EE2211 Introduction to Machine Learning

Lecture 9

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Acknowledgement: EE2211 development team
Thomas, Helen, Xinchao, Kar-Ann, Chen Khong, Robby and Haizhou

Course Contents

- Introduction and Preliminaries (Xinchao)
  - Introduction
  - Data Engineering
  - Introduction to Probability and Statistics
- Fundamental Machine Learning Algorithms I (Vincent)
  - Systems of linear equations
  - Least squares, Linear regression
  - Ridge regression, Polynomial regression
- Fundamental Machine Learning Algorithms II (Vincent)
  - Over-fitting, bias/variance trade-off
  - Optimization, Gradient descent
  - Decision Trees, Random Forest
- Performance and More Algorithms (Xinchao)
  - Performance Issues
  - K-means Clustering
  - Neural Networks

Fundamental ML Algorithms: Decision Trees, Random Forest

Module III Contents

- Overfitting, underfitting and model complexity
- Bias-variance trade-off
- Regularization
- Loss function
- Optimization
- Gradient descent
- Decision trees
- Random forest

Review

- Supervised learning: given feature(s) x, we want to predict target y to be some $f(x)$
  - If y is continuous, problem is called “regression”
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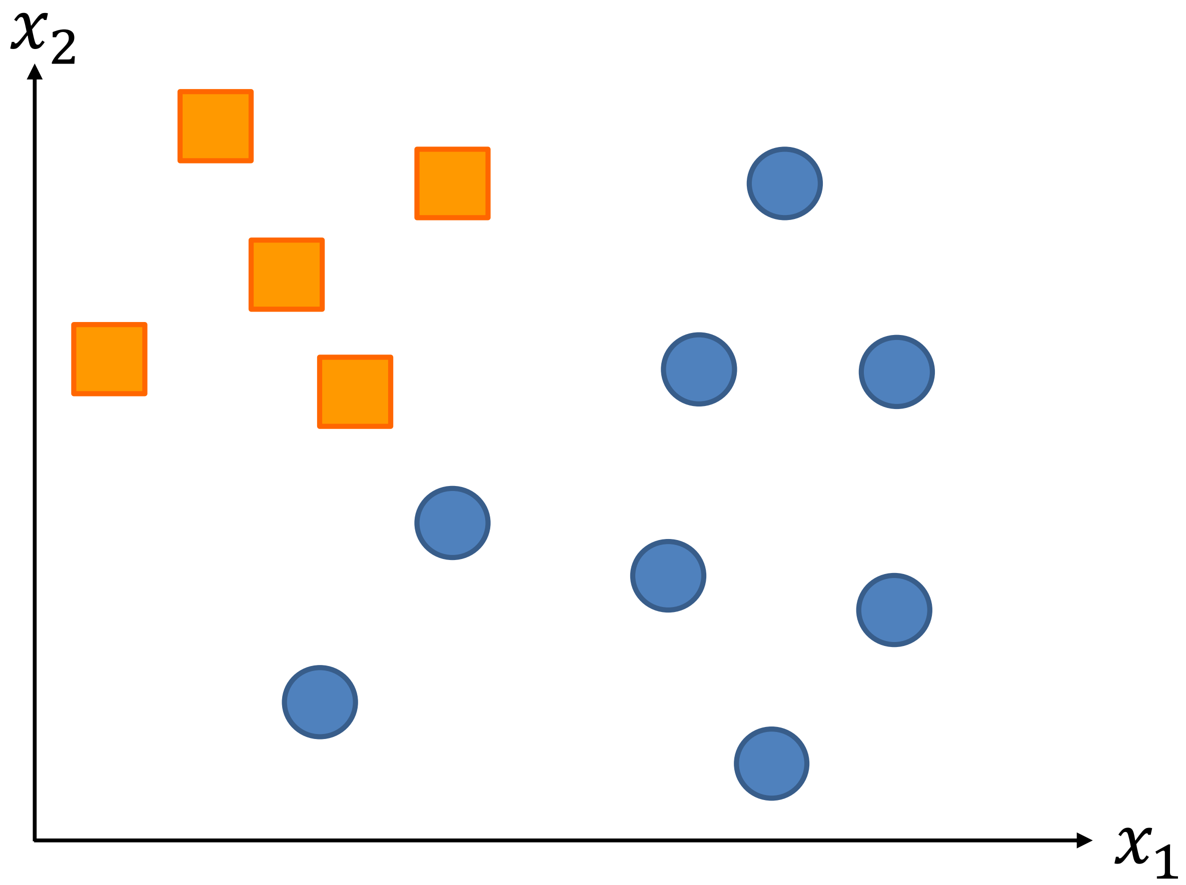
- Previous lectures used linear models for regression (and classification)
  - Nonlinearity added by using polynomial regression or other learning models
- New approach today: trees

Decision Tree Classification Example

- Goal: predict class labels using two features x_1 & x_2



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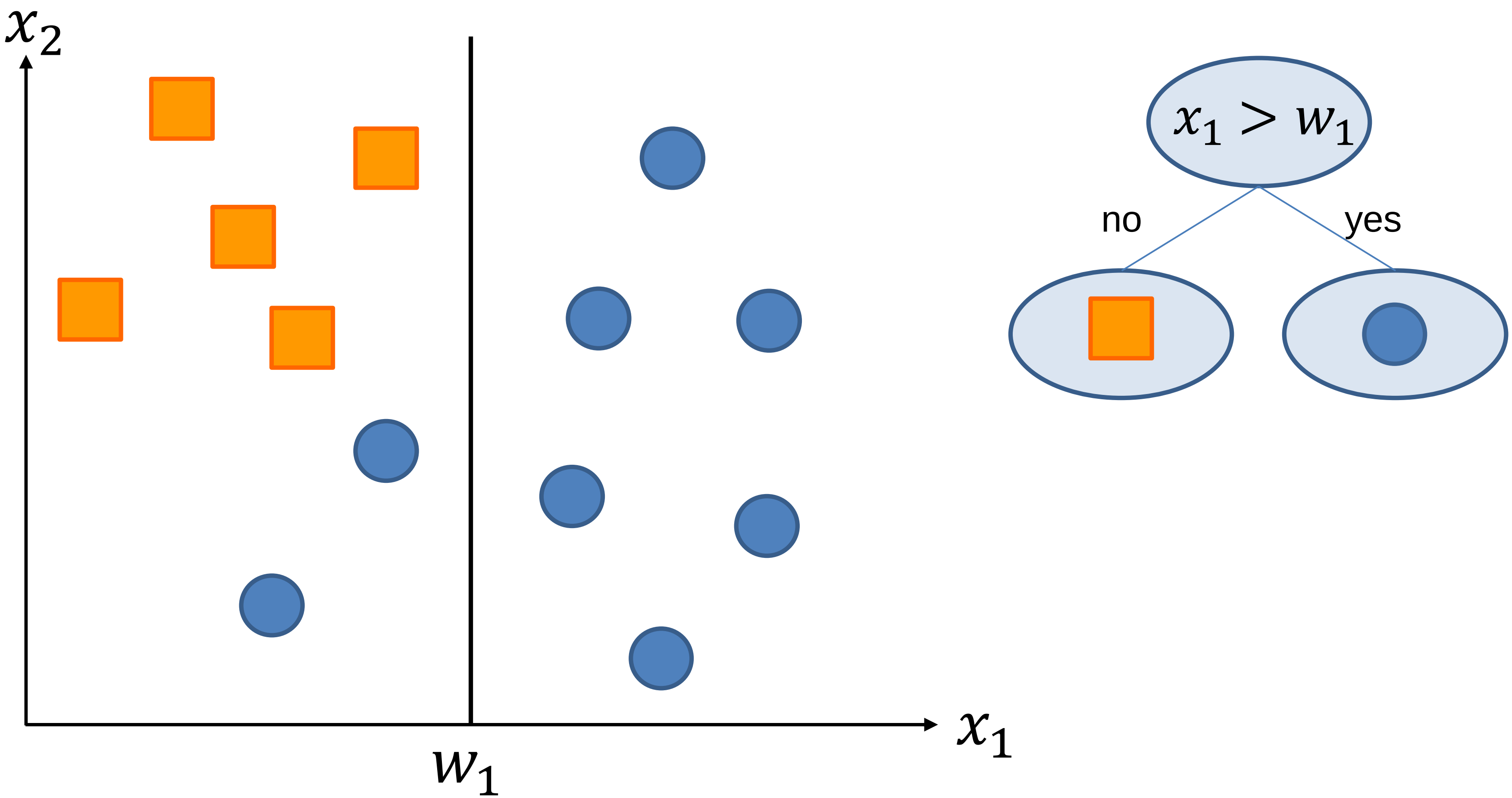

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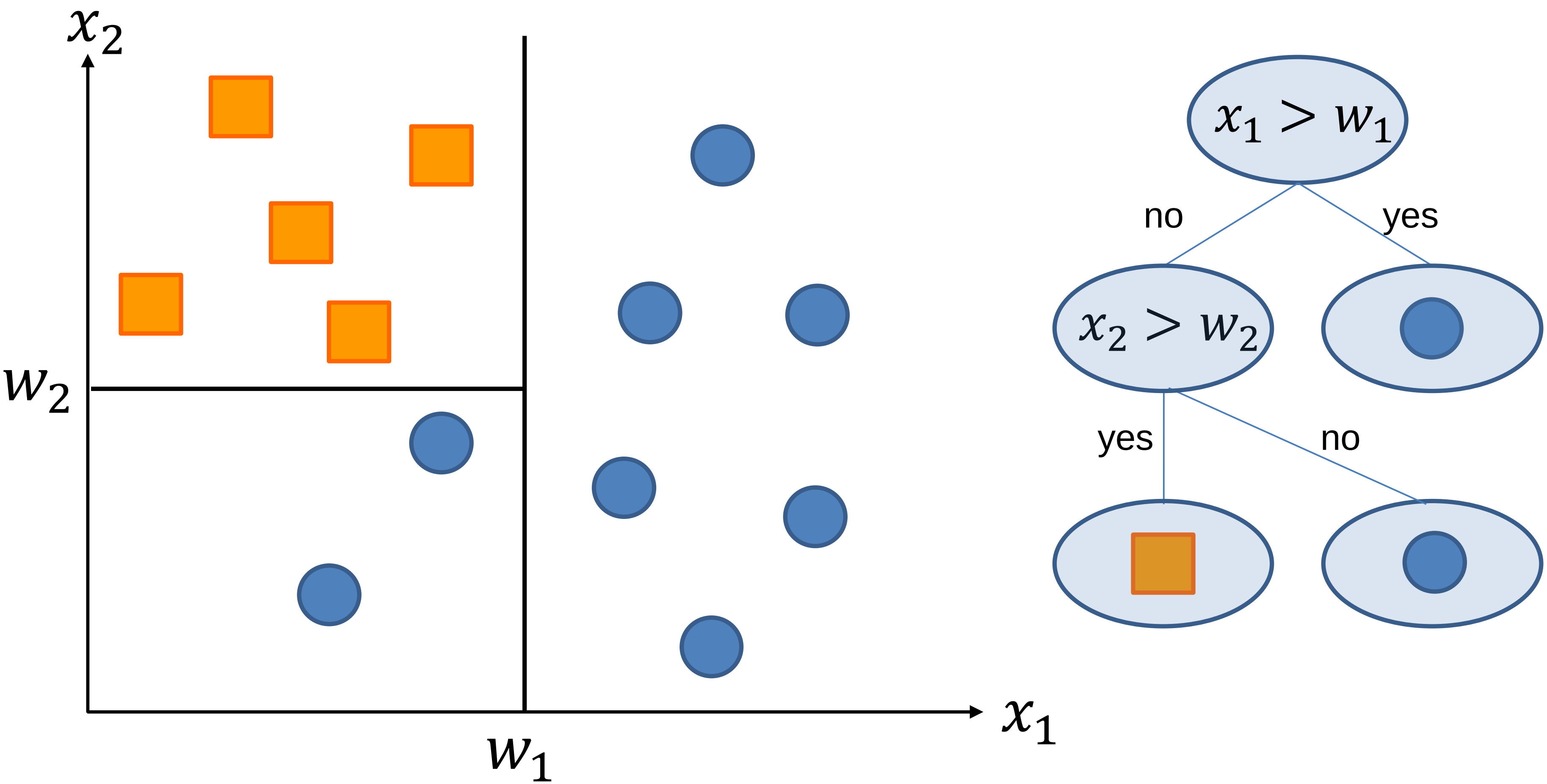
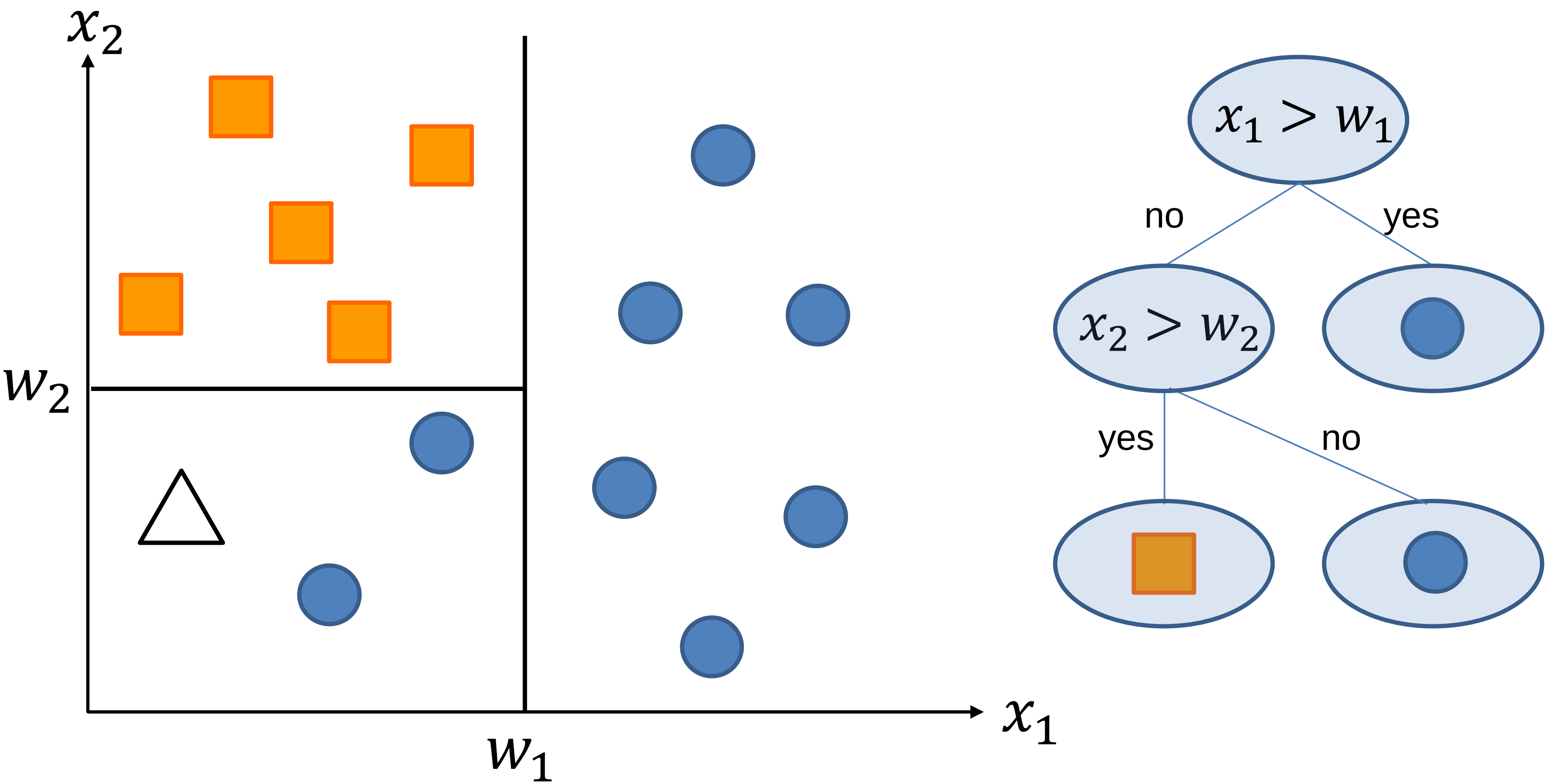


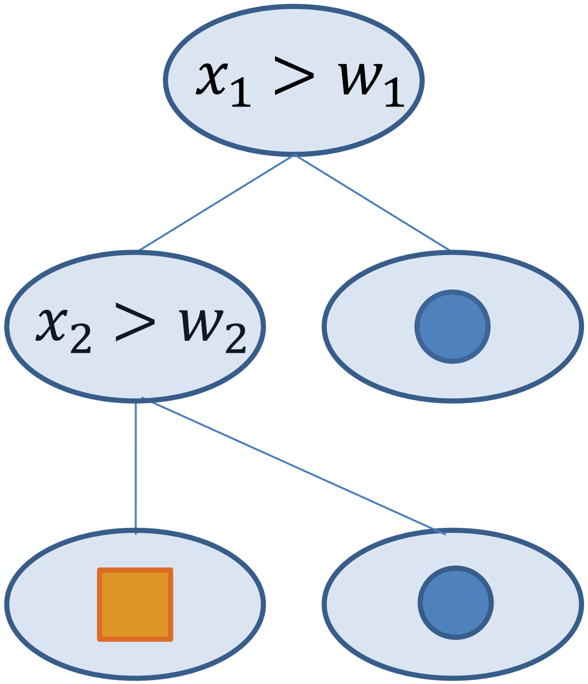
Decision Tree Classification Example

- In our test set, we observe datapoint △ shown below. How would the decision tree classify this point?



Questions?

Basic Terminologies



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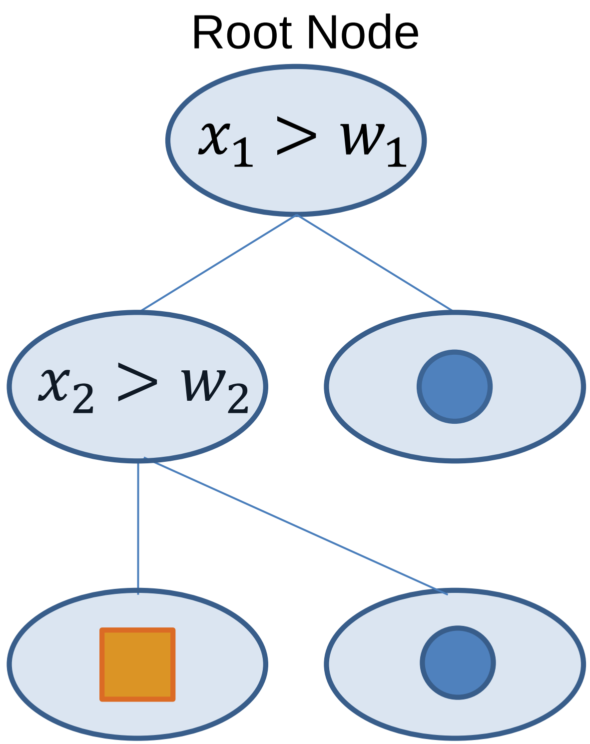

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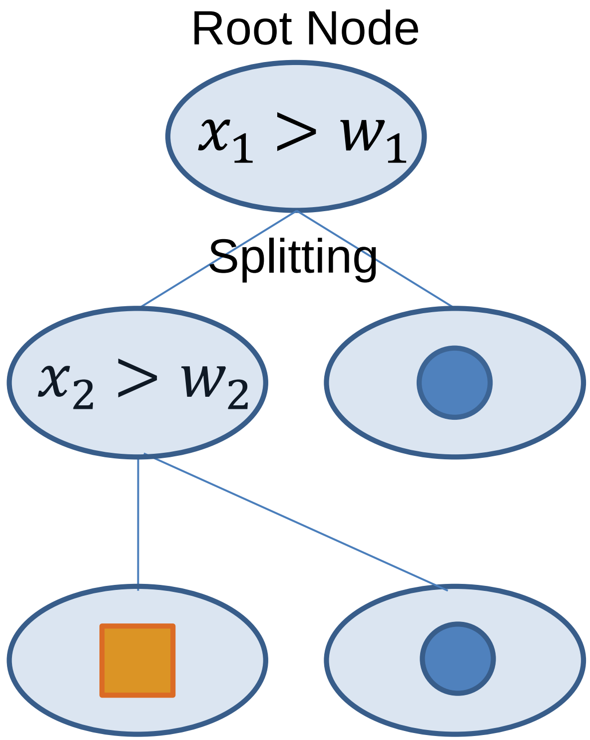

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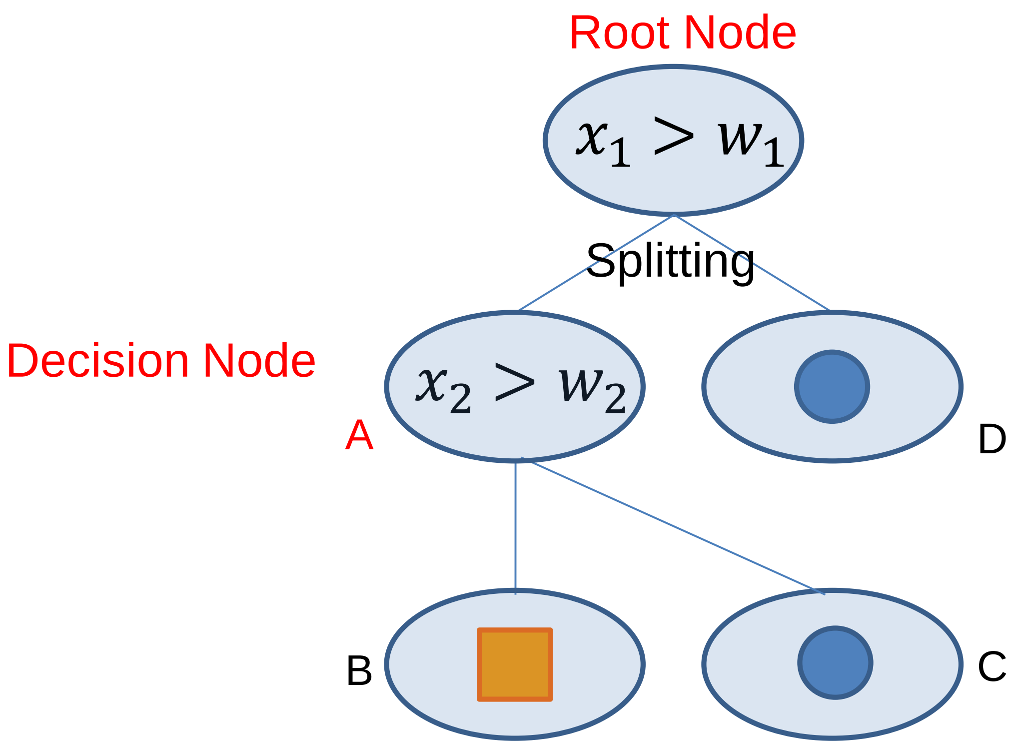

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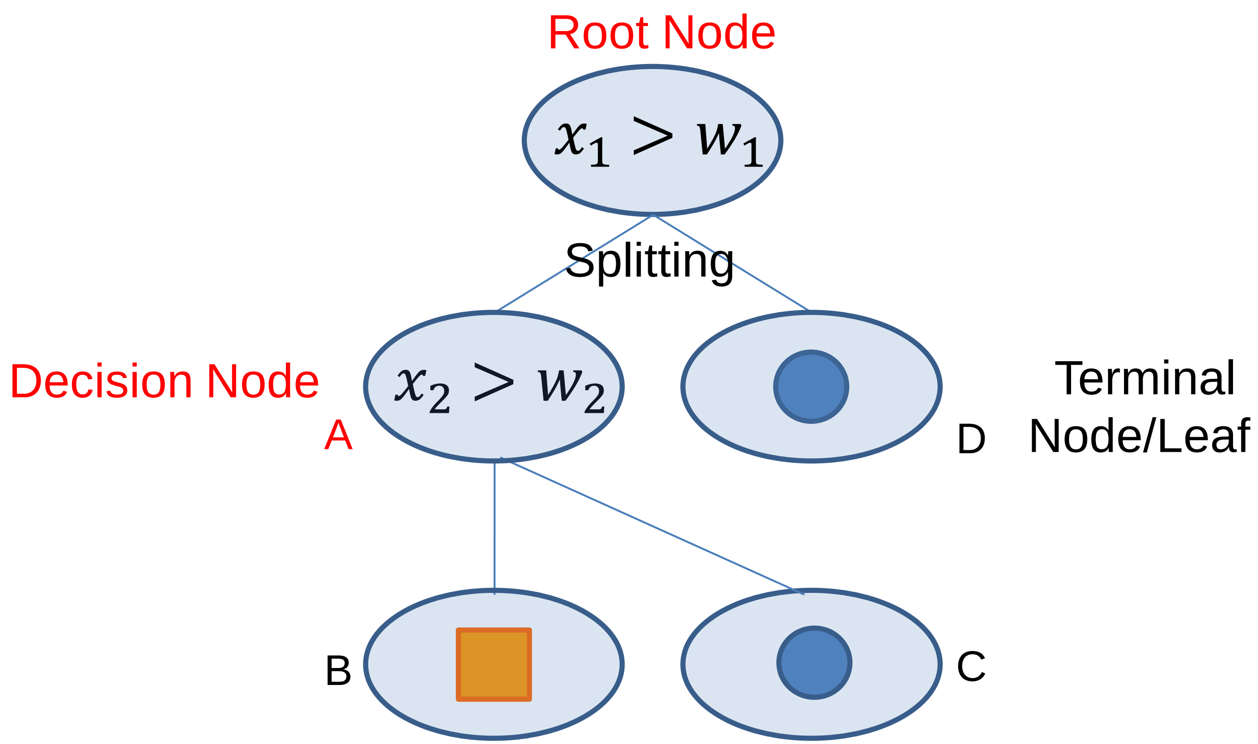
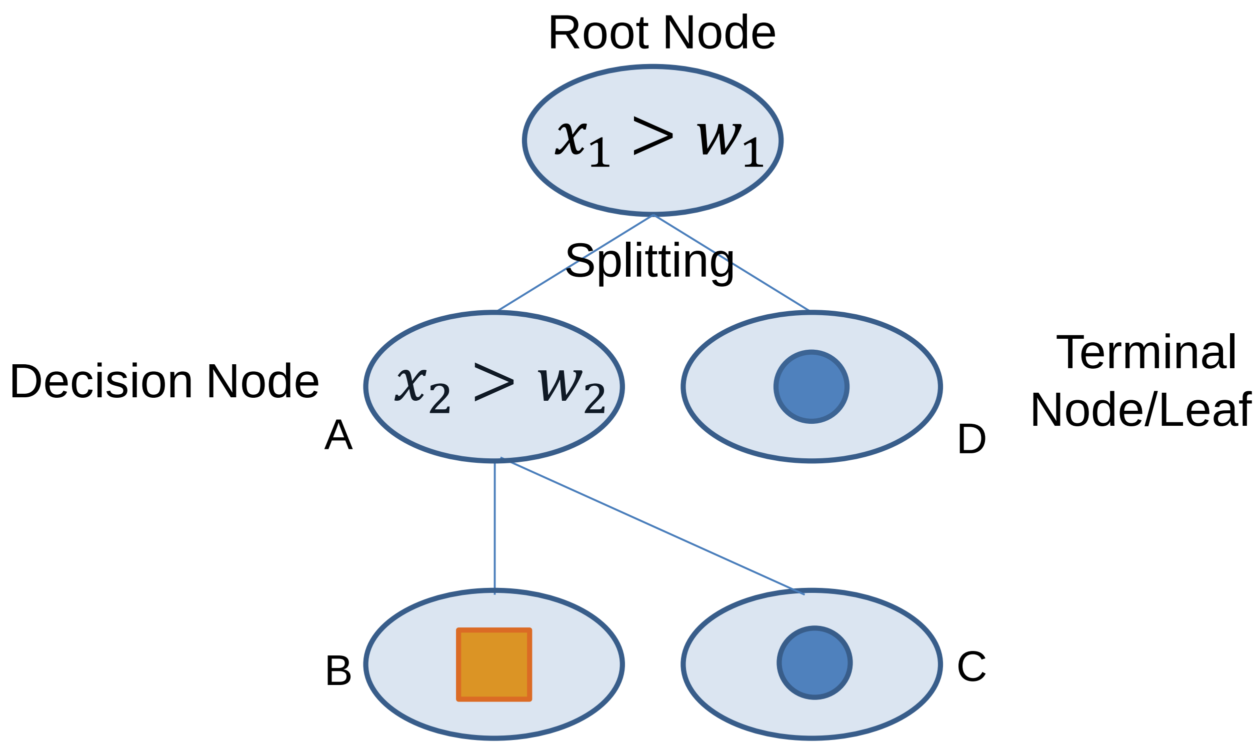


B and C are Terminal Nodes or Leaves

Basic Terminologies



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A-B-C forms a **sub-tree** or **branch**.

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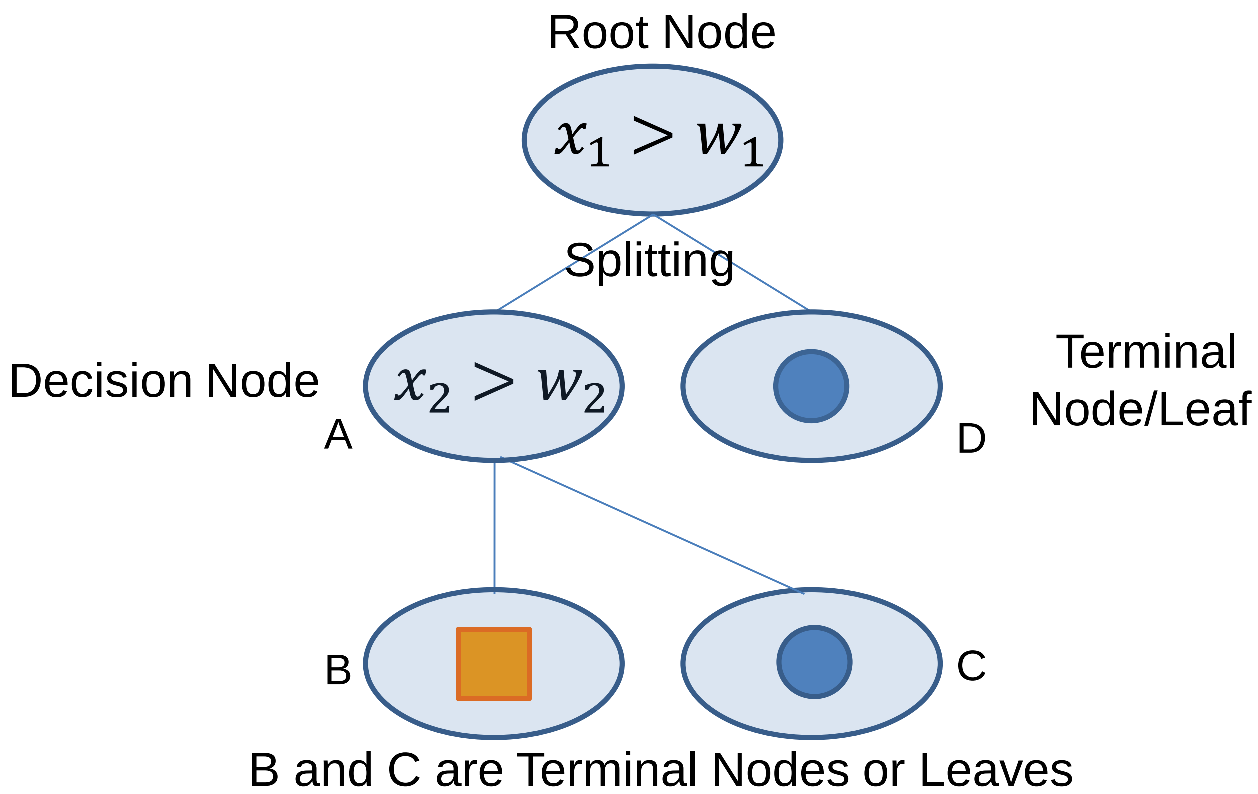

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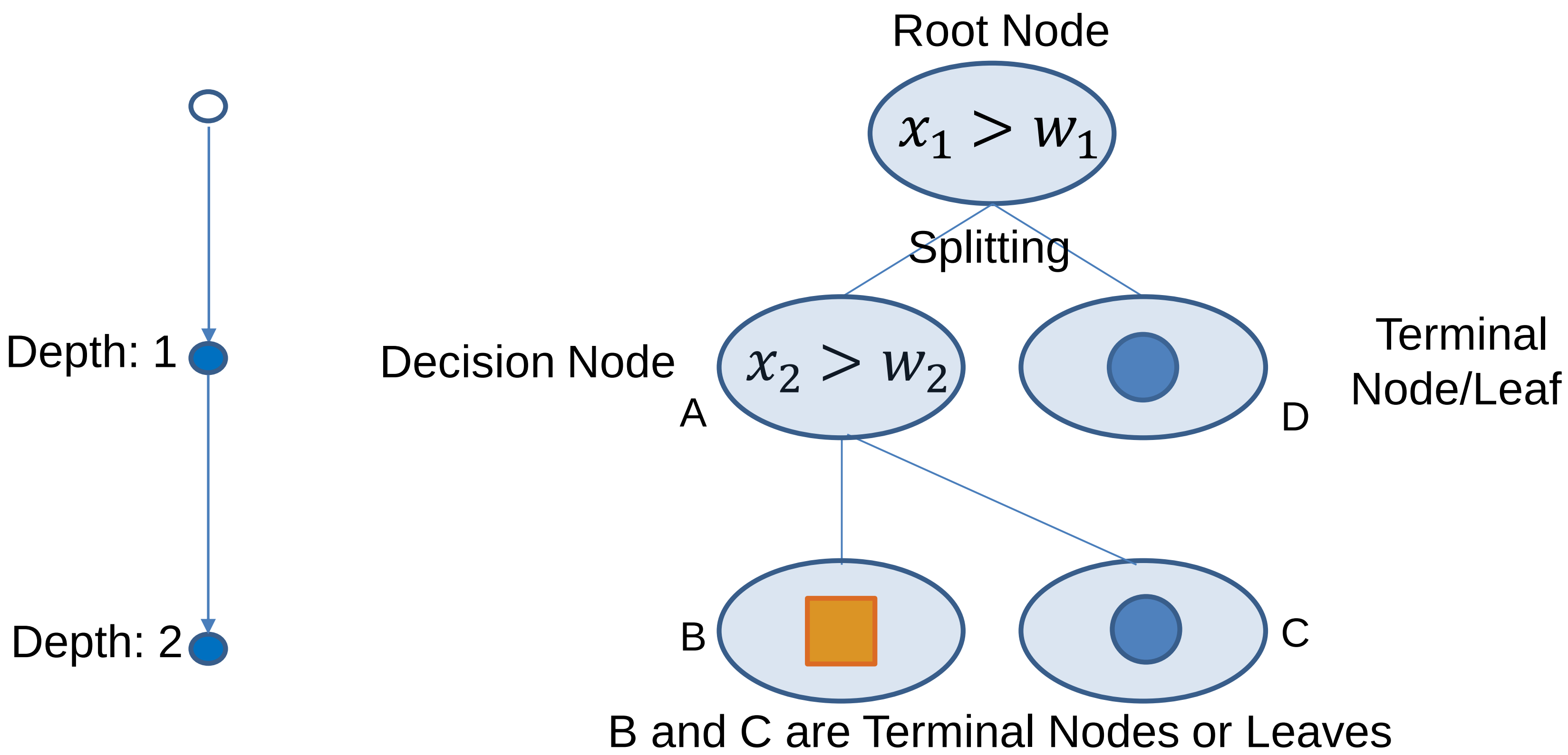

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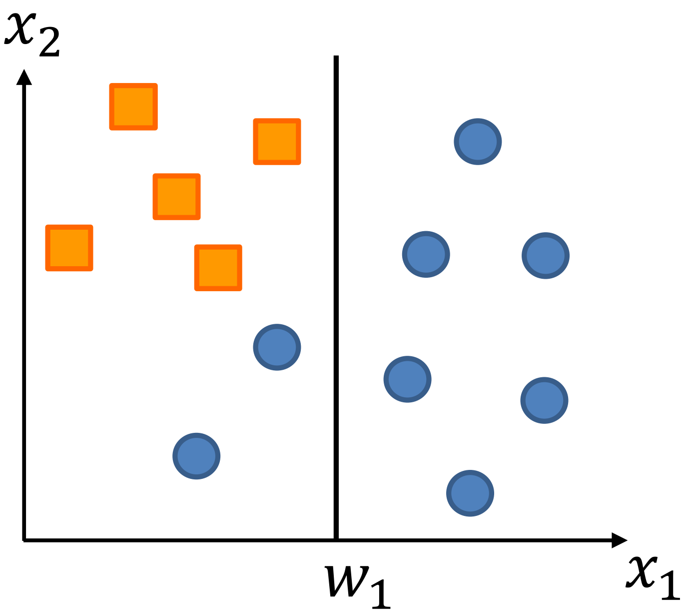
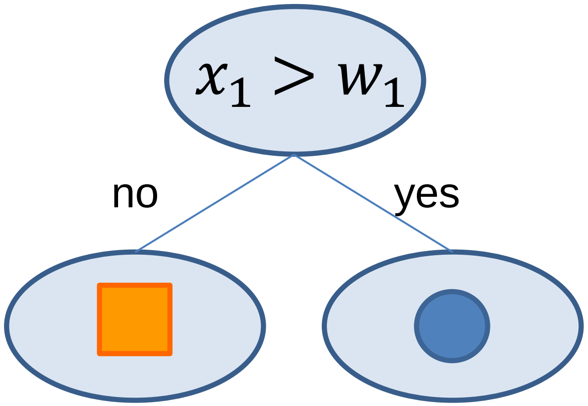
- Finding smallest tree is computationally hard, so we typically use some greedy algorithm not guaranteed to find the best tree
- We need to first define the concept of node impurity

Node Impurity





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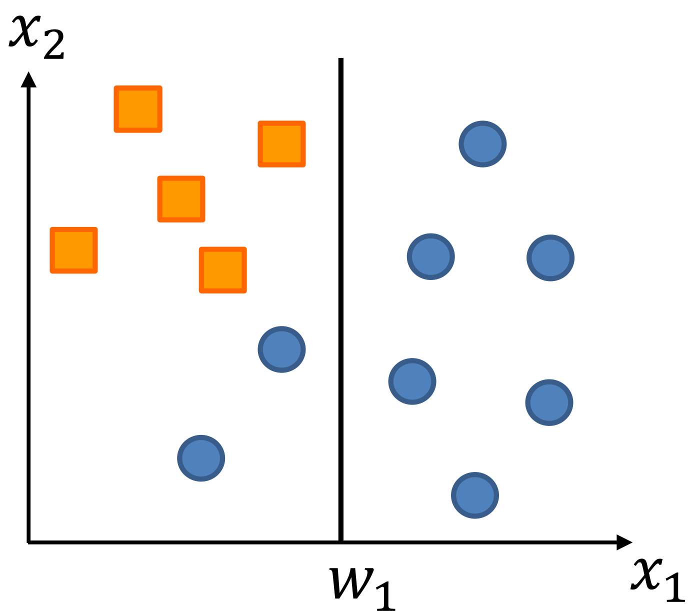

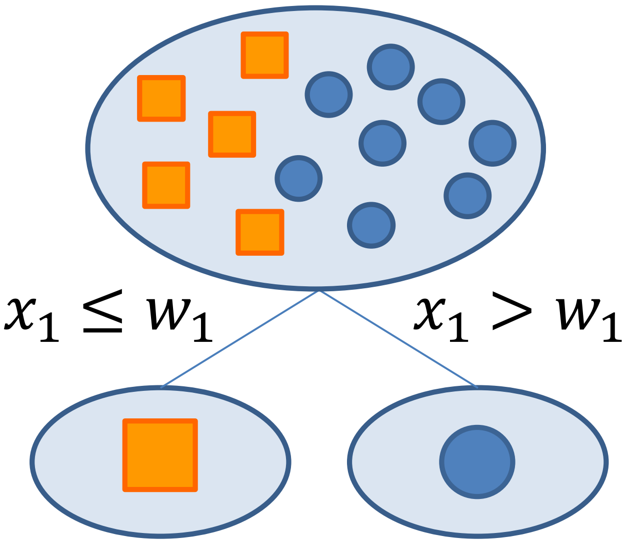

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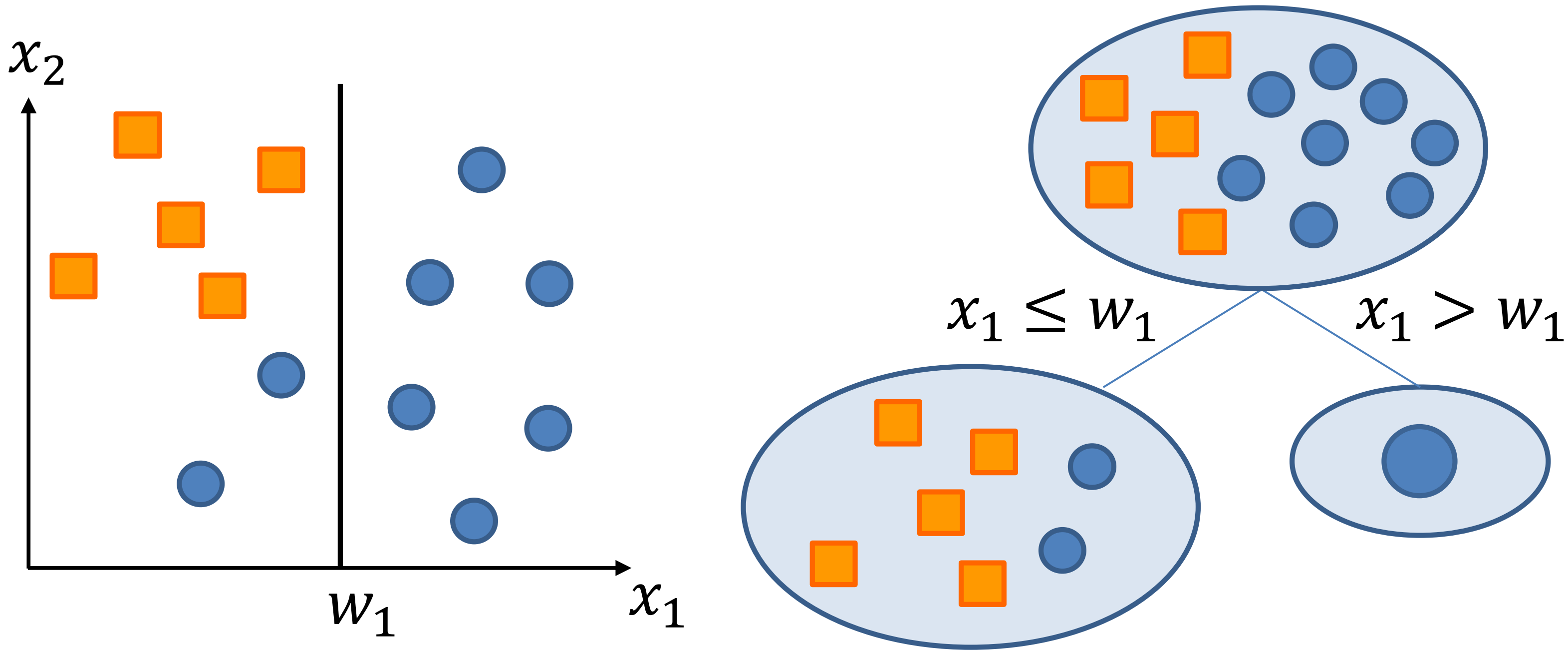

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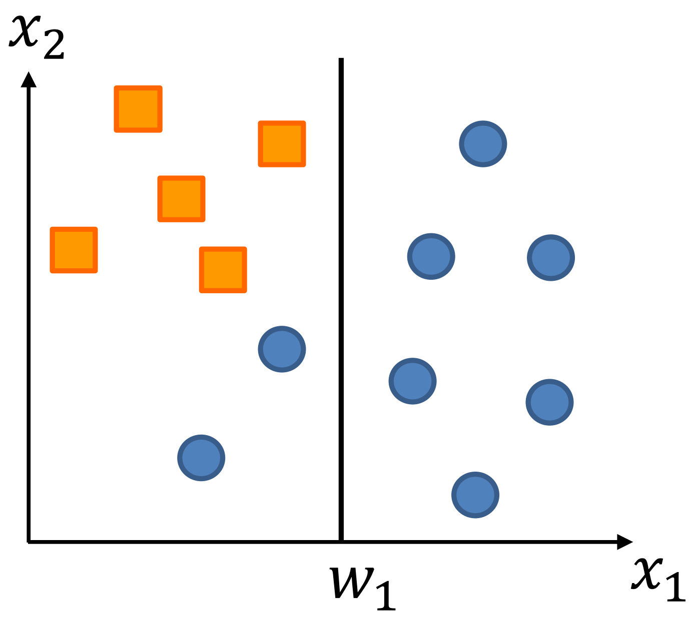

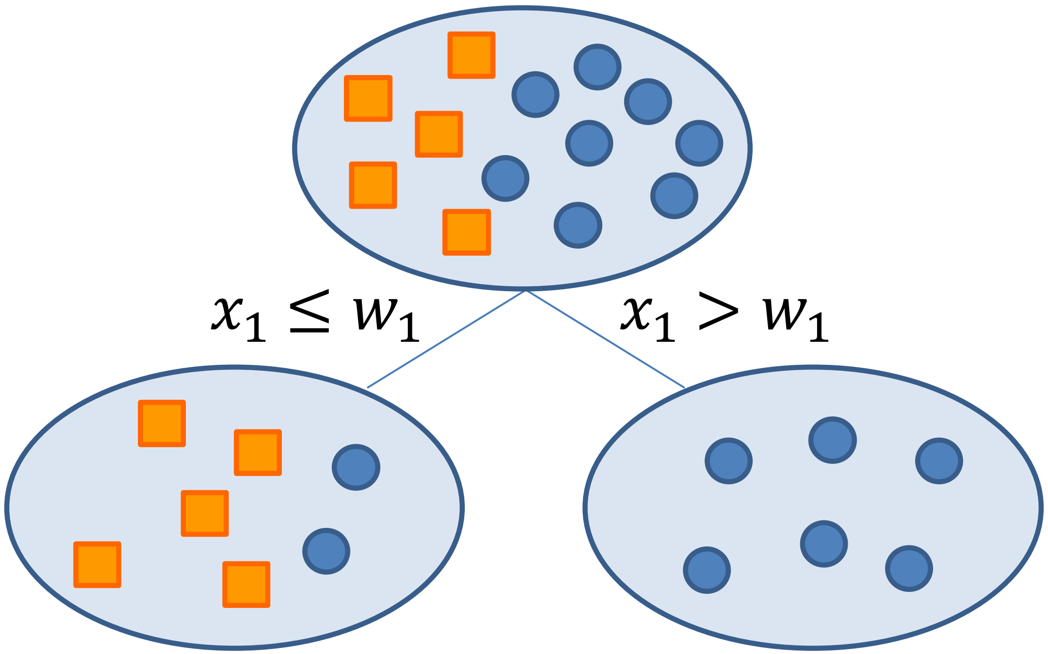

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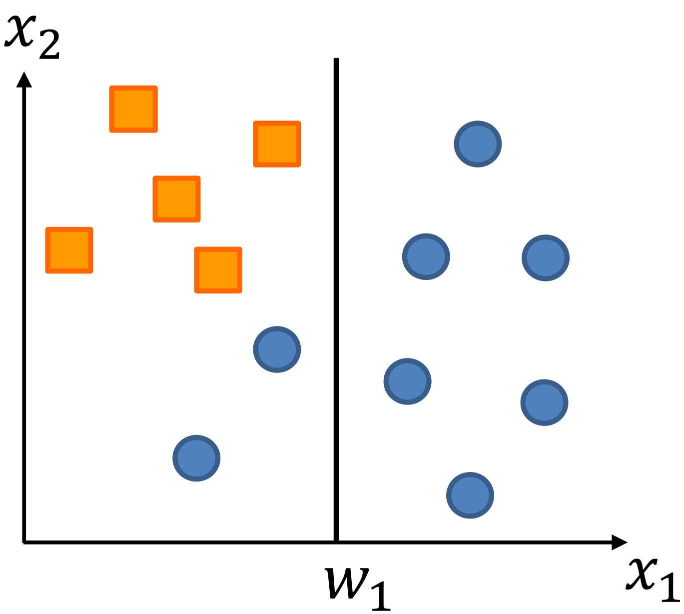

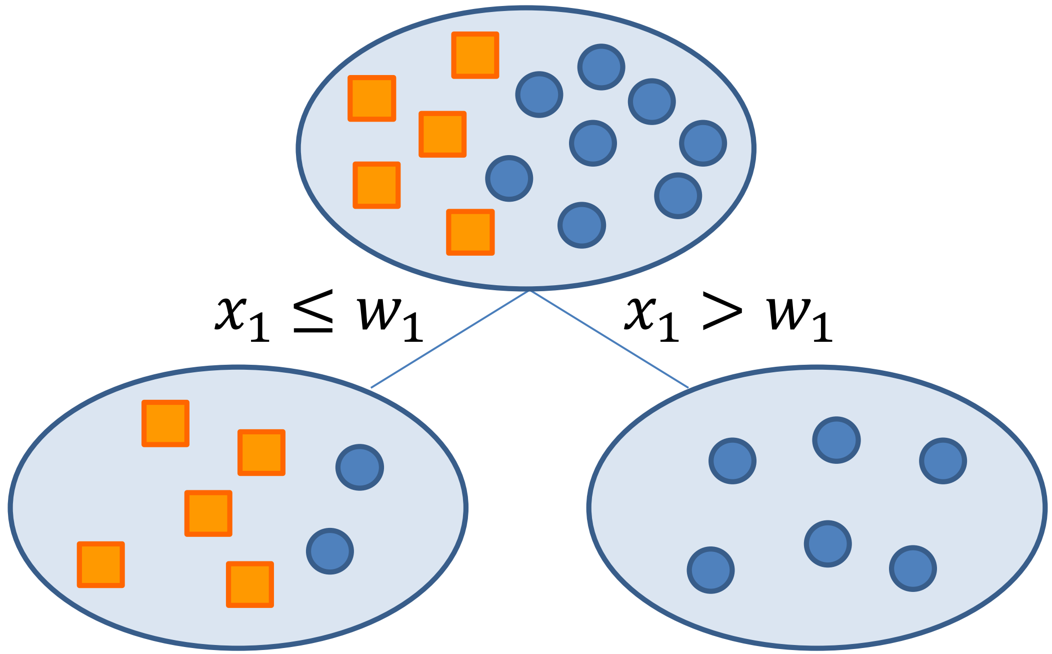

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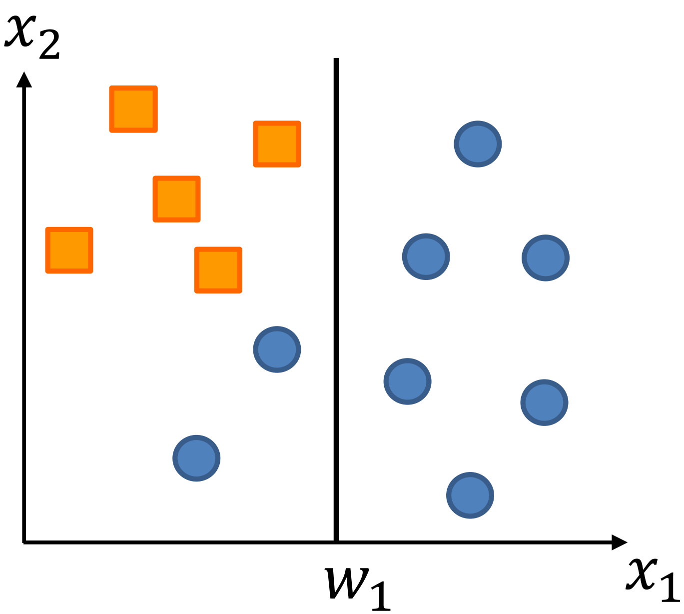
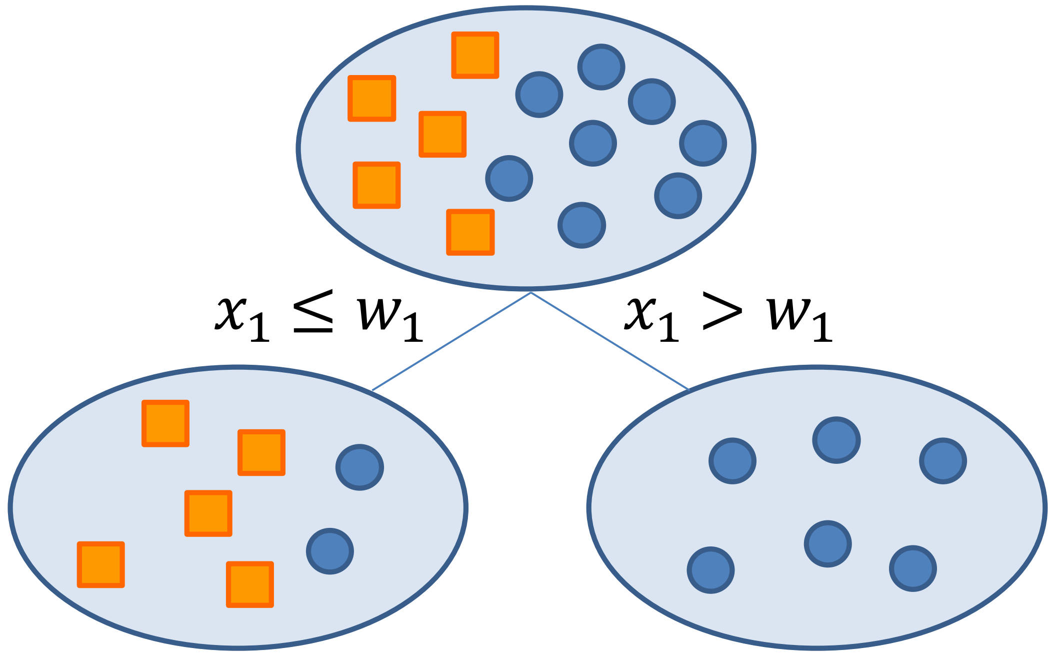




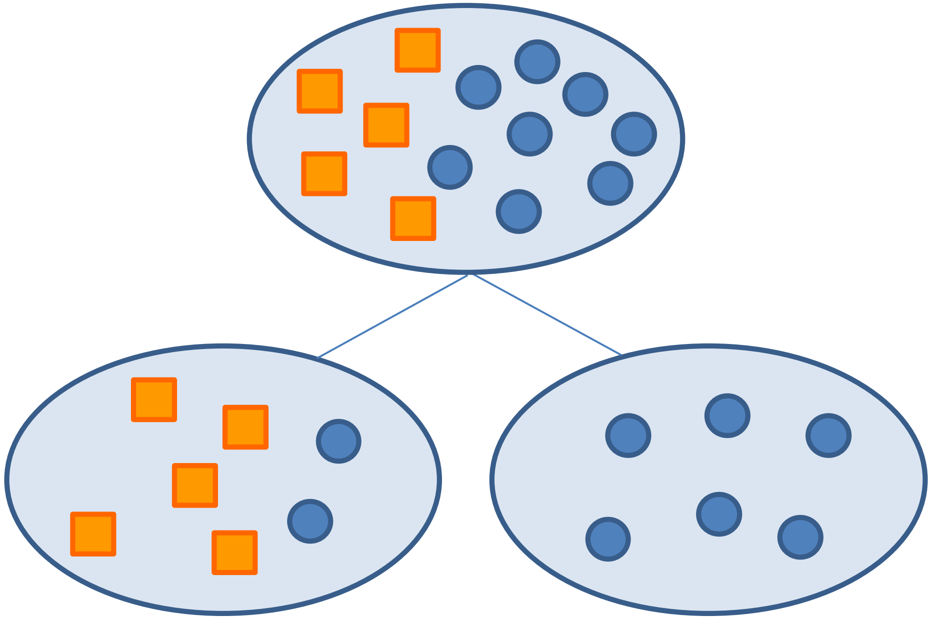
“Impure” because it contains &

“Pure” because it only contains

- “Purity” is desirable because if a node contains only training data from one class, then prediction for training data in the node is perfect

Node Impurity Measures

- Let ● be class 1 & ■ be class 2



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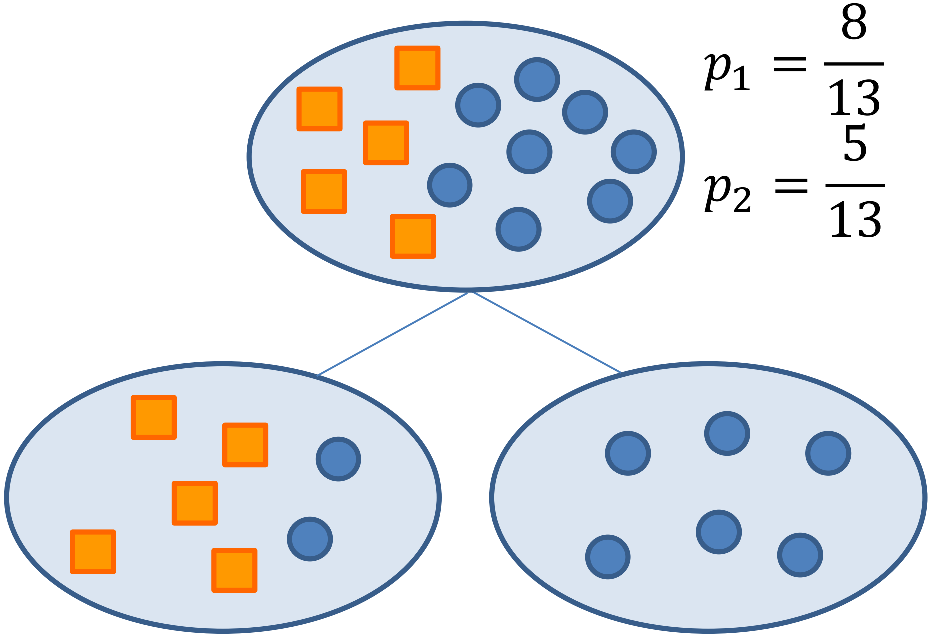

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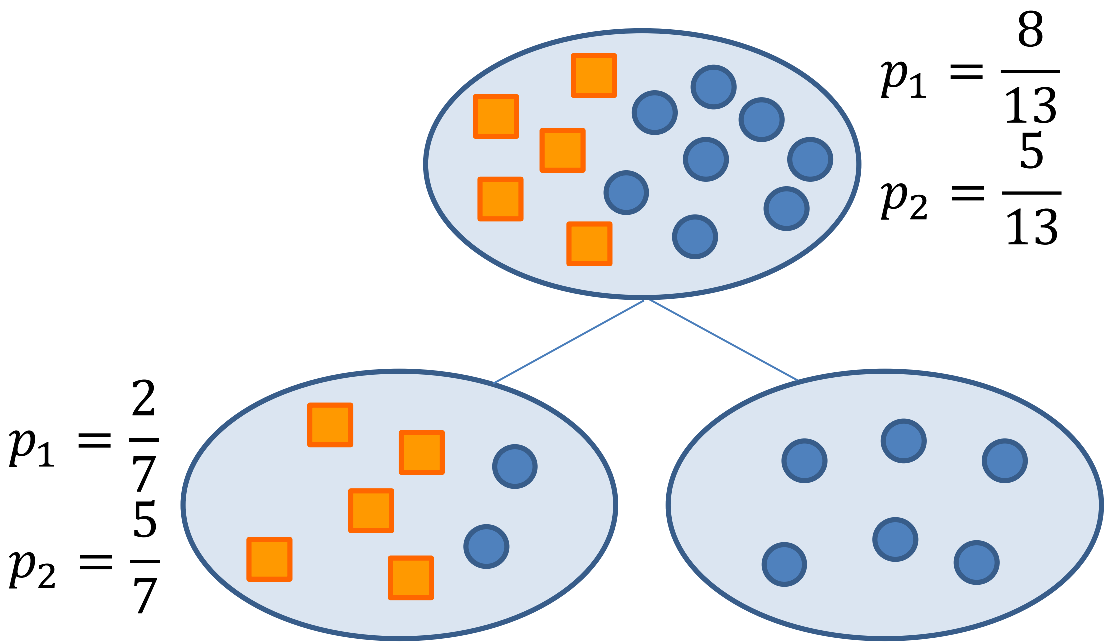

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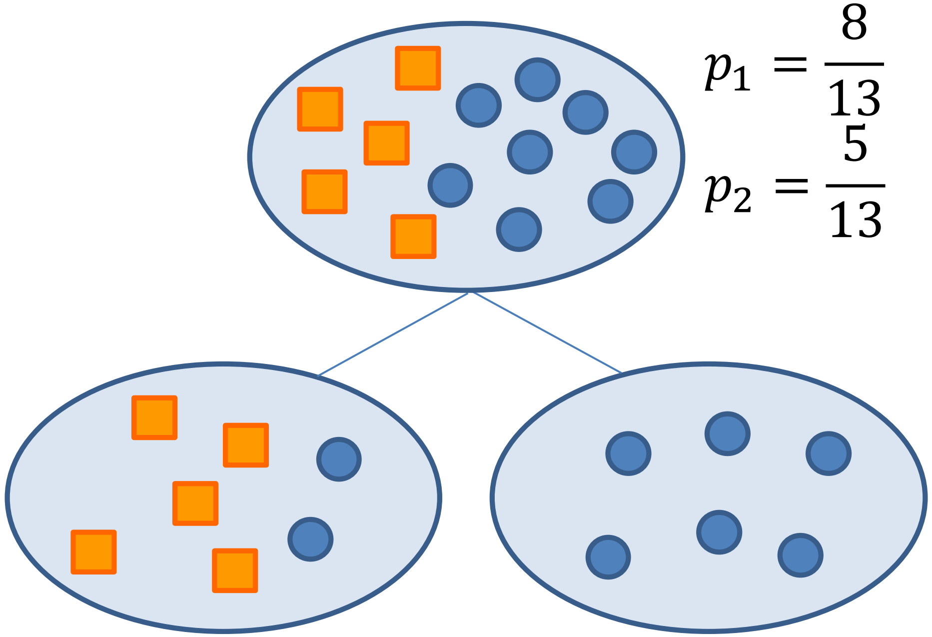

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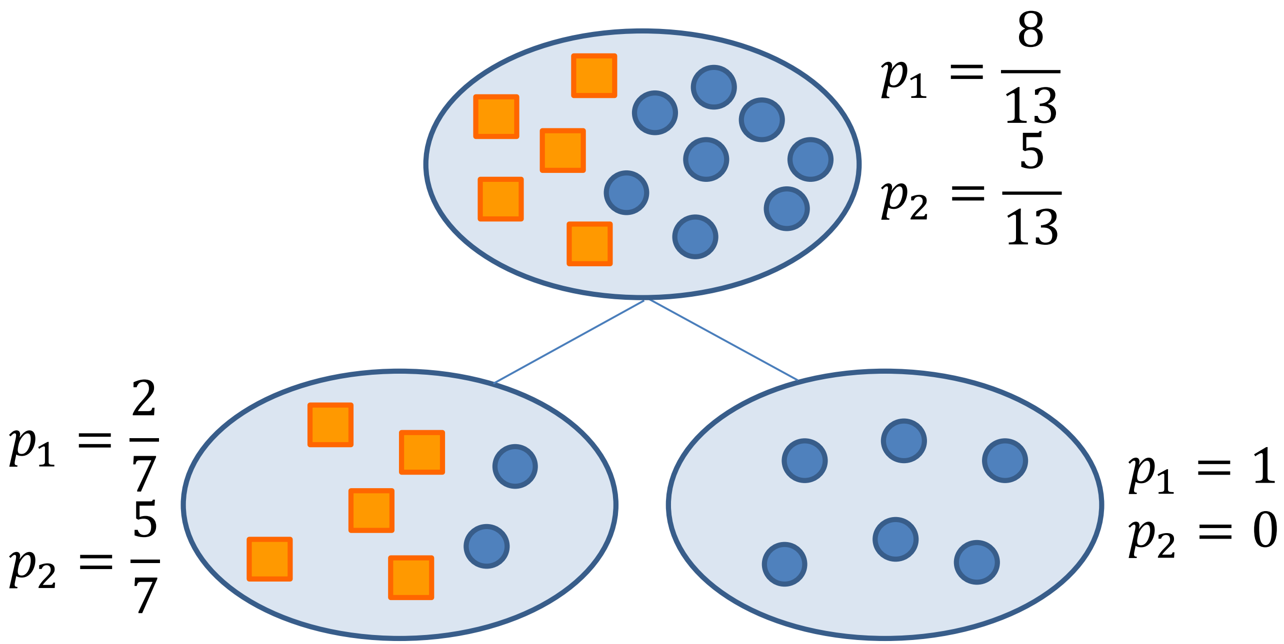
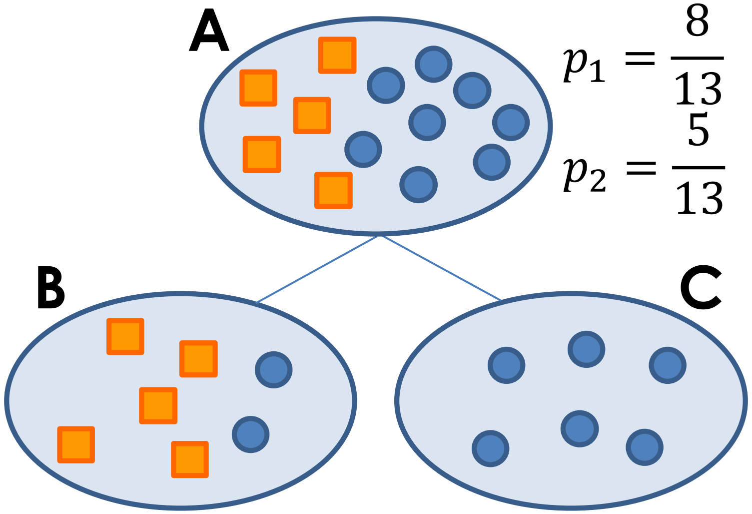
- Let Q_m be impurity of node m
- 3 impurity measures: Gini, entropy, misclassification rate



Gini Impurity



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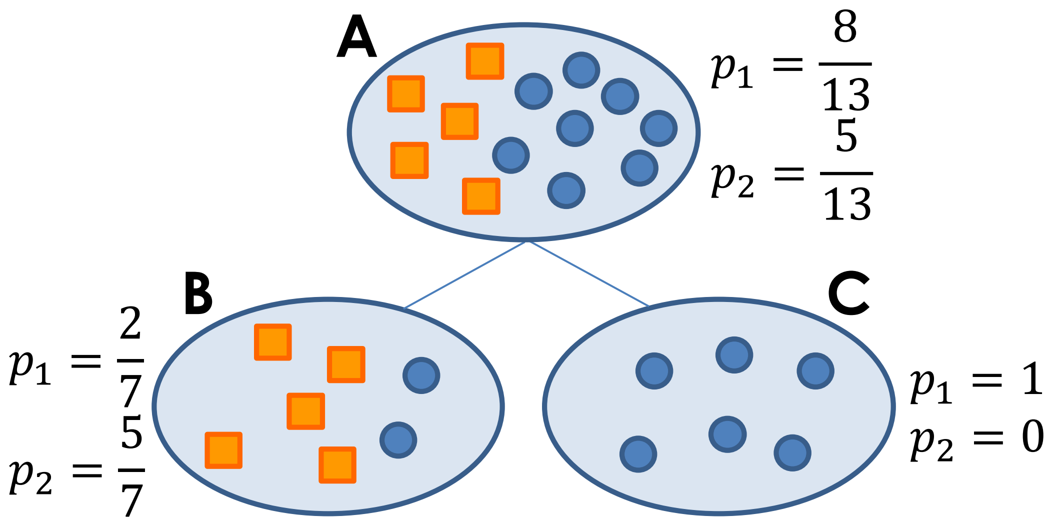

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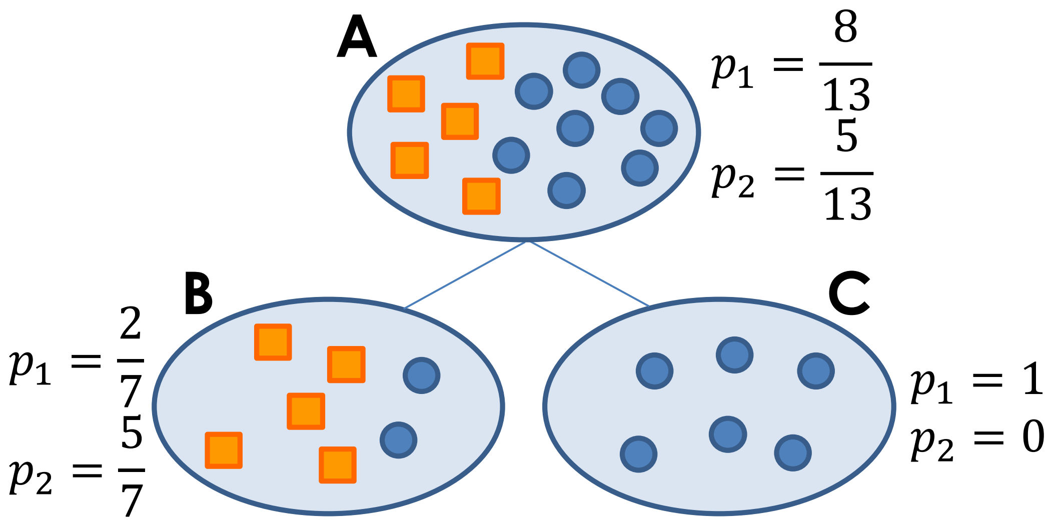

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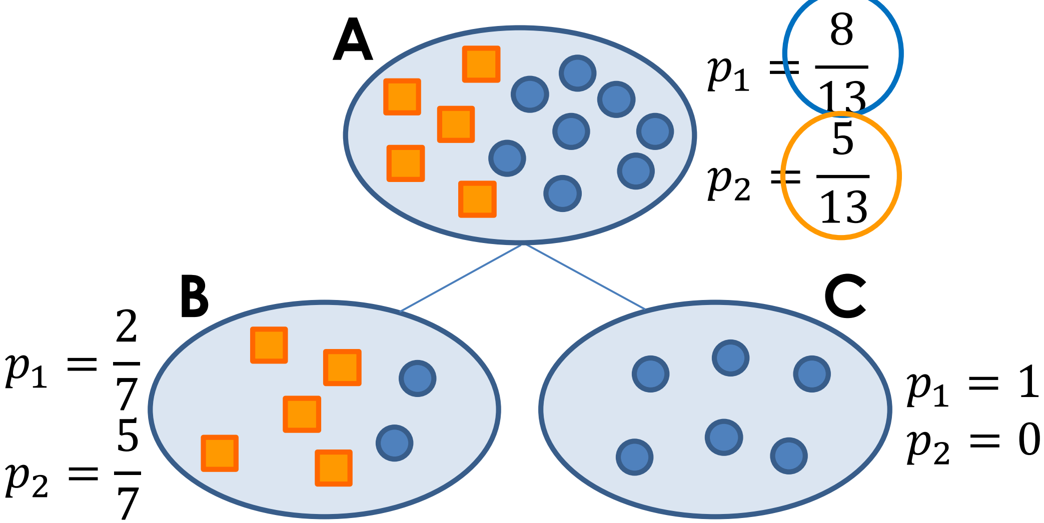

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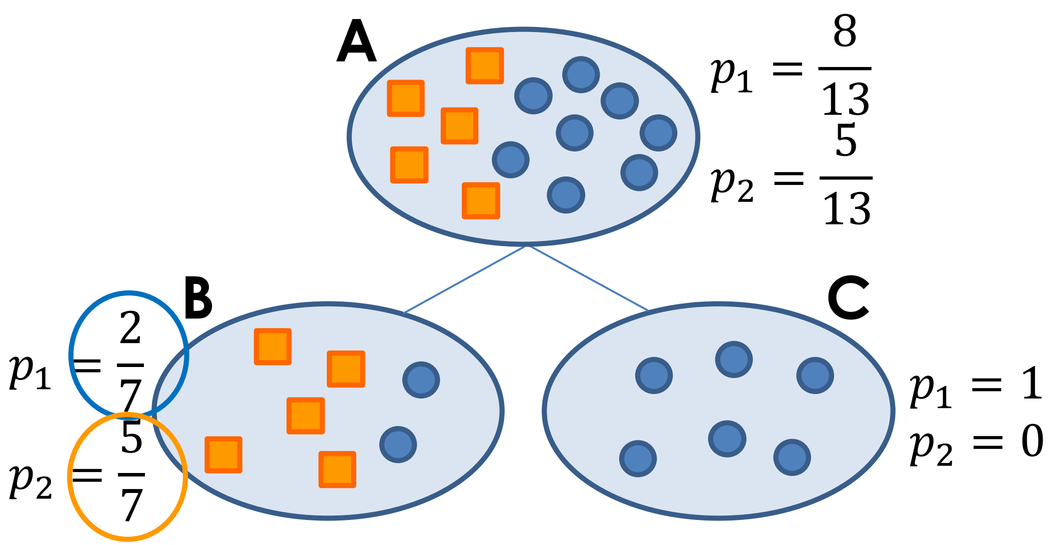

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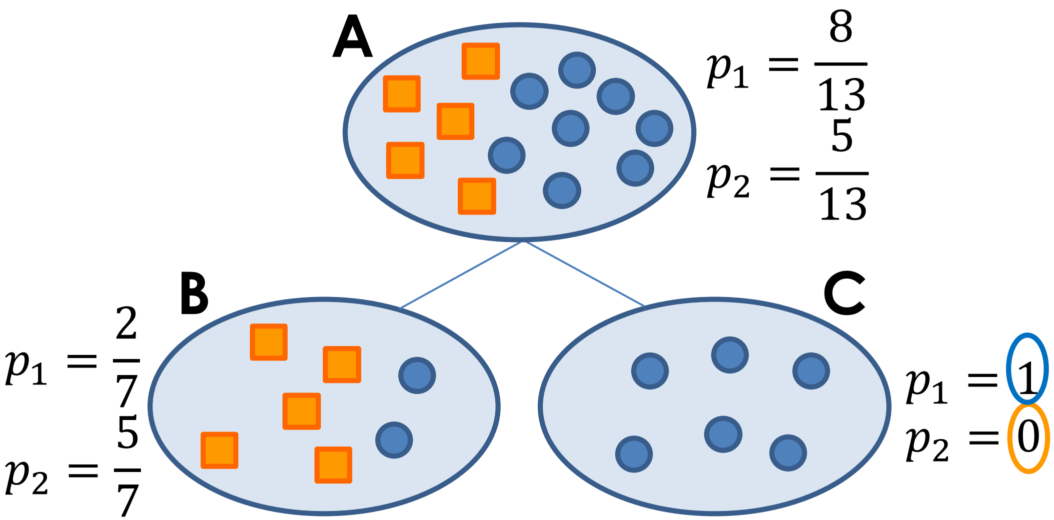

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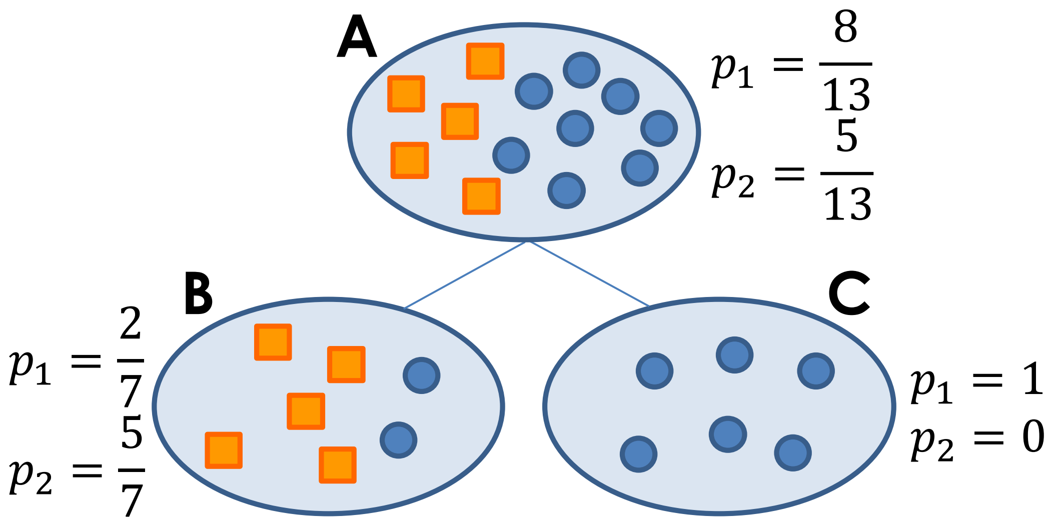

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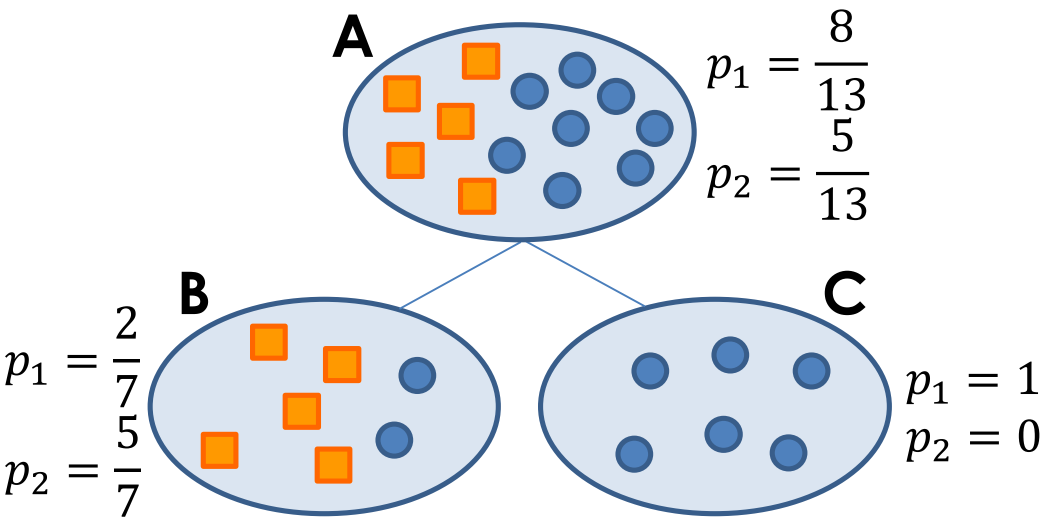

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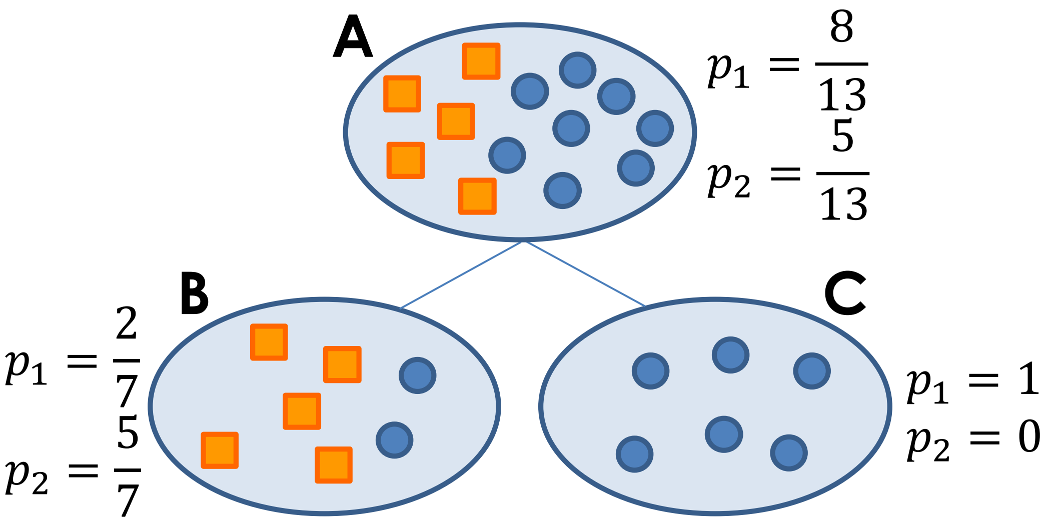

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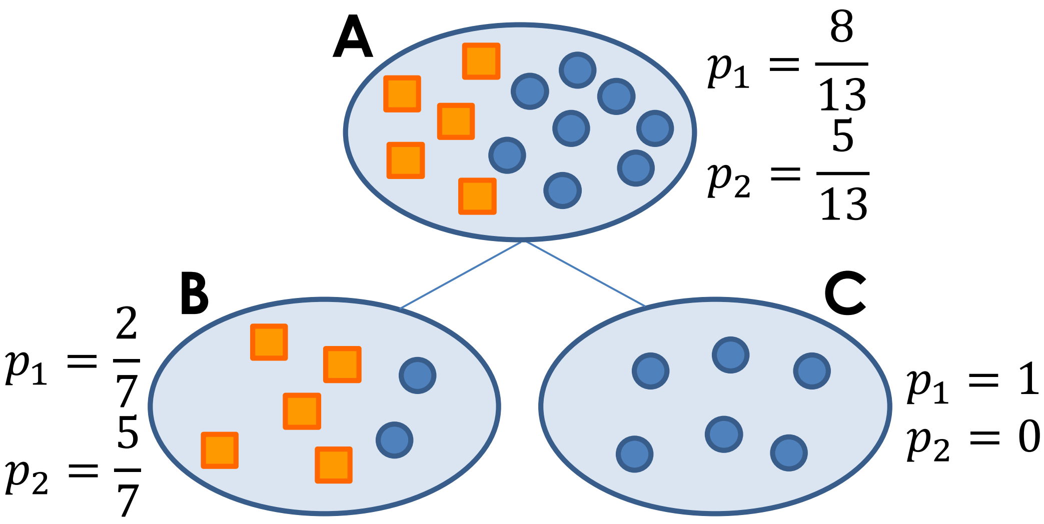
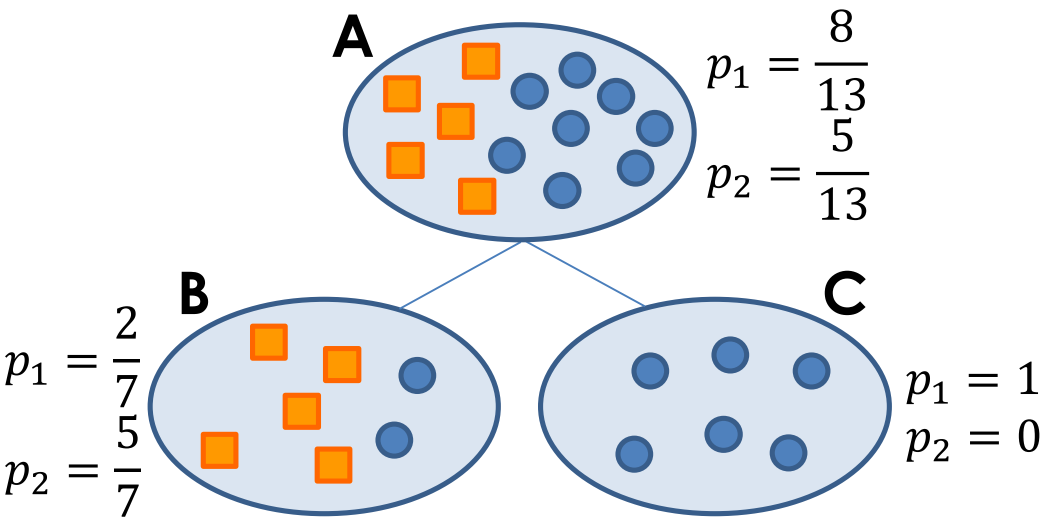
- Same Gini formula for more than 2 classes:

$$Q_m = 1 - \Sigma_{i=1}^{K} p_i^2$$



Entropy



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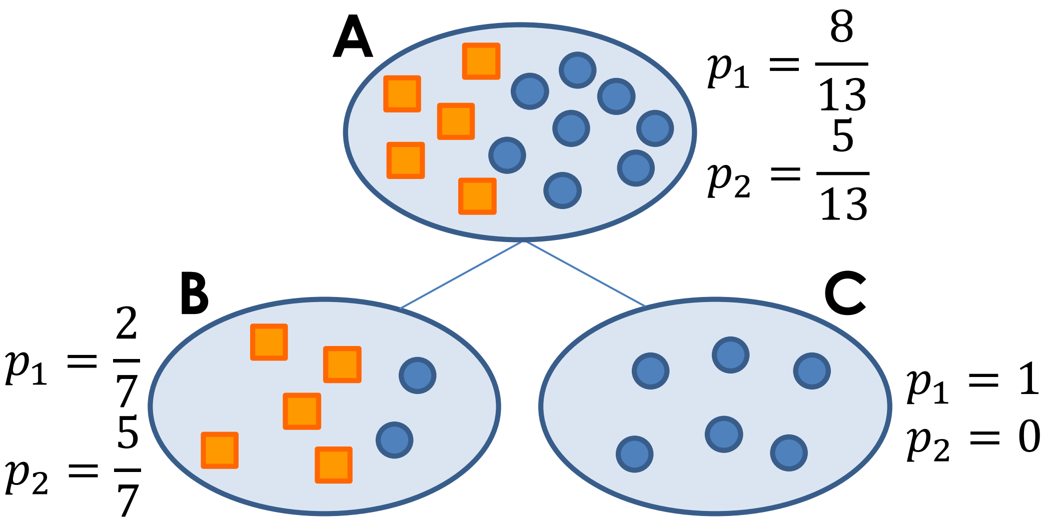

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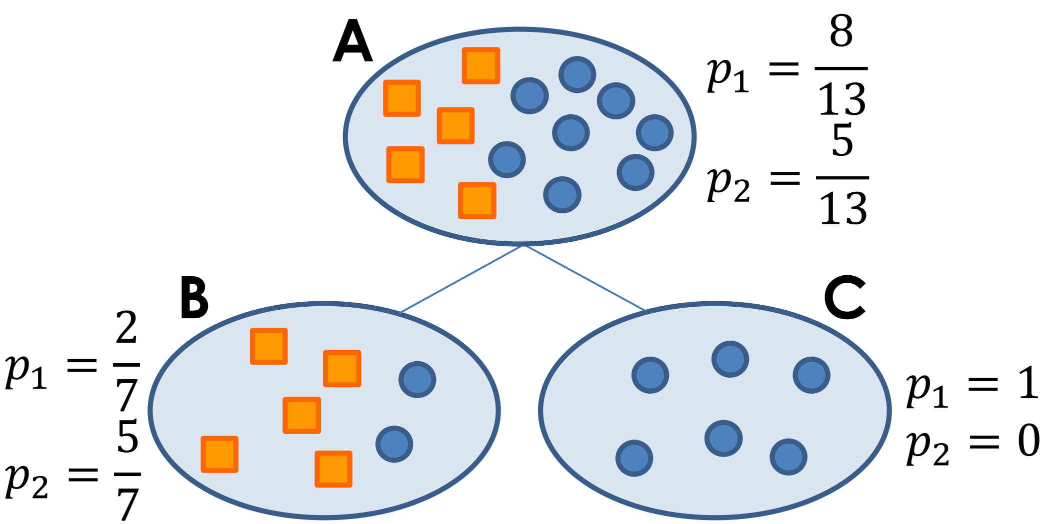

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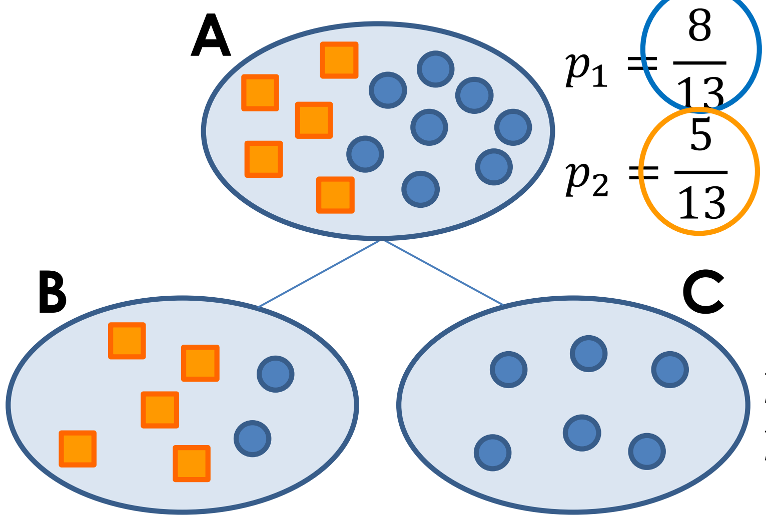

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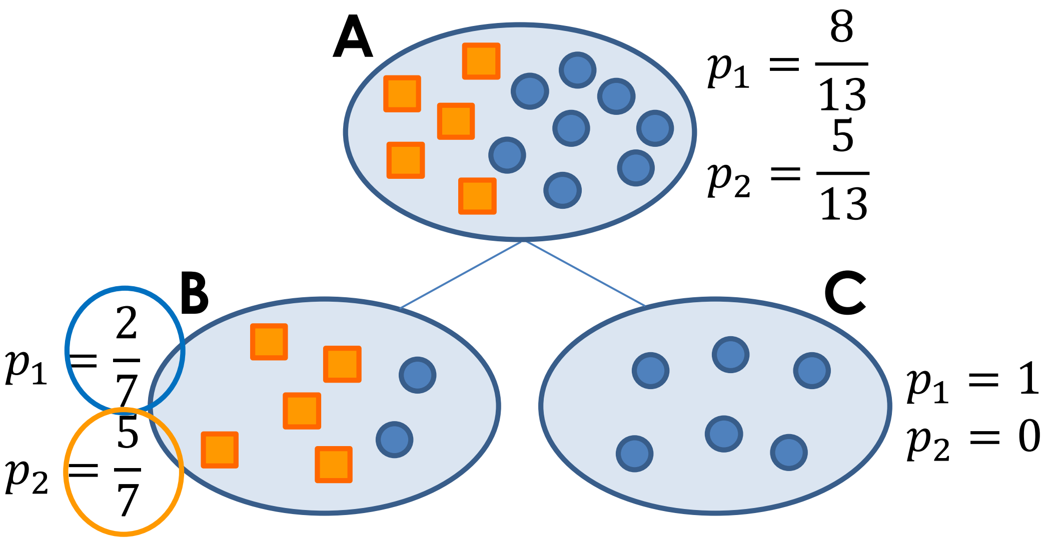

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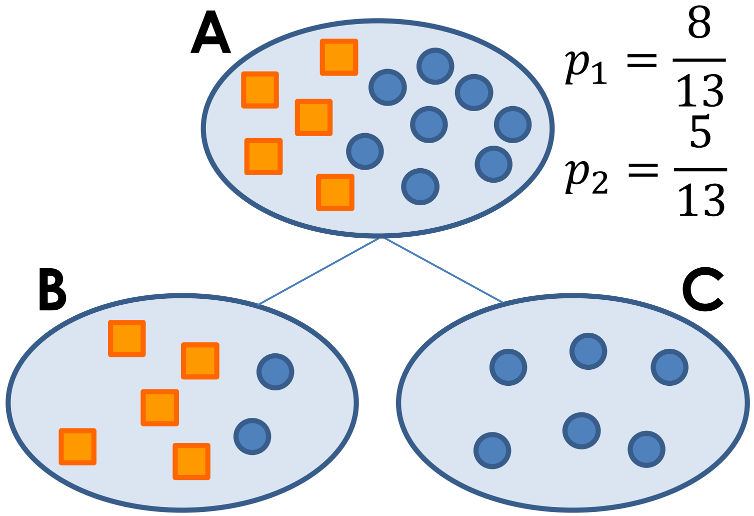

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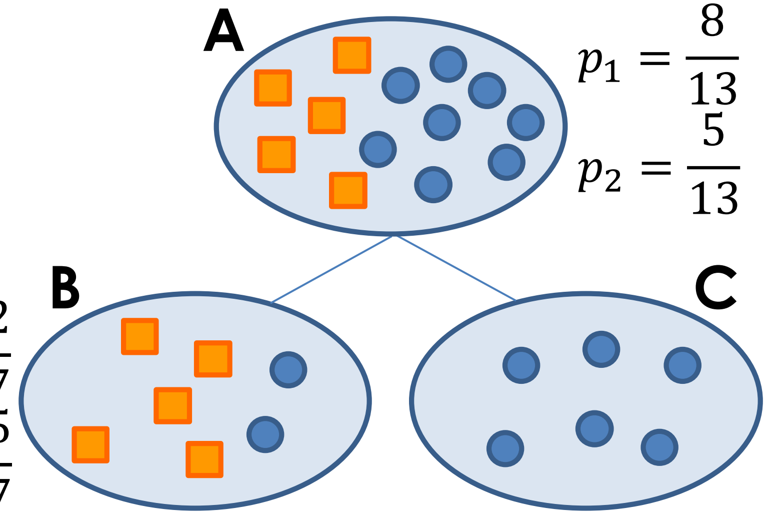

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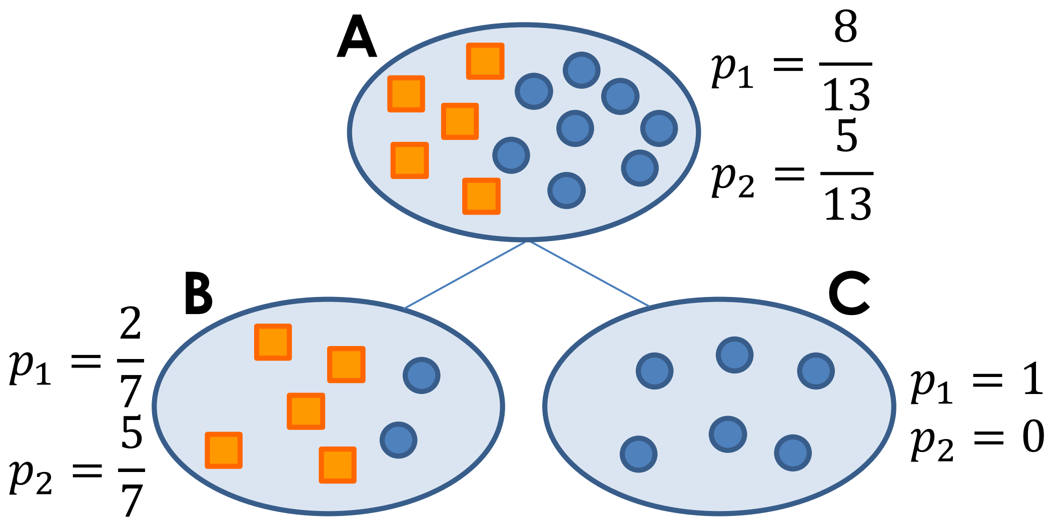

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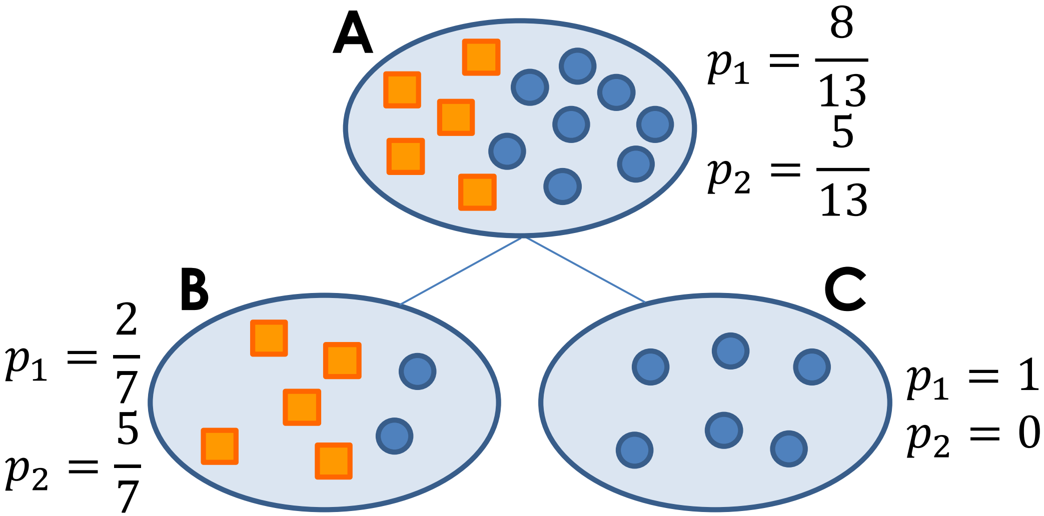
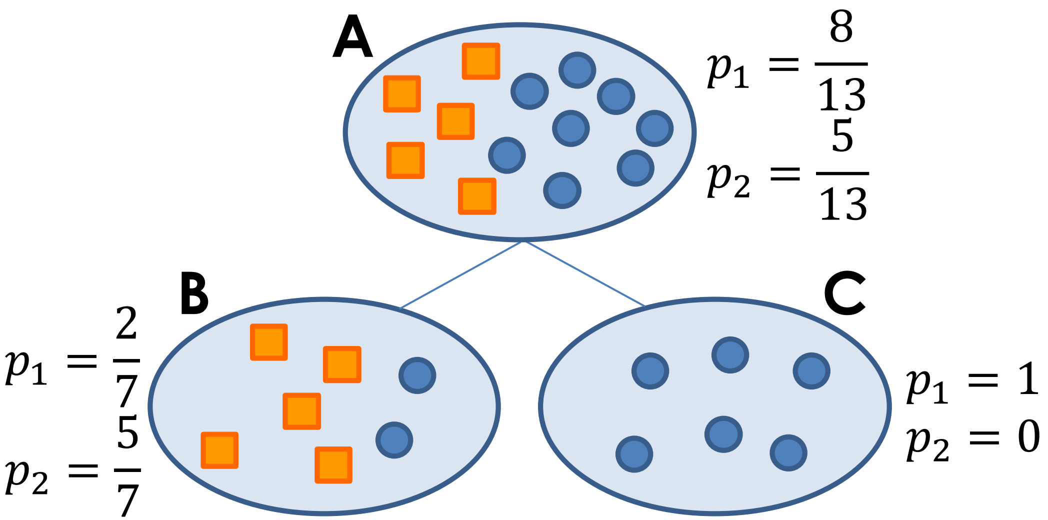


Misclassification rate



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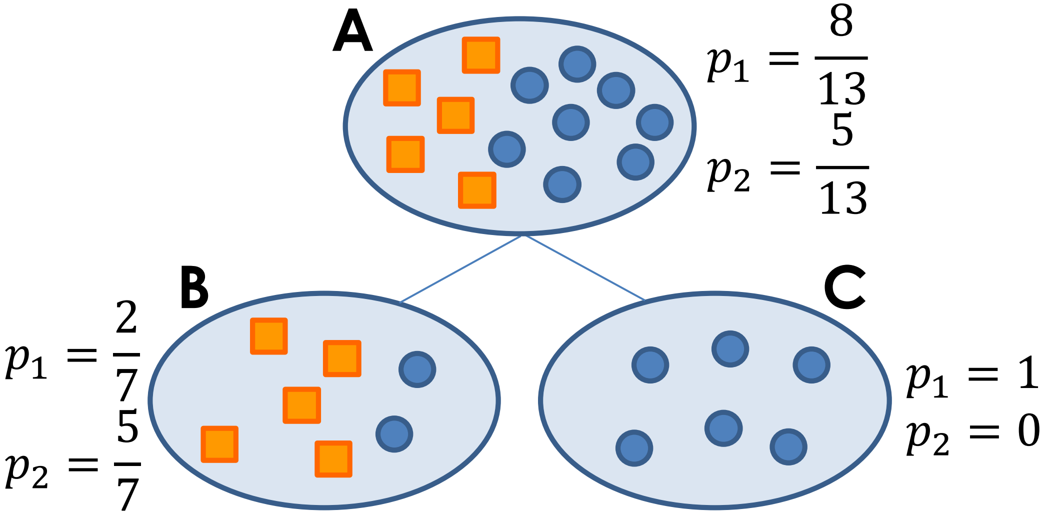

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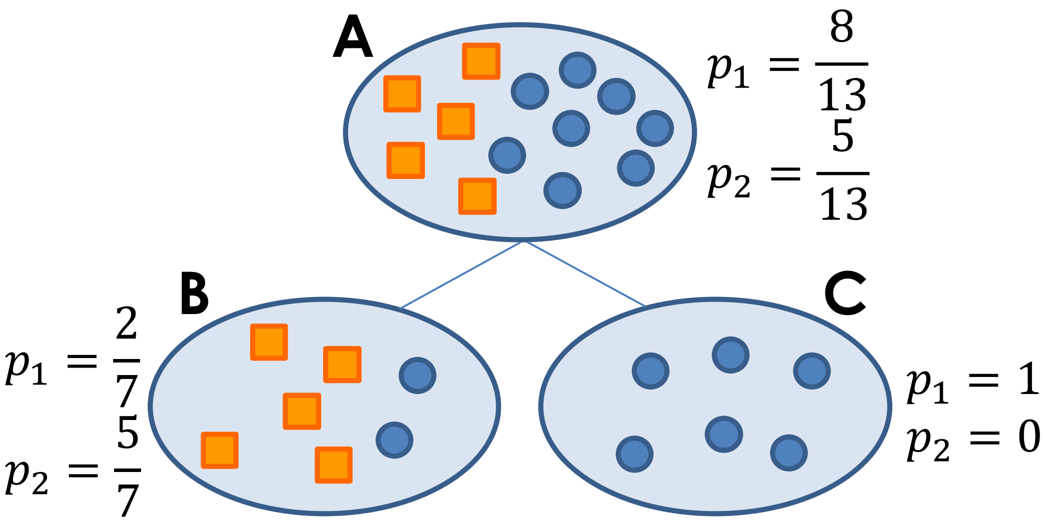

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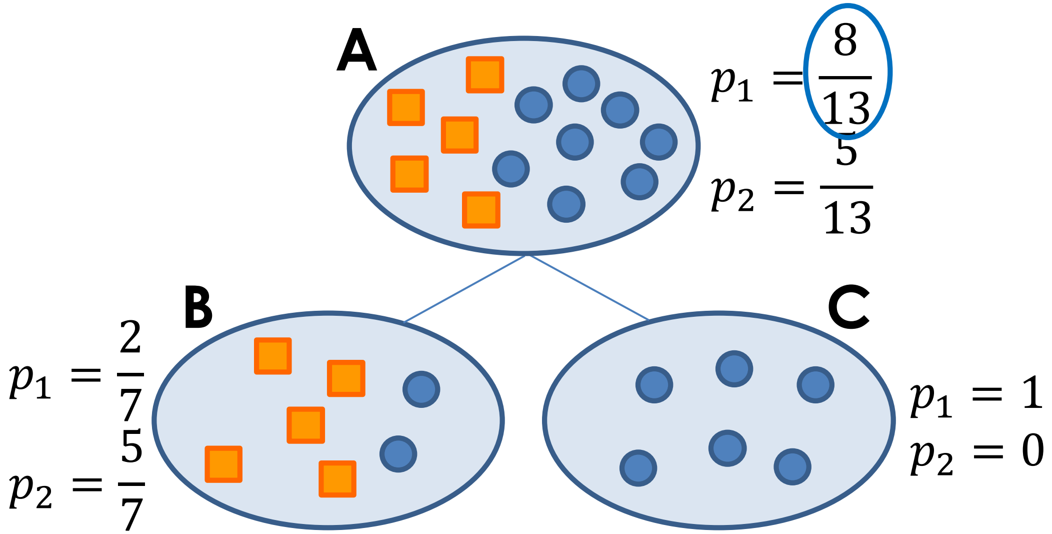

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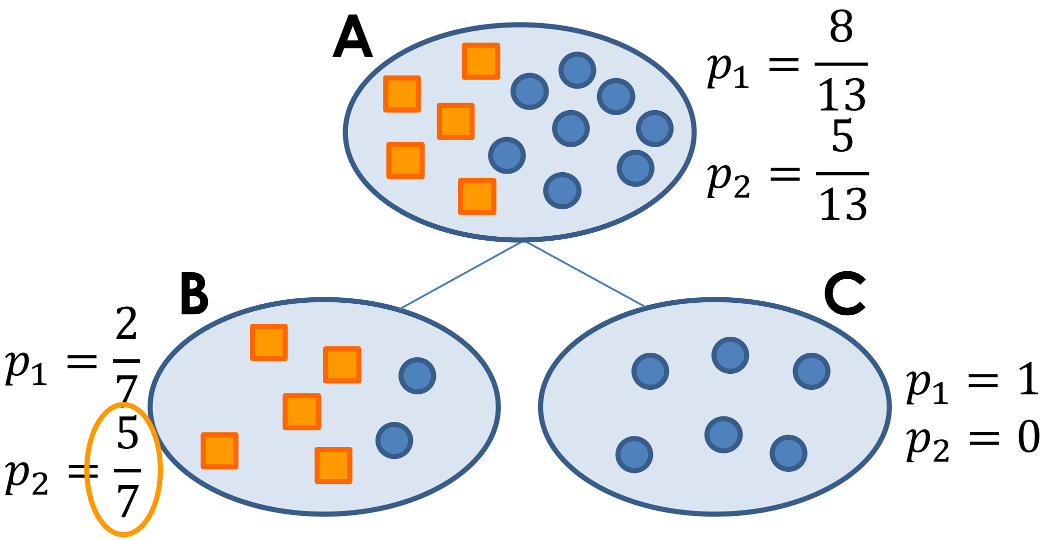

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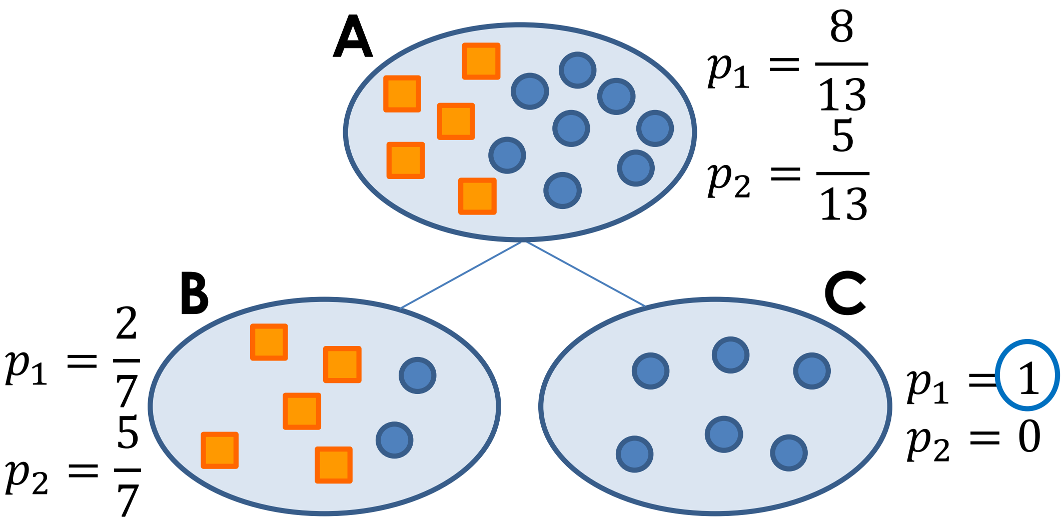

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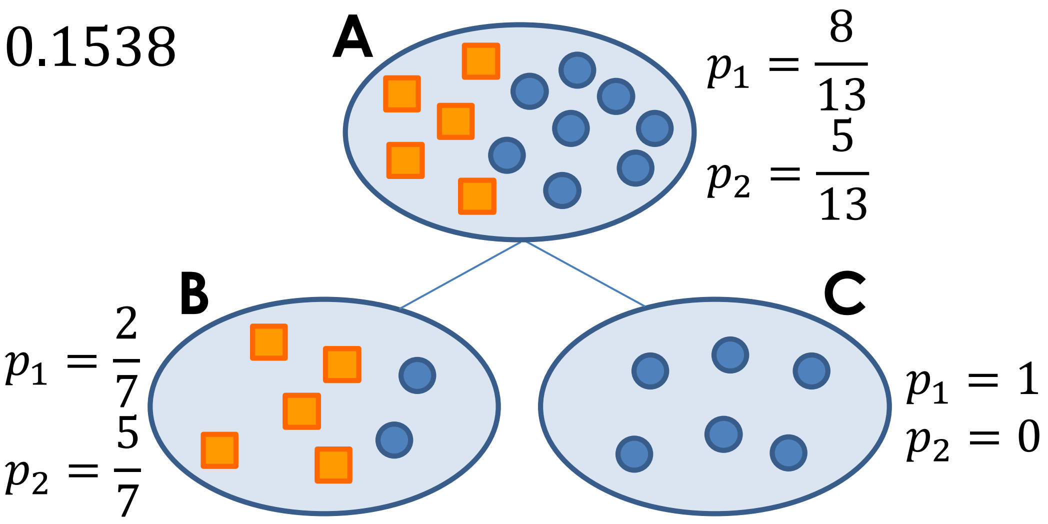

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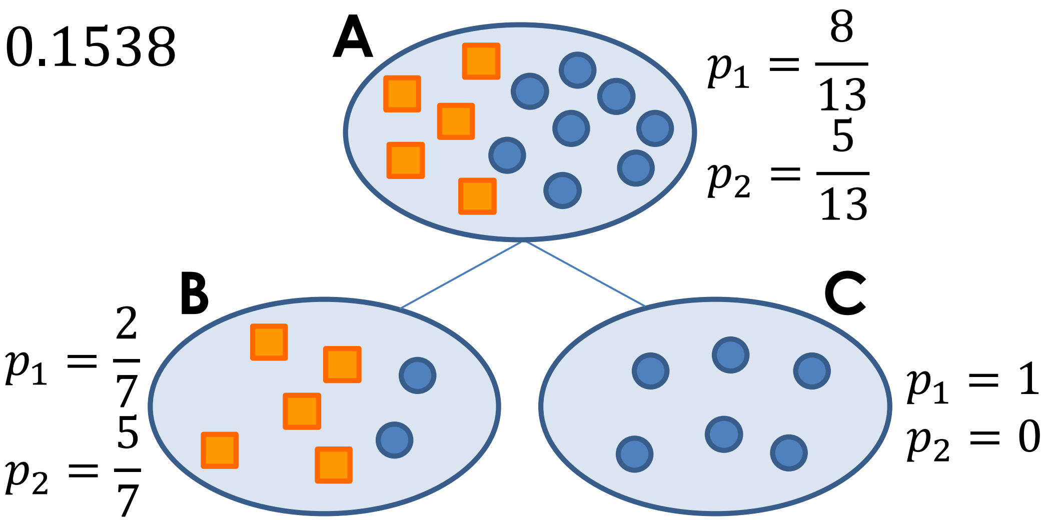

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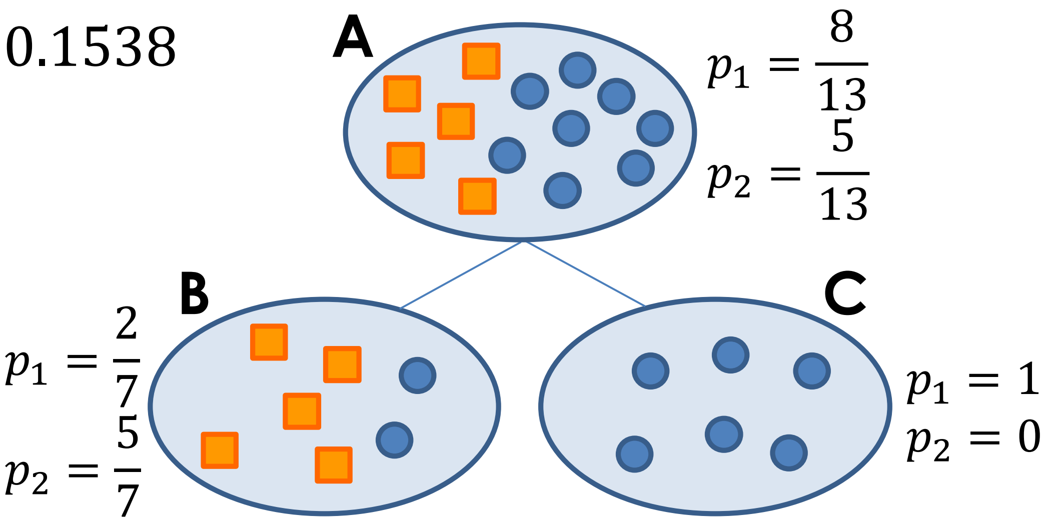

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Classification Tree Learning

Algorithm: Classification Tree Learning

Input: Impurity measure Q, parameter max_depth & training set

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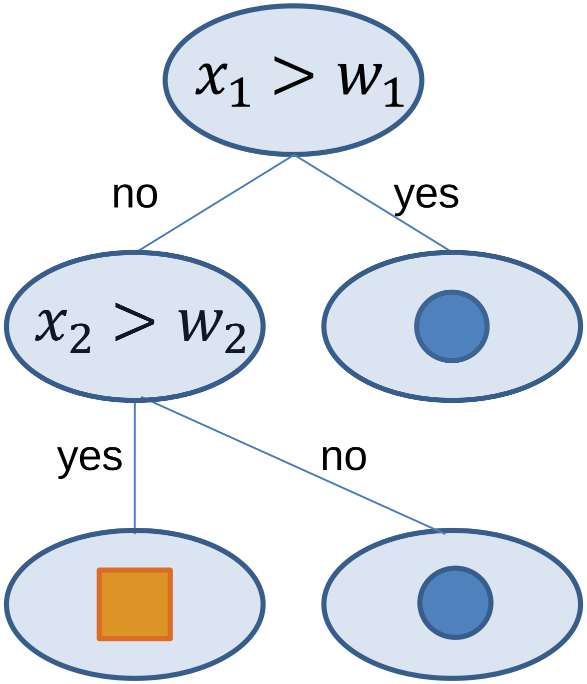

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- Across all leaf nodes, total MSE $S = \sum_m \frac{J_m}{N} S_m$, where N is the total number of data samples

Regression Tree Learning

- Algorithm is basically the same as classification tree learning

Algorithm: Regression Tree Learning

Input: parameter *max_depth* & training set

Output: Tree

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Regression Tree Learning

- Algorithm is basically the same as classification tree learning
- Various approaches to reduce overfitting also apply here

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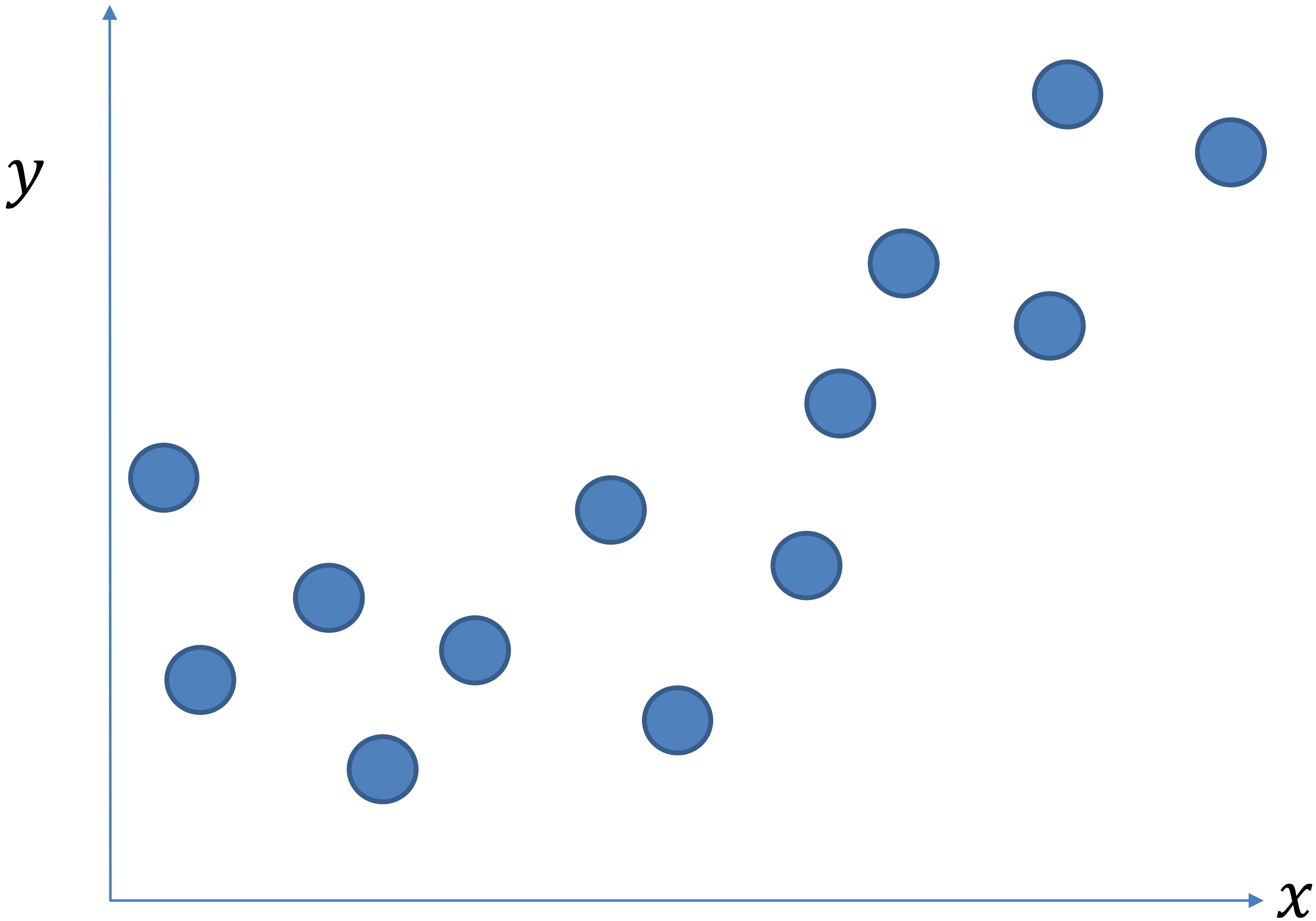
Regression Tree Example



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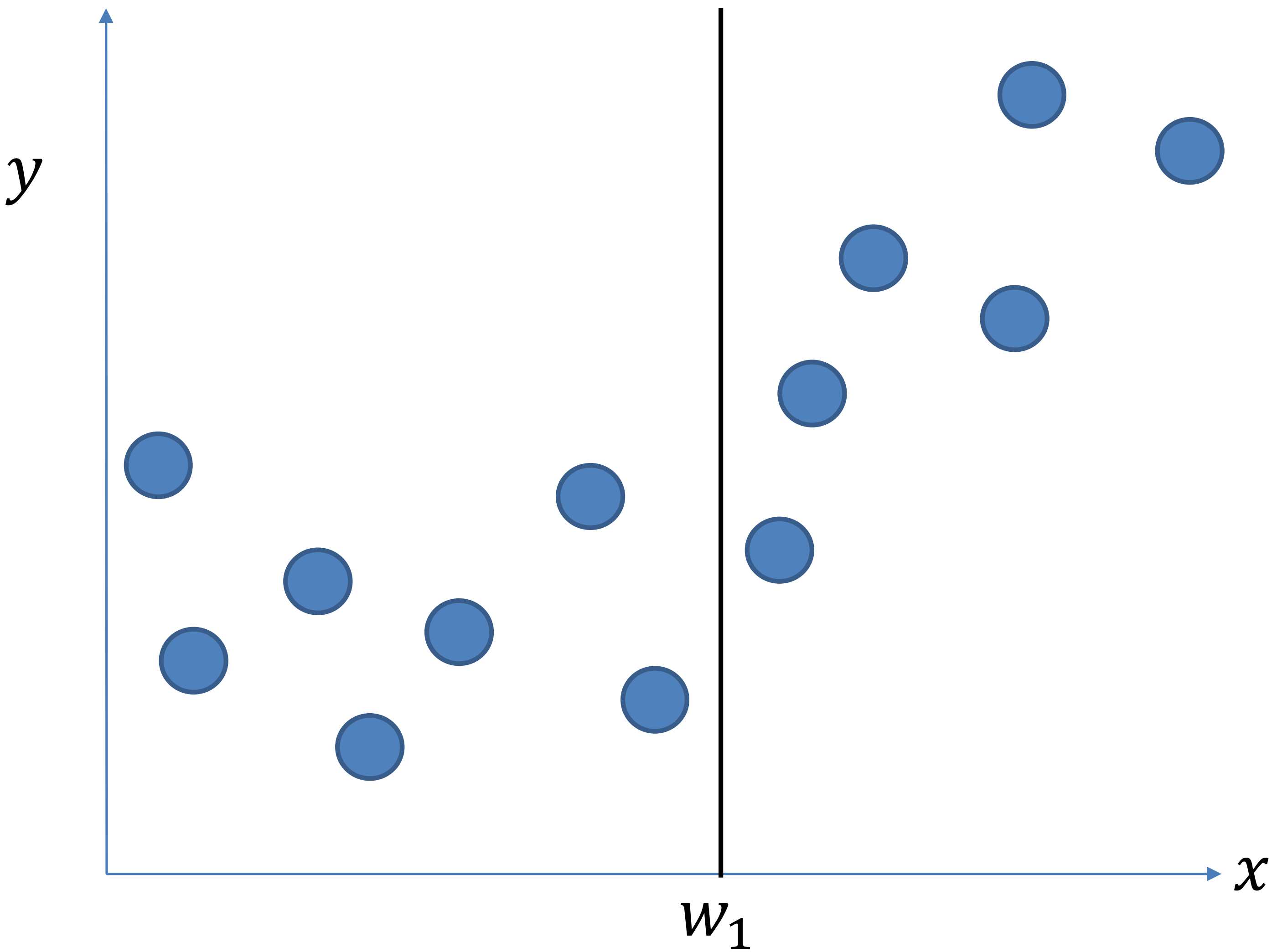

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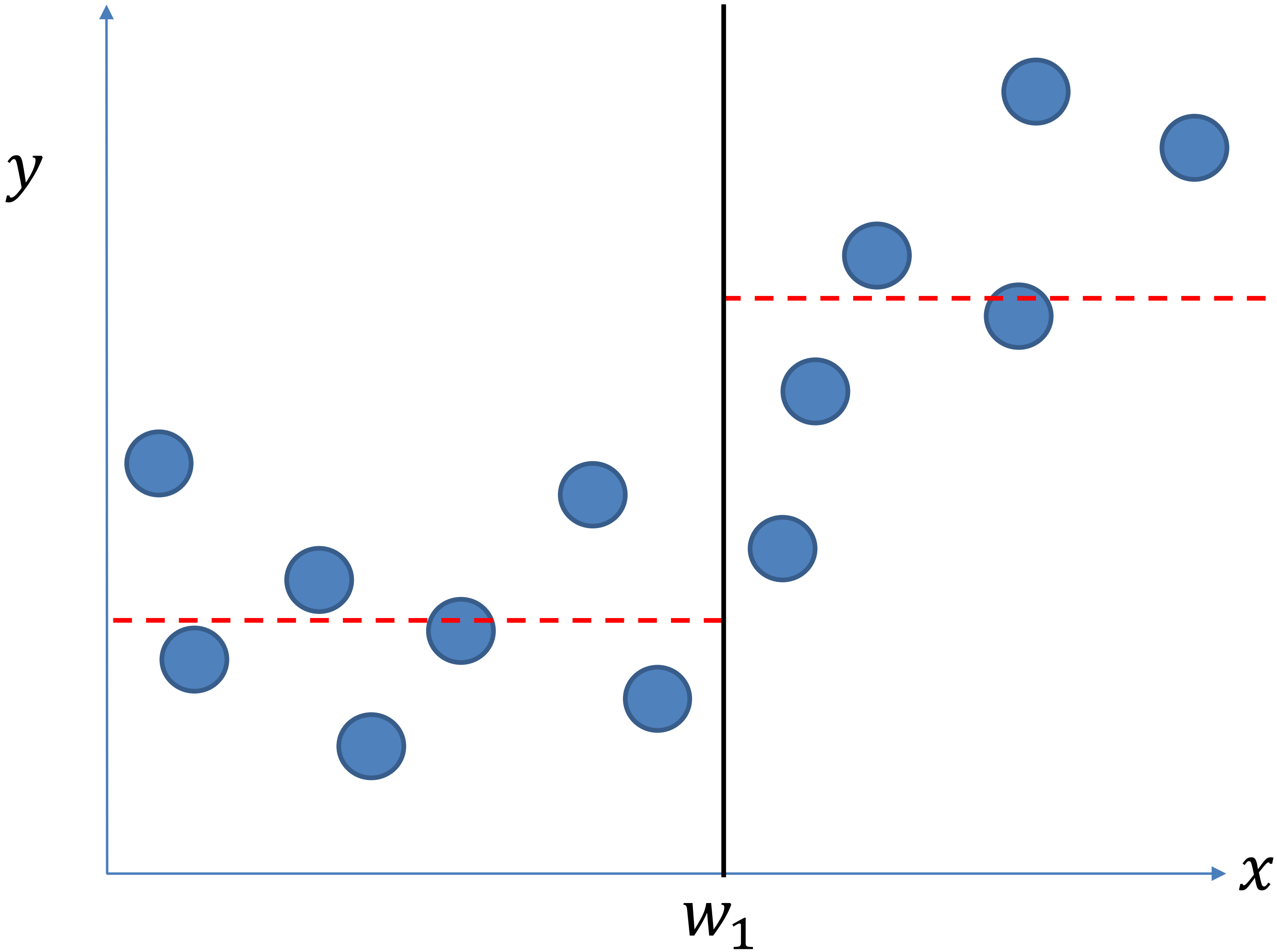

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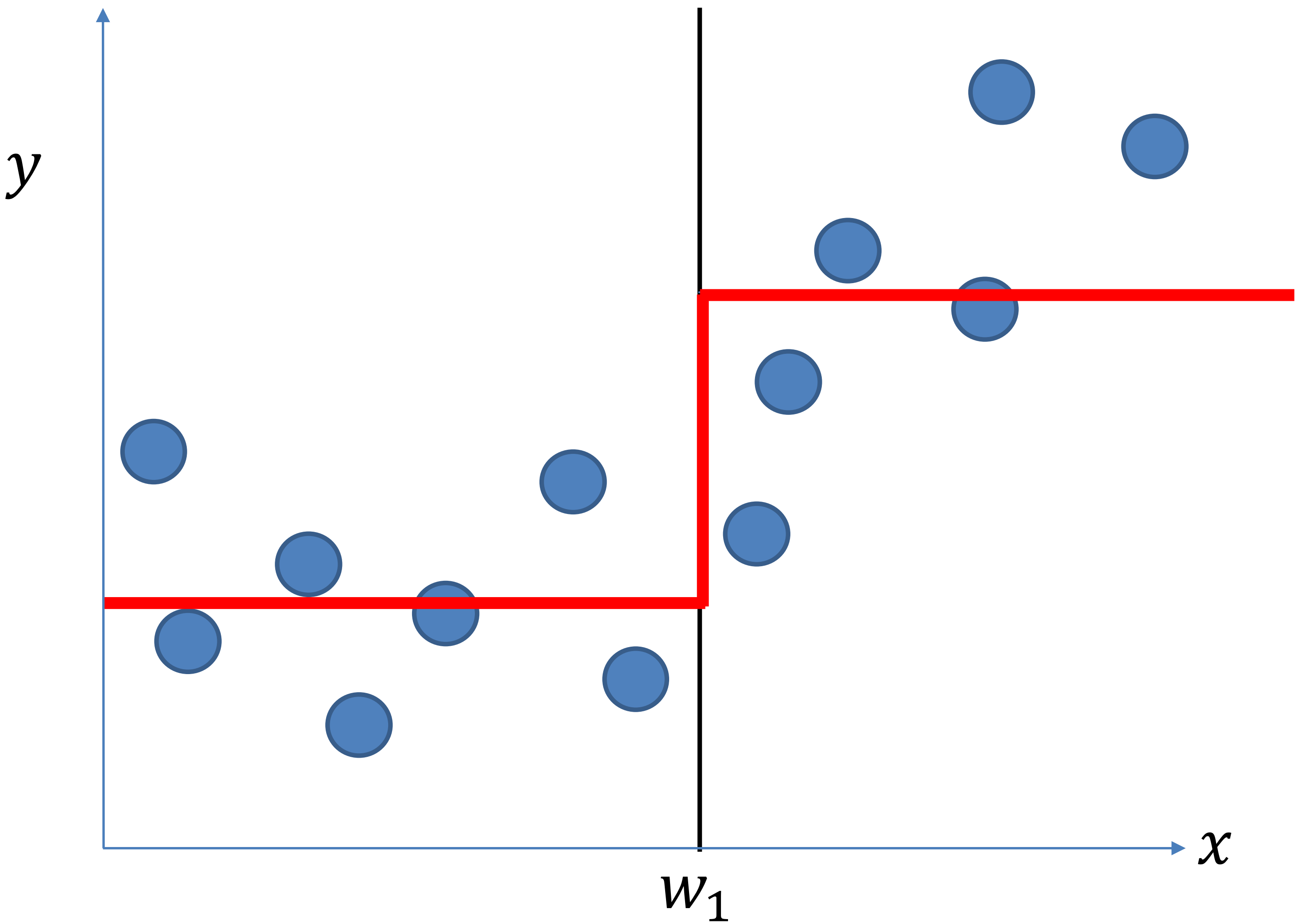

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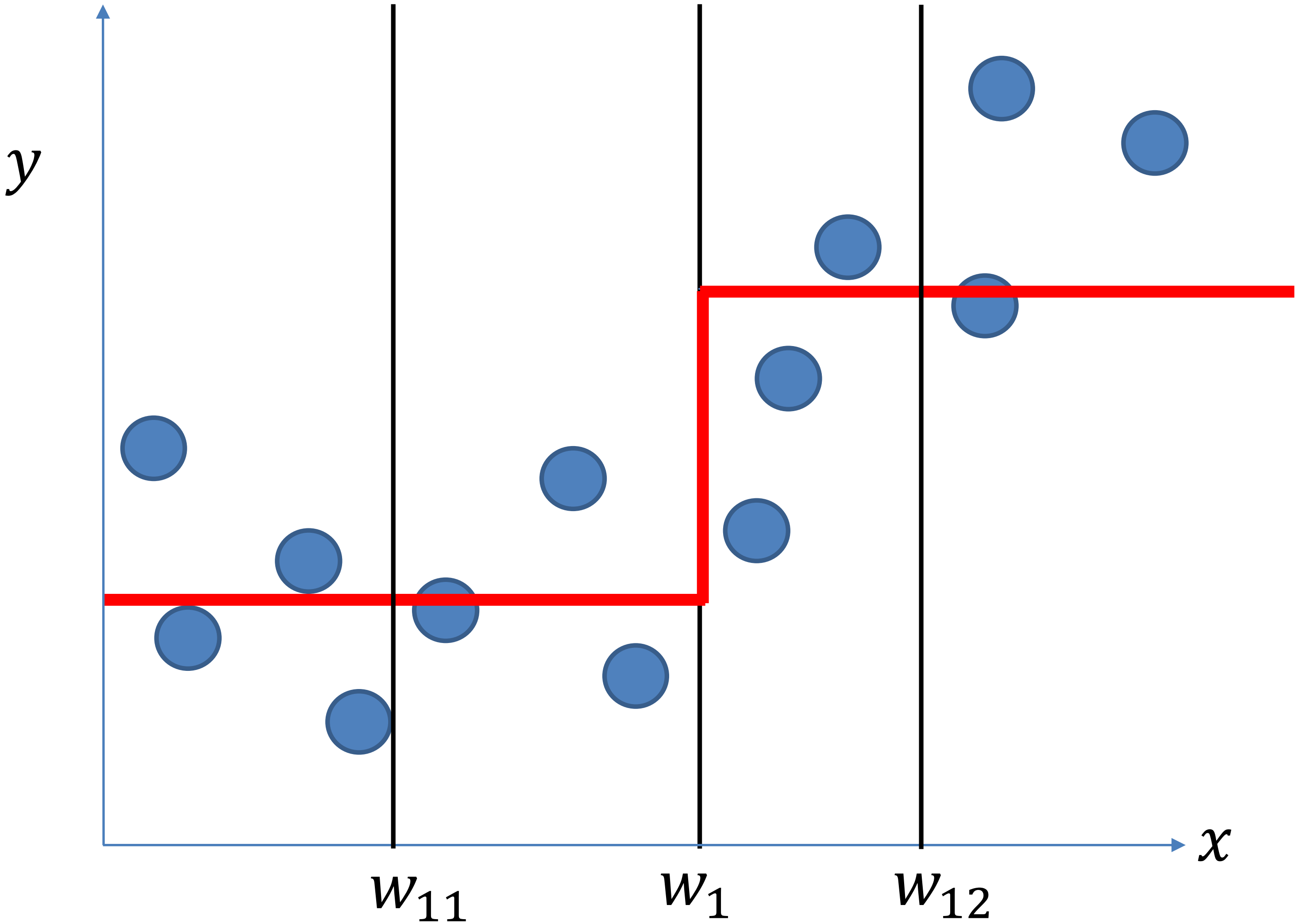

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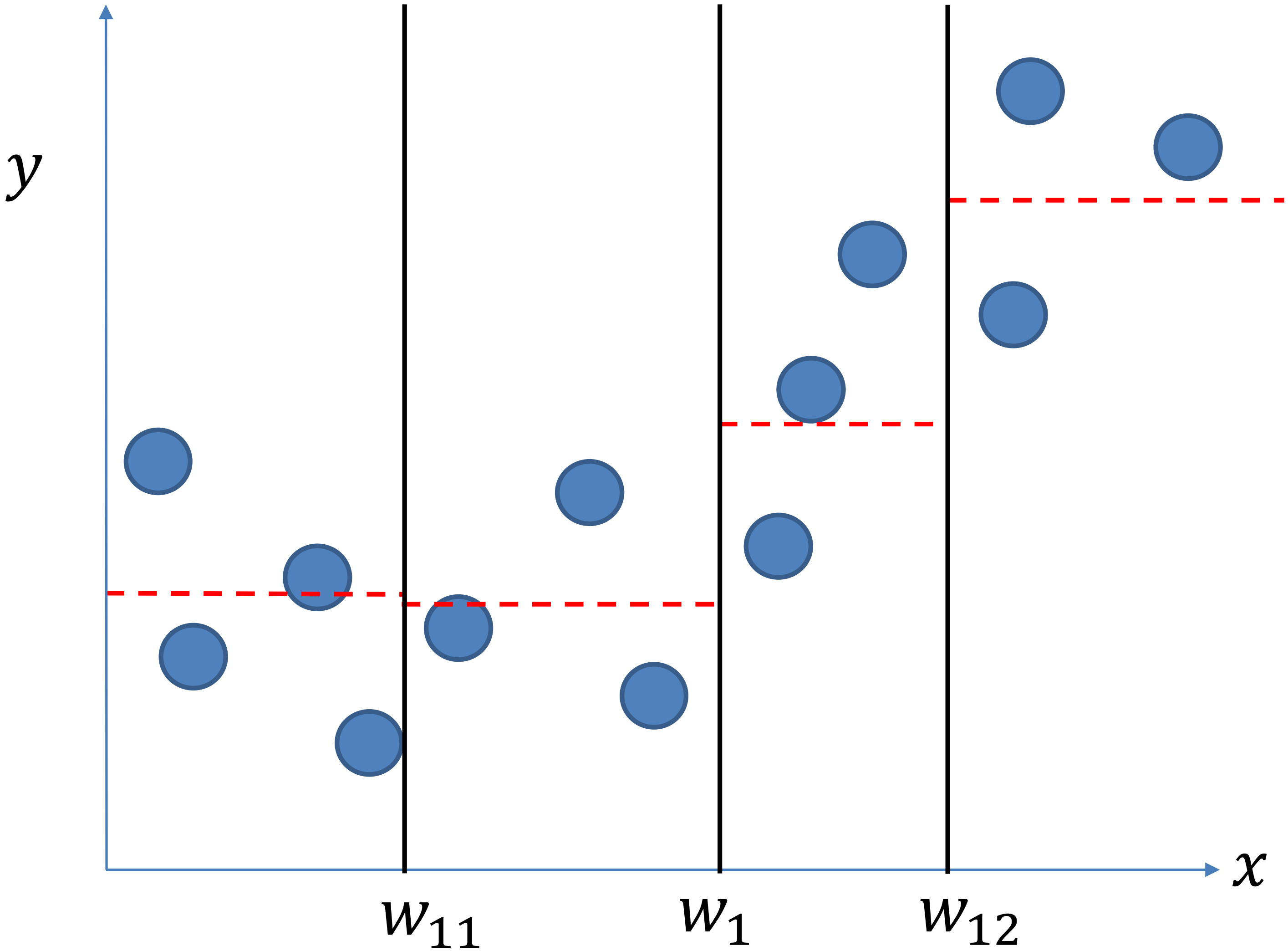

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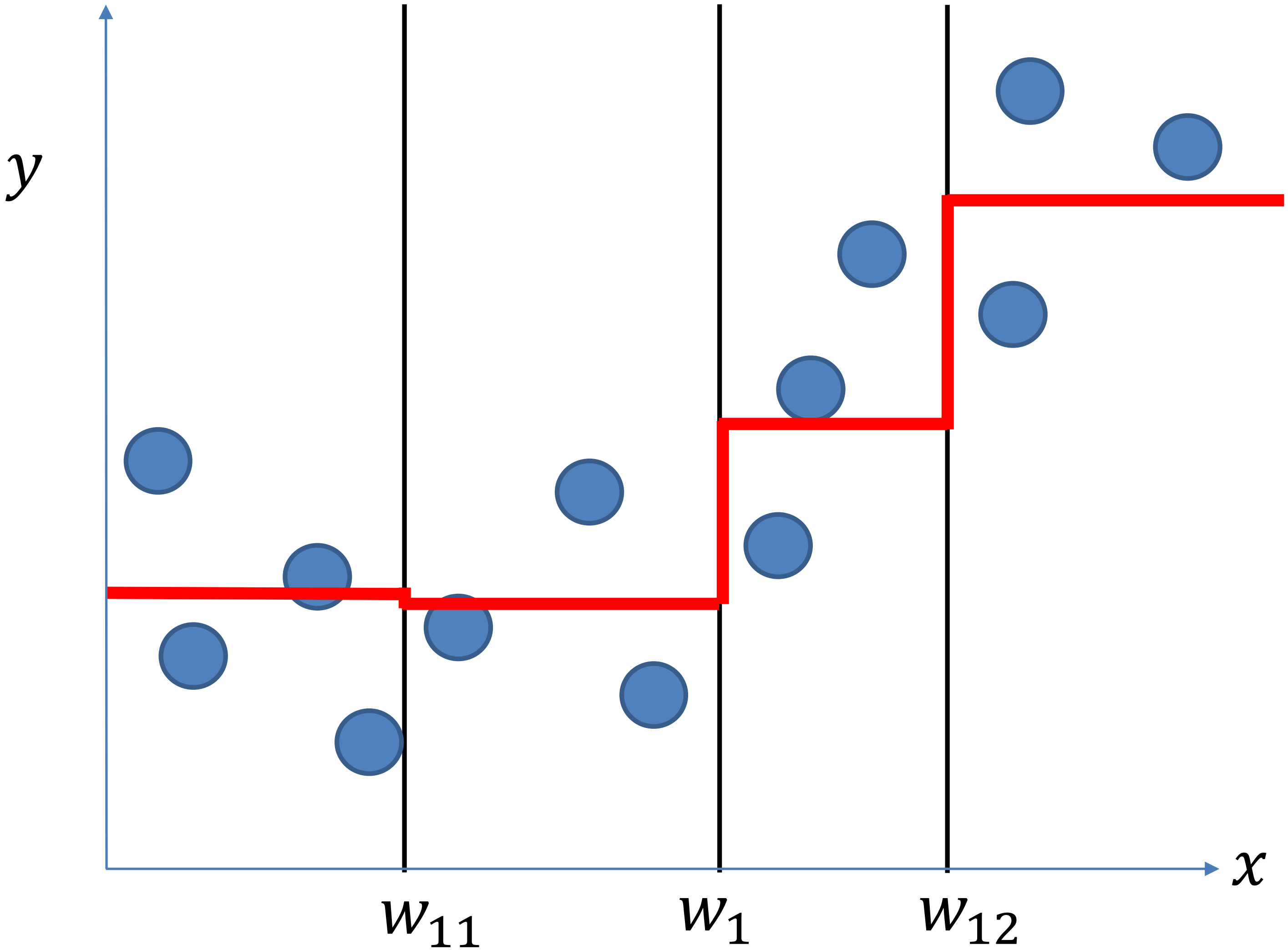

Example of Regression Tree

Example of Regression Tree

- Consider house prices in Singapore.
- Target variable is Price P.
- Attributes are House Size S and Number of Rooms R.

	House Size ('000 sq ft)	Num of Rooms	Price ('000,000 SGD)
1	0.5	2	0.19
2	0.6	1	0.23
3	1.0	3	0.28
4	2.0	5	0.42
5	3.0	4	0.53
6	3.2	6	0.75
7	3.8	7	0.80

- Note that I have arranged the data points in increasing order of P, which so happens to be increasing order of S as well. However, this is not the same order as that of R.

Example of Regression Tree

Mean Squared Error (MSE)

- The MSE for a node m with samples $\{y_i : 1 \leq i \leq J_m\}$ is

$$\mathrm{MSE}_m = \frac{1}{J_m}\sum_{i=1}^{J_m}(y_i - \hat{\mu}_m)^2 \quad \text{where} \quad \hat{\mu}_m = \frac{1}{J_m}\sum_{i=1}^{J_m} y_i.$$

- The overall MSE is $\mathrm{MSE}_P = 0.0520$.

Example of Regression Tree

Calculation of MSE for House Size Split

- Focus first on the House Size attribute S. If we set the threshold at $\tau = 0.75$, then the targets of the two classes are $\{0.19, 0.23\}$ and $\{0.28, 0.42, 0.53, 0.75, 0.80\}$. The individual conditional MSEs are

$$\text{MSE}_{P|S<0.75} = 4 \times 10^{-4} \quad \text{and} \quad \text{MSE}_{P|S\geq 0.75} = 0.0385.$$

- Thus, the averaged conditional MSE with a split of S at 0.75 is

$$\text{MSE}_{P|S(0.75)} = \frac{2}{7}\text{MSE}_{P|S<0.75} + \frac{5}{7}\text{MSE}_{P|S\geq 0.75} = 0.0276.$$

- Sweep through all possible thresholds τ to determine the best threshold for attribute S.

$\text{MSE}_{P\|S(0.55)}$	$\text{MSE}_{P\|S(0.75)}$	$\text{MSE}_{P\|S(1.5)}$	$\text{MSE}_{P\|S(2.5)}$	$\text{MSE}_{P\|S(3.1)}$	$\text{MSE}_{P\|S(3.5)}$
0.0402	0.0276	0.0145	0.0102	0.0116	0.0325

Example of Regression Tree

Calculation of MSE for $\#$ Rooms Split

- Rearrange the target variables in order of the house sizes. Doing so we get $(0.23, 0.19, 0.28, 0.53, 0.42, 0.75, 0.80)$. Now we sweep through all possible thresholds τ for R to get the following averaged conditional MSEs.

- We get the following table.

$\mathrm{MSE}_{P\|R(1.5)}$	$\mathrm{MSE}_{P\|R(2.5)}$	$\mathrm{MSE}_{P\|R(3.5)}$	$\mathrm{MSE}_{P\|R(4.5)}$	$\mathrm{MSE}_{P\|R(5.5)}$	$\mathrm{MSE}_{P\|R(6.5)}$
0.0435	0.0276	0.0145	0.0222	0.0116	0.0325

Example of Regression Tree

Where is the First Split?

- Minima of the split of the S and R variables at different thresholds τ are shaded.
- Choose the minimum MSE as doing so and keeping in mind that MSE_P is the same throughout.
- Gain which is

$$\mathrm{Gain}(S(\tau);P) = \mathrm{MSE}_P - \mathrm{MSE}_{P|S(\tau)}$$

  or

$$\mathrm{Gain}(R(\tau);P) = \mathrm{MSE}_P - \mathrm{MSE}_{P|R(\tau)}$$

  for various τ.

- Minimum MSE is attained for the split of the S attribute at $\tau = 2.5$.

Example of Regression Tree

Where is the First Split?

- We should first split the dataset into two branches, the left branch indicating $S < 2.5$ and the right with $S \geq 2.5$.
- Split the dataset into two sub-datasets and we may decide to stop or split the R feature.
- If we decide to stop, then for any new/test house with a house size of < 2.5, we will predict that its price is the average of the houses in our training set whose size is < 2.5, i.e.,

$$(0.19 + 0.23 + 0.28 + 0.42)/4 = 0.28.$$

- For a new/test house with a house size of ≥ 2.5, we will predict that its price is the average of the houses in our training set whose size is ≥ 2.5, i.e.,

$$(0.53 + 0.75 + 0.80)/3 = 0.6933.$$

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Random Forest

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for t ← 1 to max_trees do
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- To increase randomness, when training the trees, instead of looking at all features when considering how to split a node, we can randomly look at a subset (e.g., square root of the total number of features)

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