
- Why a logistic function?
  - It produces a value between 0 and 1 (range of the probability values)
  - It can be viewed as a differentiable and smoothed alternative to sign.
- Allows gradient-based learning of parameters
- A model for classification (not regression).

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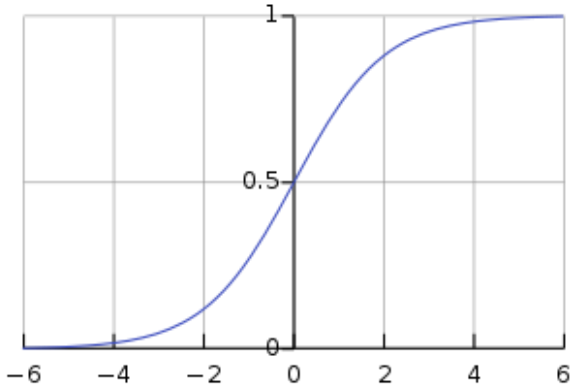
Logistic Function

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



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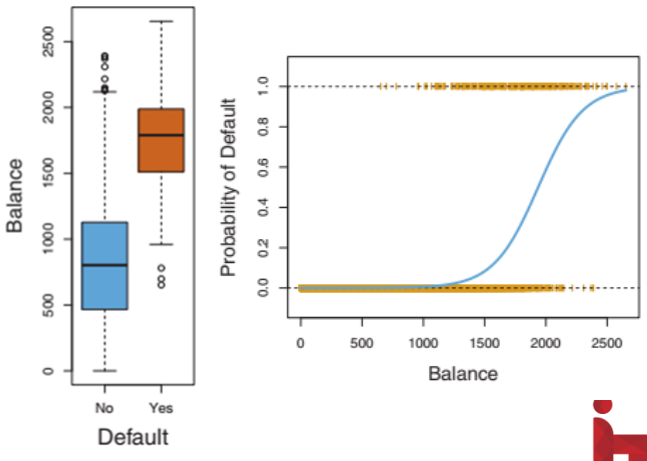
In the credit card payments example

- $\Pr(default = Yes|blanace) = \sigma(\theta_0 + \theta_1 * blance)$
- One might predict default = Yes for any individual for whom $\Pr(default = Yes|blanace) > 0.5$.
- Alternatively, a more conservative approach in predicting whether an individual will default (fail to repay) on his or her credit card payment $\Pr(default = Yes|blanace) > 0.1$



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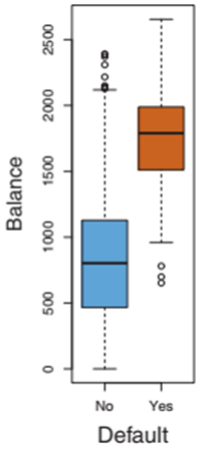
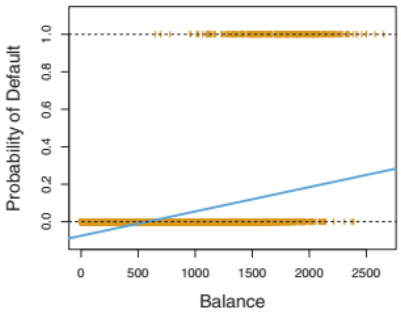
Assume you use a linear model (without a logistic function)

- $\Pr(default = Yes|blanace) = \theta_0 + \theta_1 * blance$
- For balances close to zero we predict a negative probability of default; if we were to predict for very large balances, we would get values bigger than 1 (not sensible).





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