Introduction to Data Mining

Chapter 4 Classification – Alternative Techniques

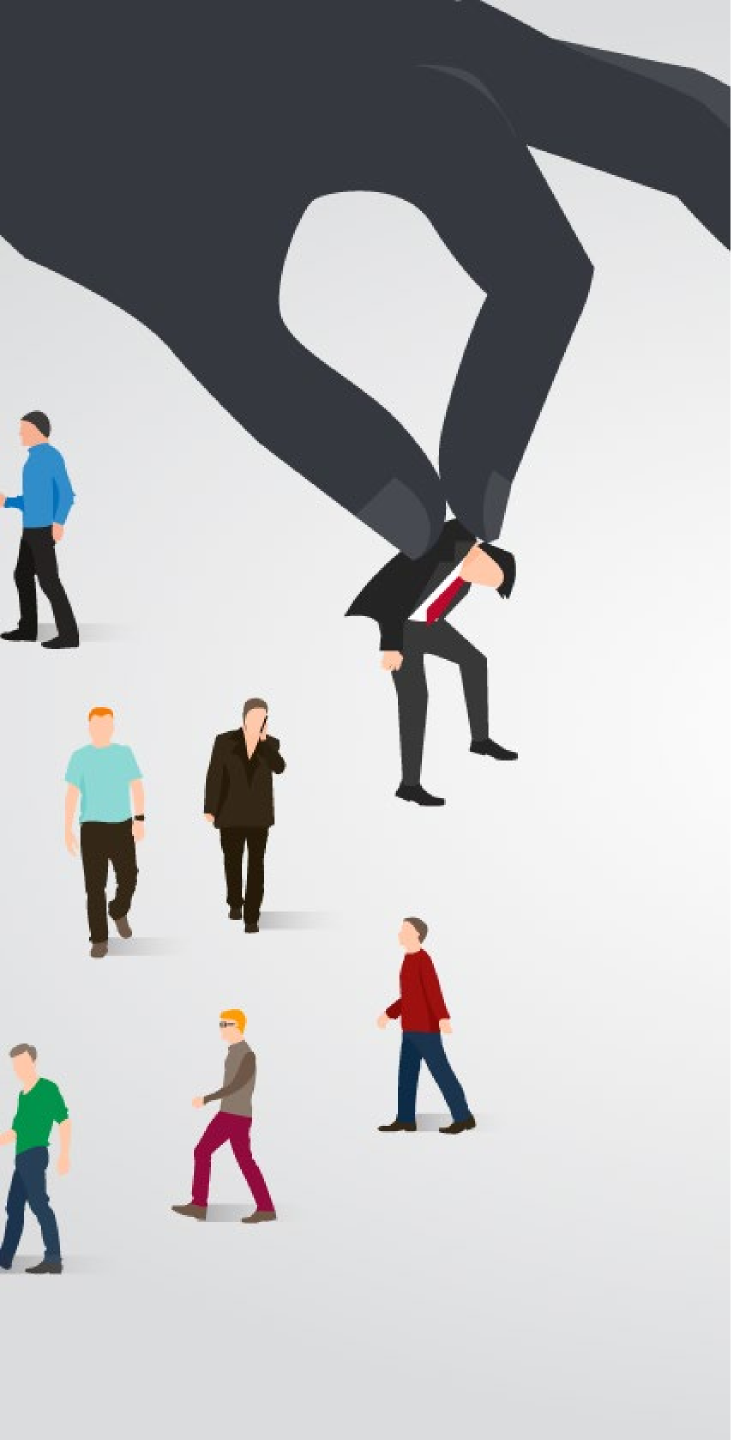
by Michael Hahsler

Based in Slides by Tan, Steinbach, Karpatne, Kumar

R Code Examples

- Available R Code examples are indicated on slides by the R logo

- The Examples are available at https://mhahsler.github.io/Introduction_to_Data_Mining_R_Examples/



Topics

- Other Classification Methods
  - **Rule-Based Classifier**
  - Nearest Neighbor Classifier
  - Naive Bayes Classifier
  - Artificial Neural Networks
  - Support Vector Machines
  - Ensemble Methods
- Class Imbalance Problem

Rule-Based Classifier

- Classify records by using a collection of “if…then…” rules
- Rule: $(Condition) \rightarrow\ y$
  - —Condition is a conjunctions of attributes called LHS, antecedent or condition
  - — y is the class label called RHS or consequent
- Examples of classification rules for an animal dataset:
  - $(Blood\ Type = Warm) \land\ (Lay\ Eggs = Yes) \rightarrow\ Birds$
  - $(Taxable\ Income\ <\ 50K) \land\ (Refund = Yes) \rightarrow\ \ Evade = No$

Using a Rule-Based Classifier

A rule R **covers** an instance x if the attributes of the instance satisfy the condition of the rule. Such a rule can be used for classification.

R1: (Give Birth = no) $\wedge$ (Can Fly = yes) $\rightarrow$ Birds

R2: (Give Birth = no) $\wedge$ (Live in Water = yes) $\rightarrow$ Fishes

R3: (Give Birth = yes) $\wedge$ (Blood Type = warm) $\rightarrow$ Mammals

R4: (Give Birth = no) $\wedge$ (Can Fly = no) $\rightarrow$ Reptiles

R5: (Live in Water = sometimes) $\rightarrow$ Amphibians

Rule base

Name	Blood Type	Give Birth	Can Fly	Live in Water	Class
hawk	warm	no	yes	no	?
grizzly bear	warm	yes	no	no	?

The rule R1 covers: $hawk \rightarrow Bird$

The rule R3 covers: $grizzly\ bear \rightarrow Mammal$

Ordered Rule Set vs. Voting

- Rules are rank ordered according to their priority
  - An ordered rule set is known as a decision list
- When a test record is presented to the classifier
  - It is assigned to the class label of the highest ranked rule it has triggered (R3 is selected below -> Amphibians)
  - If none of the rules fired, it is assigned to the default class

R1: (Give Birth = no) $\wedge$ (Can Fly = yes) $\rightarrow$ Birds

R2: (Give Birth = yes) $\wedge$ (Blood Type = warm) $\rightarrow$ Mammals

R3: (Live in Water = sometimes) $\rightarrow$ Amphibians

R4: (Give Birth = no) $\wedge$ (Can Fly = no) $\rightarrow$ Reptiles

R5: (Give Birth = no) $\rightarrow$ Amphibians

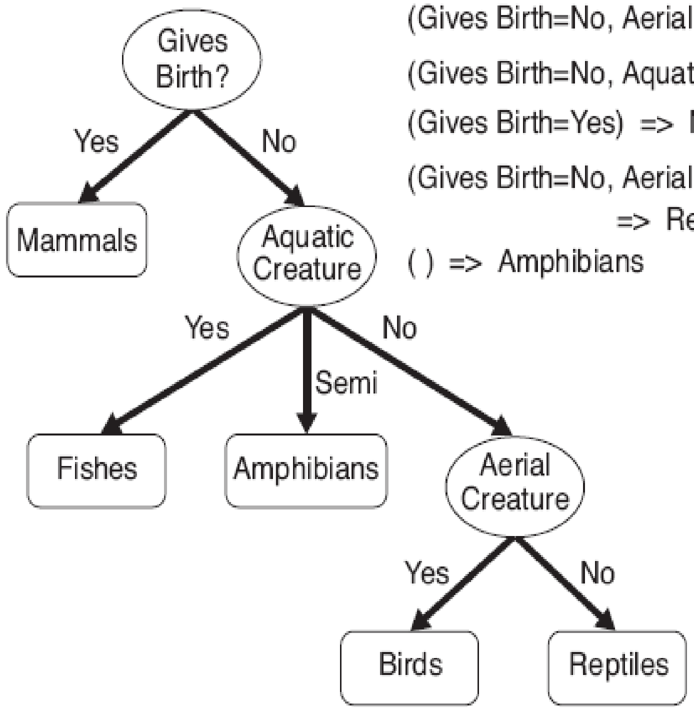
Rule base

Name	Blood Type	Give Birth	Can Fly	Live in Water	Class
turtle	cold	no	no	sometimes	?

R3, 4 and 5 cover the observation

- Alternative: (weighted) voting by all matching rules (-> Amphibians)

Rules From Decision Trees



Rule-Based Classifier:

(Gives Birth=No, Aerial Creature=Yes) => Birds

(Gives Birth=No, Aquatic Creature=Yes) => Fishes

(Gives Birth=Yes) => Mammals

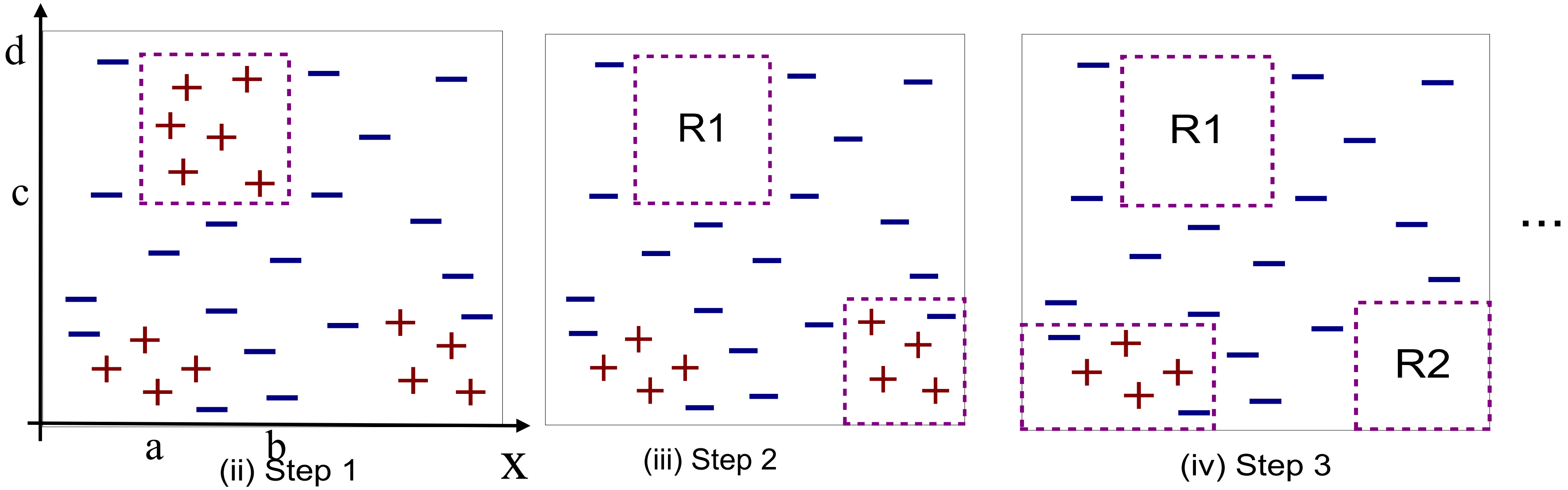
(Gives Birth=No, Aerial Creature=No, Aquatic Creature=No) => Reptiles

( ) => Amphibians

- Rules are created by reading the decisions in tree branches from the root to a final node.
- Rule set contains as much information as the tree.
- Rules can be simplified (similar to pruning of the tree).
- Example: C4.5rules

Direct Methods of Rule Generation

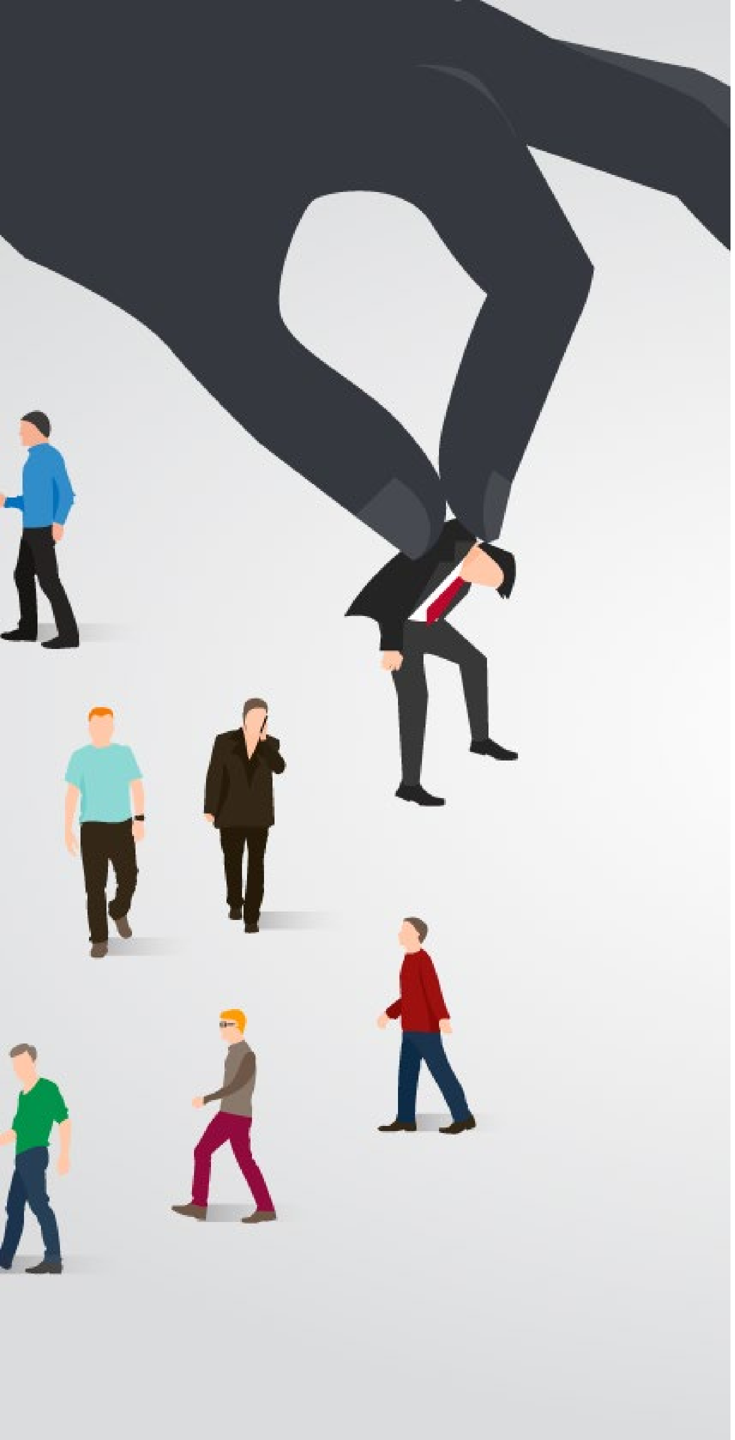
- Extract rules directly from the data
- Sequential Covering (Example: try to cover class +)



R1: $a>x>b \wedge c>y>d \longrightarrow class +$

Advantages of Rule-Based Classifiers

- As expressive as decision trees
- Easy to interpret
- Easy to generate
- Can classify new instances rapidly
- Performance comparable to decision trees



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- **Nearest Neighbor Classifier**
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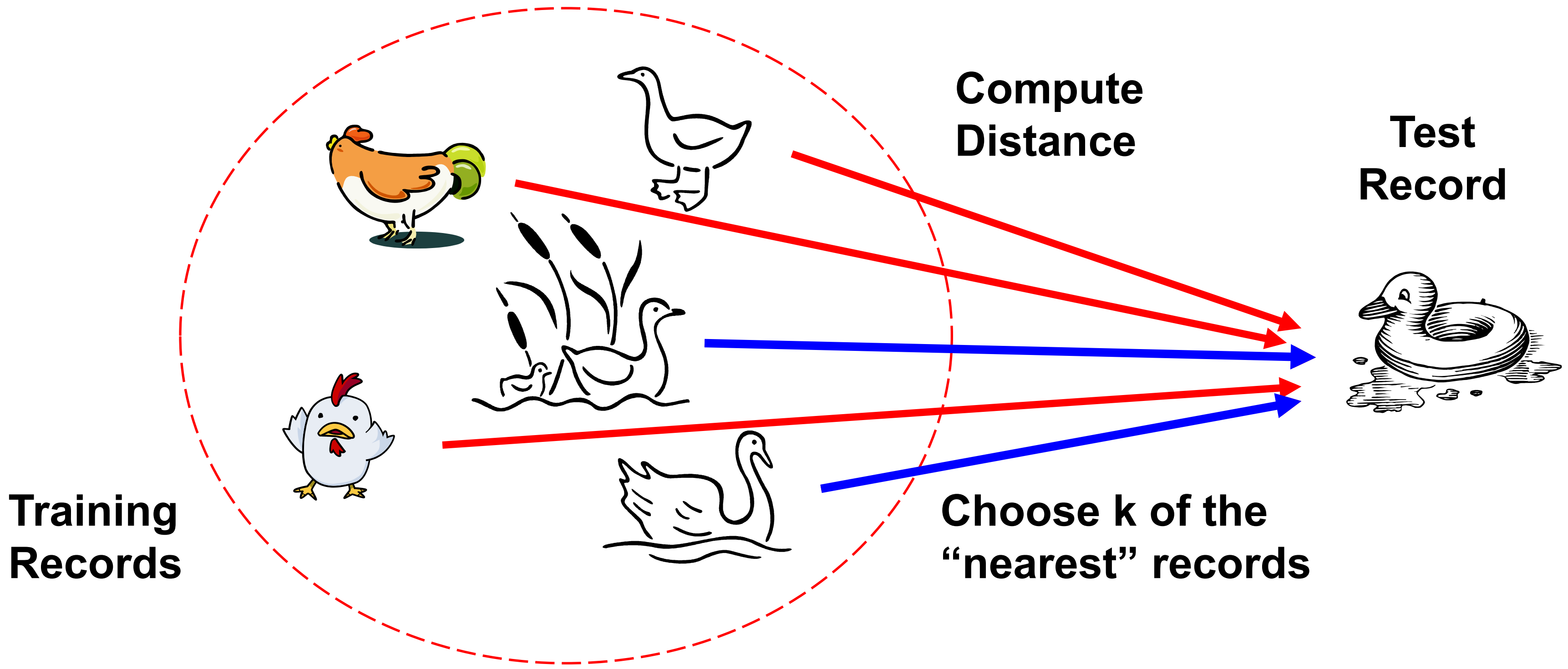
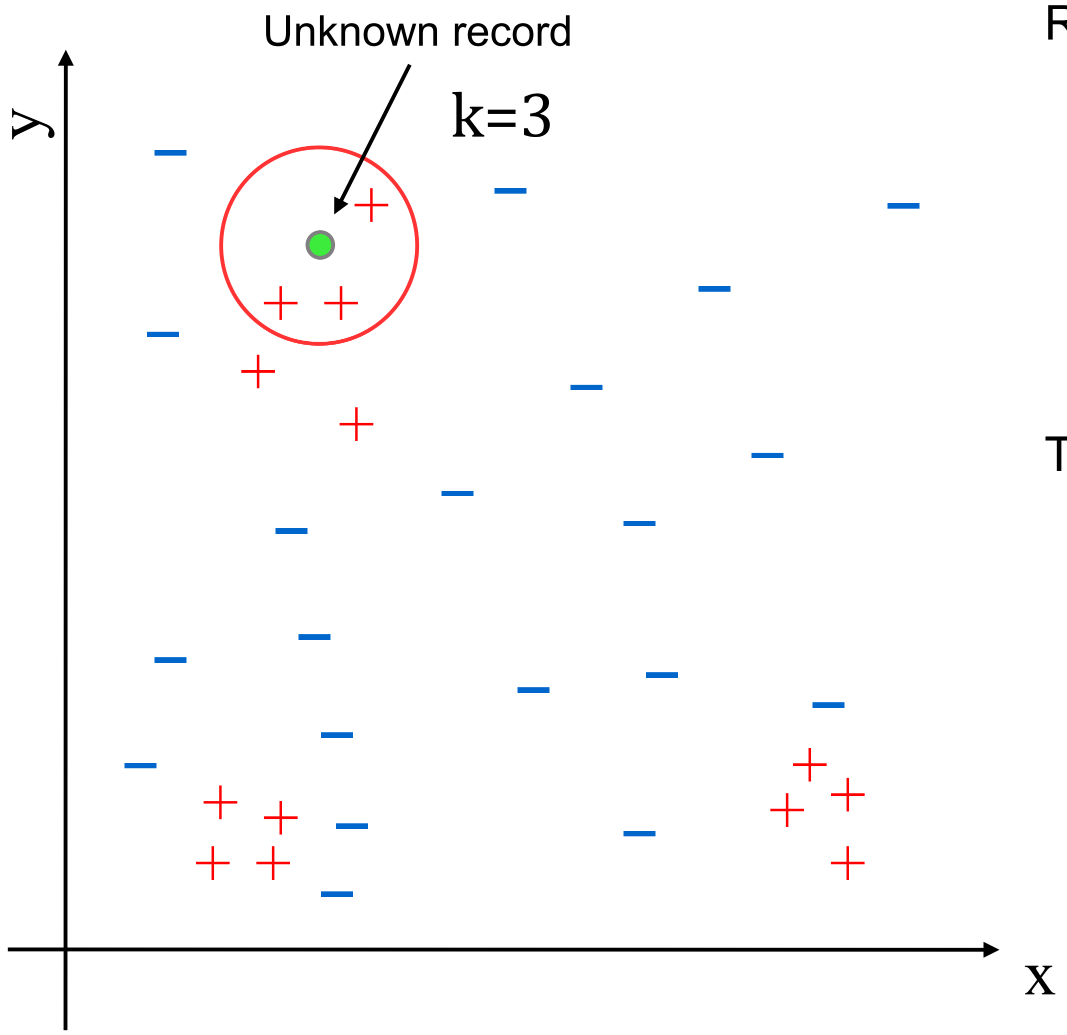
Nearest Neighbor Classifiers

- Basic idea:
  - If it walks like a duck, quacks like a duck, then it’s probably a duck



Nearest-Neighbor Classifiers



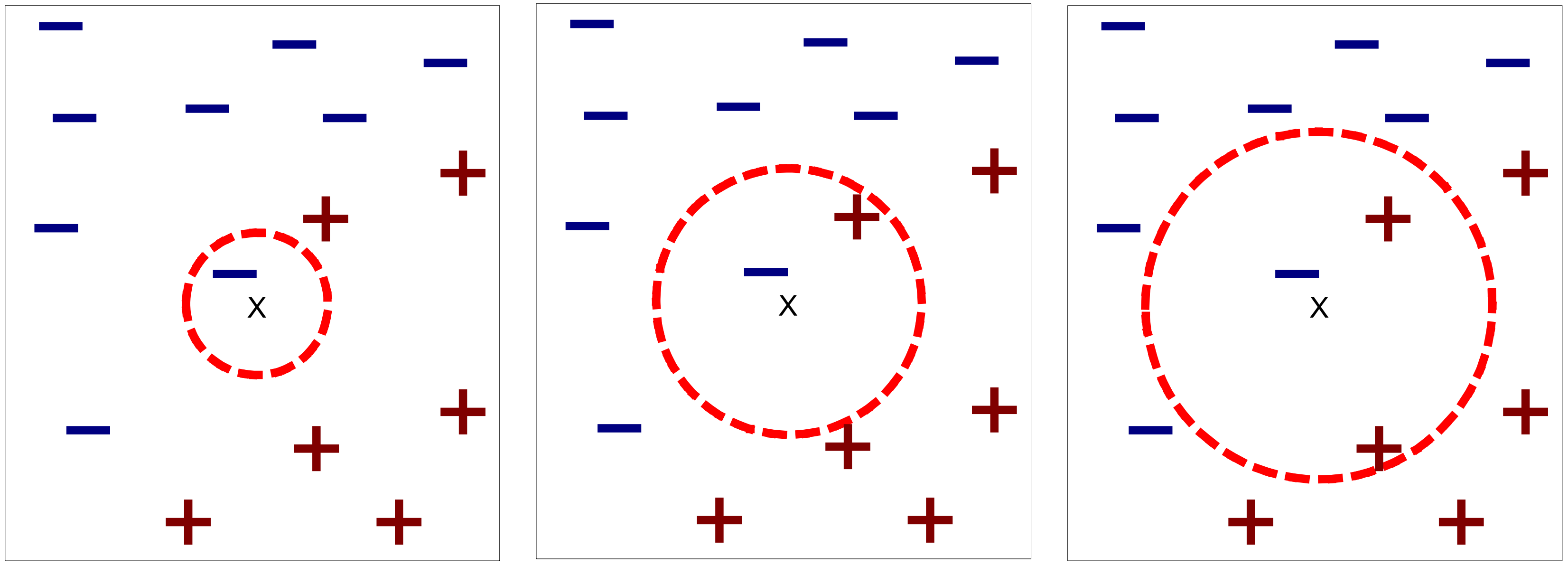
Requires three things

- The set of stored records
- Distance Metric to compute distance between records
- The value of k, the number of nearest neighbors to retrieve

To classify an unknown record:

- Compute distance to other training records
- Identify k nearest neighbors
- Use class labels of nearest neighbors to determine the class label of unknown record (e.g., by taking majority vote)

Definition of Nearest Neighbor



(a) 1-nearest neighbor (b) 2-nearest neighbor (c) 3-nearest neighbor

k-nearest neighbors of a record x are data points that have the k smallest distance to x. k is a hyperparameter.

Nearest Neighbor Classification

- Compute distance between two points:
  - Typically Euclidean distance

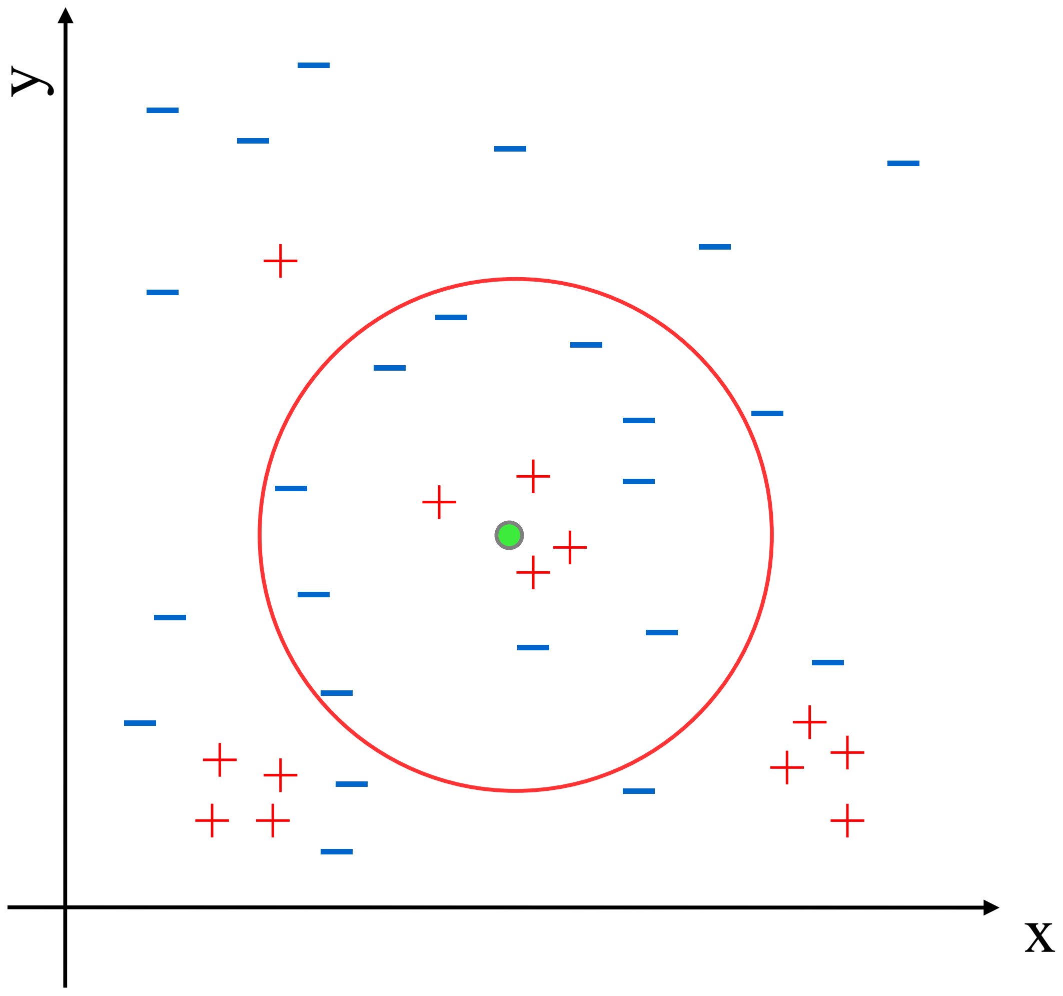
$$d(\boldsymbol{p},\boldsymbol{q}) = \sqrt{\sum_i (p_i - q_i)^2}$$

Note: This means that the data needs to be **scaled**!

- Determine the class from nearest neighbor list
  - Take the majority vote of class labels among the k-nearest neighbors.
  - Weigh the vote according to distance (e.g., weight factor $w = 1/d^2$).

Nearest Neighbor Classification

- Choosing the value of k:
  - If k is too small, sensitive to noise points
  - If k is too large, neighborhood may include points from other classes



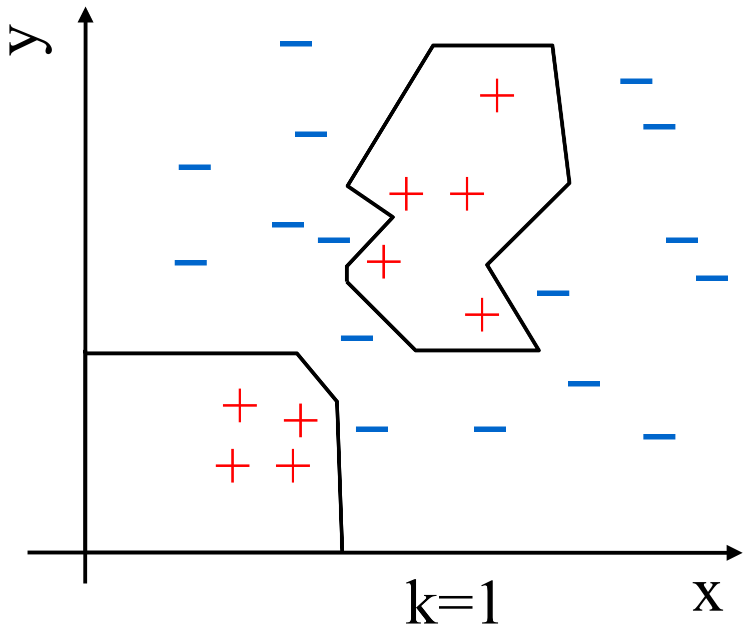
k is too large!

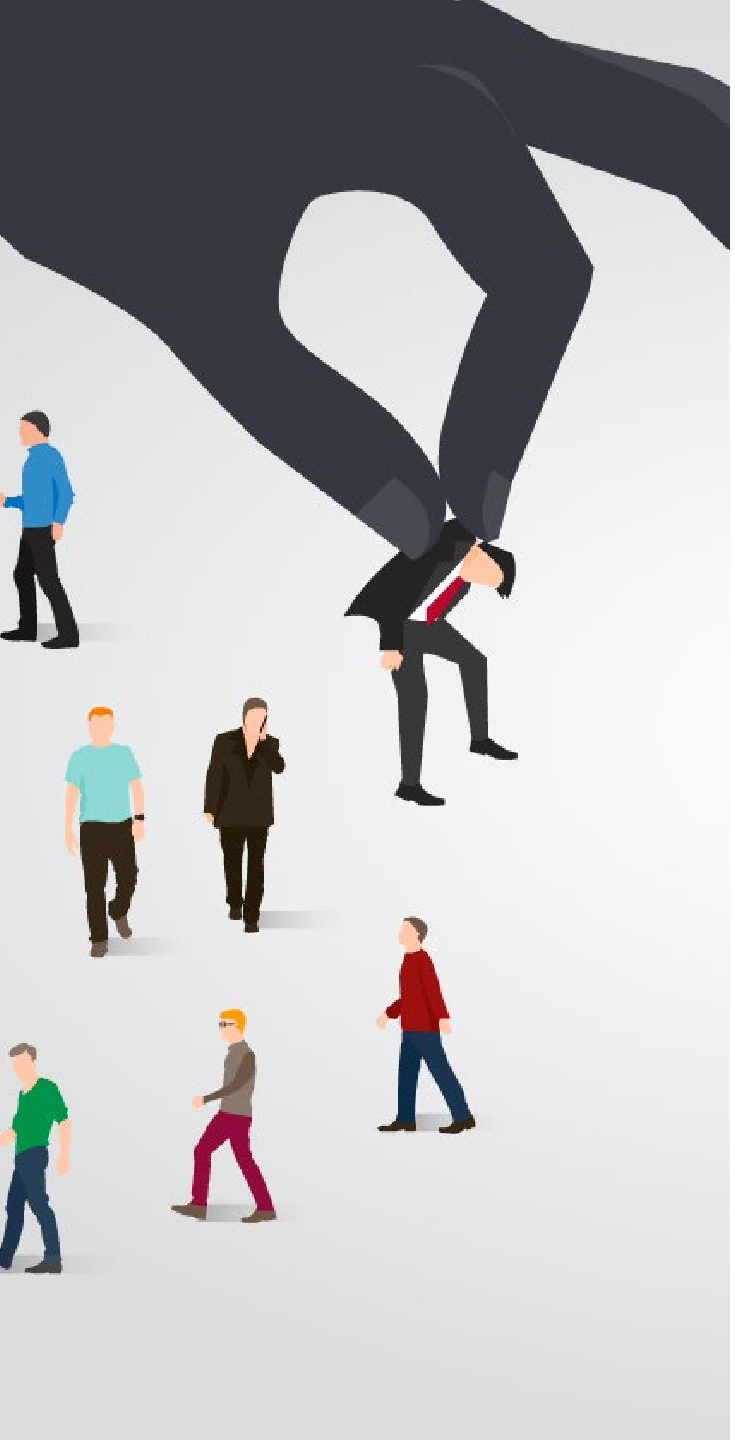
Nearest neighbor Classification…

k-NN classifiers are lazy learners

- It does not build models explicitly (unlike eager learners such as decision trees).
- Needs to store all the training data.
- Classifying unknown records are relatively expensive (find the k-nearest neighbors). Space partitioning data structures like k-d trees can help.

Advantage: Can create arbitrary non-linear decision boundaries.





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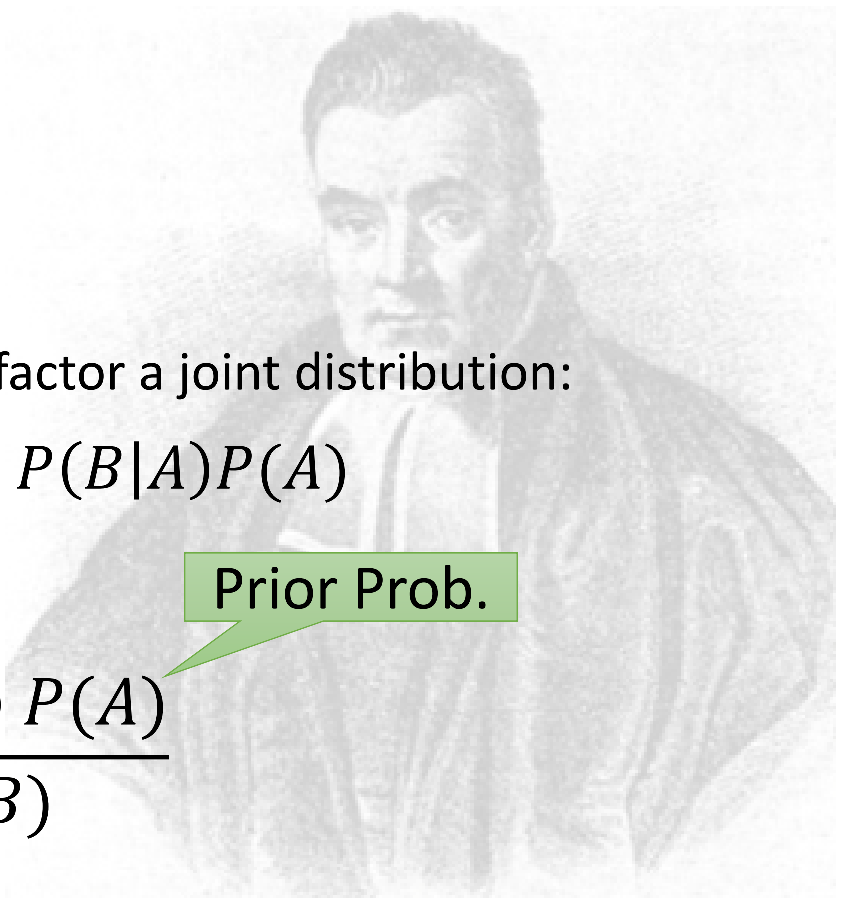
Bayes' Rule



- The product rule gives us two ways to factor a joint distribution:

$$P(A,B) = P(A|B)P(B) = P(B|A)P(A)$$

- Therefore,

Posterior Prob.

Prior Prob.

$$P(A|B) = \frac{P(B|A)\,P(A)}{P(B)}$$

- Why is this useful?
  - Can get diagnostic probability $P(\text{cavity} \mid \text{toothache})$ from causal probability $P(\text{toothache} \mid \text{cavity})$
  - We can update our beliefs based on evidence.
  - Important tool for probabilistic inference .

Example of Bayes Theorem

- A doctor knows that meningitis causes stiff neck 50% of the time → P(S|M)=.5
- Prior probability of any patient having meningitis is P(M) = 1/50,000 = **0.00002**
- Prior probability of any patient having stiff neck is P(S) = 1/20=0.05

- If a patient has stiff neck, what's the probability he/she has meningitis?

$$P(M \mid S) = \frac{P(S \mid M)\, P(M)}{P(S)} = \frac{.5 \times 0.00002}{0.05} = \mathbf{0.0002}$$

Increases the probability by x10!

Bayesian Classifiers

- Consider each attribute and class label as a random variable.
- Classification problem: Given a record with attributes $(A_1, A_2, \dots, A_n)$ predict class C.
- This can be done by finding the most likely class that has the largest

$$\text{argmax}_C \, P(C \mid A_1, A_2, \dots, A_n)$$

- This classification rule is guaranteed to be **optimal** for the accuracy measure!

Bayesian Classifiers

- Compute the posterior probability $P(C \mid A_1, A_2 \; \ldots, A_n)$ for all values of C using the Bayes theorem

$$\underset{C}{\operatorname{argmax}} P(C \mid A_1, A_2, \ldots, A_n) = \operatorname{argmax}_C \frac{P(A_1, A_2, \ldots, A_n \mid C)\, P(C)}{P(A_1, A_2, \ldots, A_n)}$$

This is a constant! We don't need it for the max.

- Equivalent to choosing value of C that maximizes

$$\underset{C}{\operatorname{argmax}} P(A_1, A_2, \ldots, A_n \mid C)\, P(C)$$

- Estimating $P(C)$ is easy, but how do we estimate $P(A_1, A_2, \ldots, A_n \mid C)$?

  Unfortunately, this table is very large and can only be estimated for a small number of attributes.

Naïve Bayes Classifier

Assume independence among attributes A given the class. Now we can factor the probability distribution into the product of a few independent probabilities.

$$P(A_1, A_2, \dots, A_n \,|C) = P(A_1|\, C)\, P(A_2|\, C) \dots P(A_n|\, C) = \prod_i P(A_i \mid C)$$

We can estimate $P(A_i \mid C_j)$ for all A_i and C_j.

A new observation is classified to C_j such that:

$$\operatorname*{argmax}_j \; P\left(C_j\right) \prod_i P(A_i \,|C_j)$$

How to Estimate Probabilities from Data?

- Use the maximum likelihood estimate.
- Class: $P(C_j) = N_{C_j} / N$

  e.g., P(C=No) = 7/10,
  P(C=Yes) = 3/10
- For discrete attributes:

$$P(A_i | C_j) = \frac{|A_{ij}|}{N_{C_j}}$$

where $|A_{ij}|$ is number of instances having attribute A_i and belongs to class C_j

e.g.
P(Status=Married | C=No) = 4/7
P(Refund=Yes | C=Yes)=0

Tid	**Refund**	**Marital Status**	**Taxable Income**	**Class**
1	Yes	**Single**	125K	**No**
2	No	Married	100K	**No**
3	No	**Single**	70K	**No**
4	Yes	Married	120K	**No**
5	No	Divorced	95K	**Yes**
6	No	Married	60K	**No**
7	Yes	Divorced	220K	**No**
8	No	**Single**	85K	**Yes**
9	No	Married	75K	**No**
10	No	**Single**	90K	**Yes**

How to Estimate Probabilities from Data?

For continuous attributes there are several options:

- Discretize the range into bins
  - one ordinal attribute per bin
  - violates independence assumption

- Two-way split: (A < v) or (A > v)
  - choose only one of the two splits as new attribute

- Probability density estimation.
  - Assume attribute follows a normal distribution.
  - Use data to estimate parameters of distribution (e.g., mean and standard deviation).
  - Once probability distribution is known, can use it to estimate the conditional probability $P(A_i \mid C_j)$.
  - Most implementations will do this automatically. This is called a Gaussian Naïve Bayes Classifier.

Example of Naïve Bayes Classifier

Given a Test Record what is the most likely class?

$$X = (Refund = No, Married, Income = 120K)$$

naive Bayes Classifier:

P(Refund=Yes|No) = 3/7
P(Refund=No|No) = 4/7
P(Refund=Yes|Yes) = 0
P(Refund=No|Yes) = 1
P(Marital Status=Single|No) = 2/7
P(Marital Status=Divorced|No)=1/7
P(Marital Status=Married|No) = 4/7
P(Marital Status=Single|Yes) = 2/7
P(Marital Status=Divorced|Yes)=1/7
P(Marital Status=Married|Yes) = 0

For taxable income:

If class=No:	sample mean=110
	sample variance=2975
If class=Yes:	sample mean=90
	sample variance=25

P(X|Class=No) = P(Refund=No|Class=No)
** P(Married| Class=No)*
** P(Income=120K| Class=No)*
*= 4/7 * 4/7 * 0.0072 = 0.0024*

P(X|Class=Yes) = P(Refund=No| Class=Yes)
** P(Married| Class=Yes)*
** P(Income=120K| Class=Yes)*
$= 1 * 0 * 1.2 * 10^{-9} = 0$

0 are an issue!

Since *P(X|No)P(No) > P(X|Yes)P(Yes)*

Therefore *P(No|X) > P(Yes|X)*

=> Class = No

Naïve Bayes Classifier: Dealing With Low Counts

Probability estimation:

Original: $P(A_i \mid C_j) = \frac{N_{ij}}{N_j}$

Issue: If one of the conditional probabilities is zero, then the entire expression becomes zero.

Laplace: $P(A_i \mid C_j) = \frac{N_{ij}+1}{N_j+c}$

m-estimate: $P(A_i \mid C_j) = \frac{N_{ij}+mp}{N_j+m}$

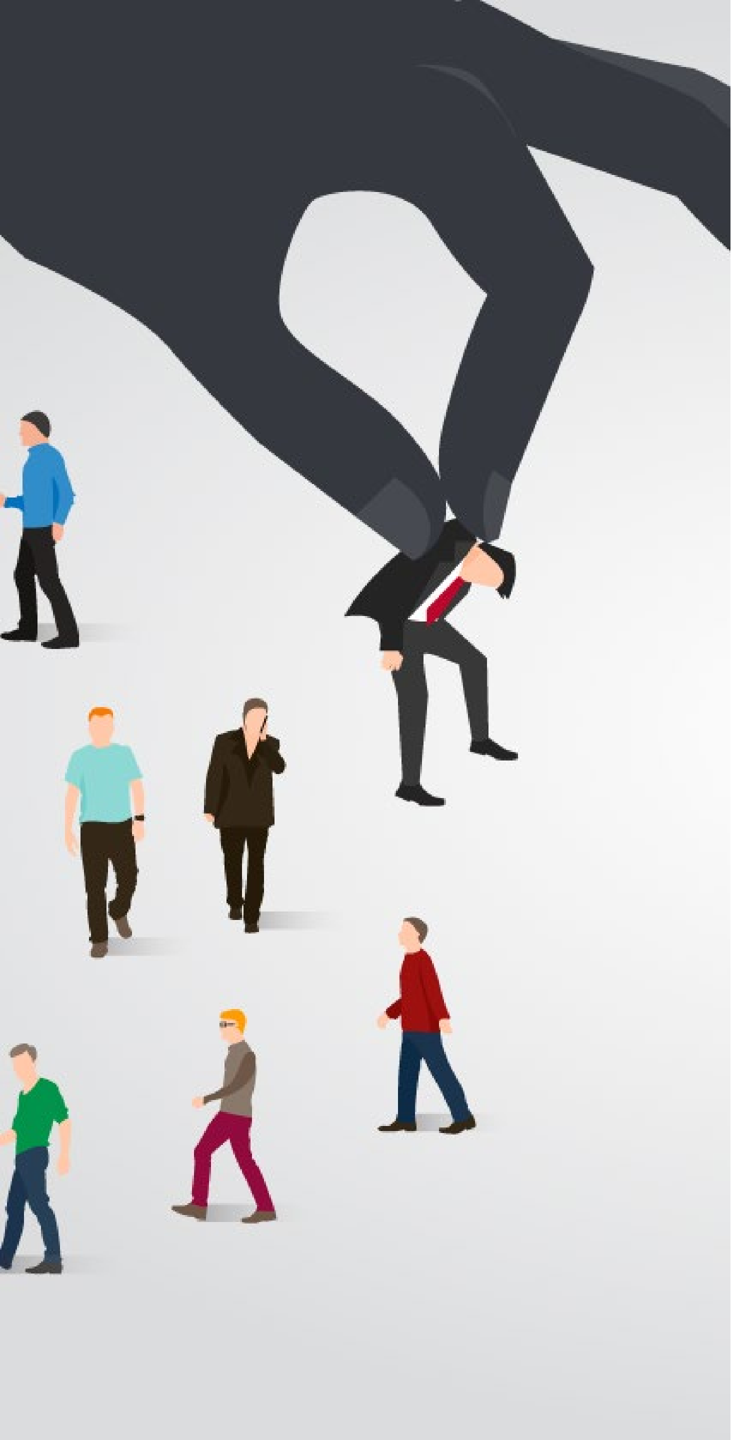
c: number of classes

p: prior probability

m: parameter

Naïve Bayes (Summary)

- **Robust to outliers** and isolated noise points since it is not based on distances.
- **Can handle missing value** during prediction: Ignore the attribute during probability estimate calculations.
- **Robust to irrelevant attributes**: They will just get a probability of $1/|C|$.
- **Independence assumption** may not hold for some attributes
  - Typically, the classifiers still work well when the assumption is slightly violated.
  - You can remove highly correlated attributes.
  - Use other techniques such as Bayesian Belief Networks (BBN)



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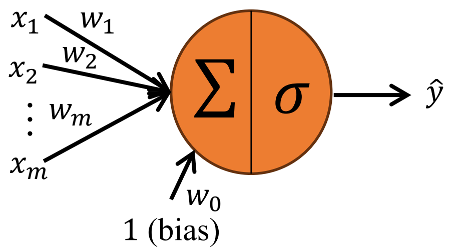
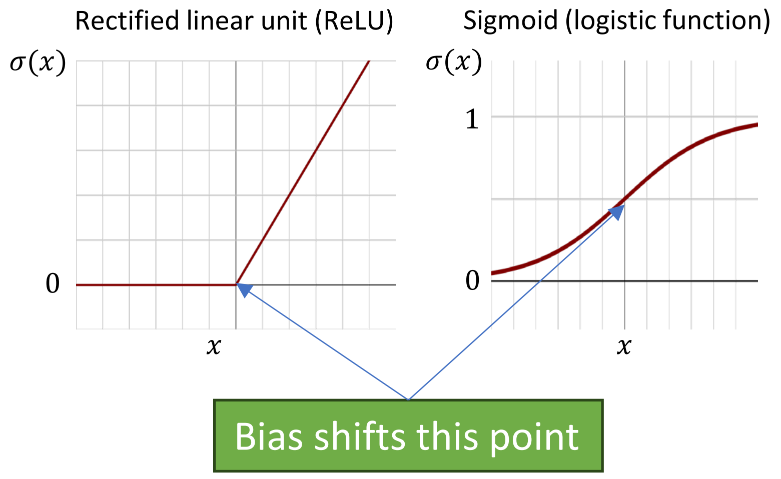
The Artificial Neuron



$$\hat{y} = \sigma\left(w_0 + \sum_{i=1}^{m} x_i w_i\right) = \sigma(\boldsymbol{w}^T \boldsymbol{x})$$

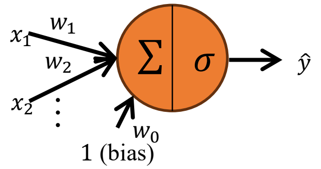
- Input vector: $\boldsymbol{x} = (1, x_1, x_2, \ldots, x_m)$, where the first element is for the bias.
- Weight vector: $\boldsymbol{w} = (w_o, w_1, w_2, \ldots, w_m)$
- Activation function: $\sigma(\cdot)$ is a nonlinear function that transforms the weighted sum of inputs into an output value called the activation of the neuron. Typical activation functions are:

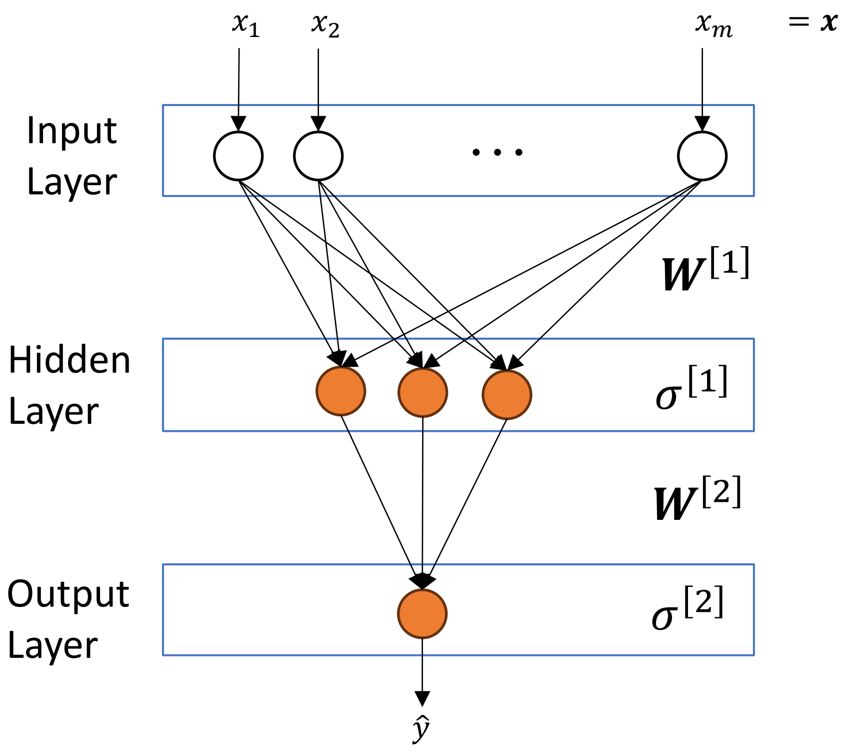


Training: Find $\boldsymbol{w}$ that minimizes the loss $L(\hat{y}, y)$ using gradient descent.

Relationship to Logistic regression to predict a binary outcome: Artificial neuron with logistic activation function and binary cross-entropy loss.

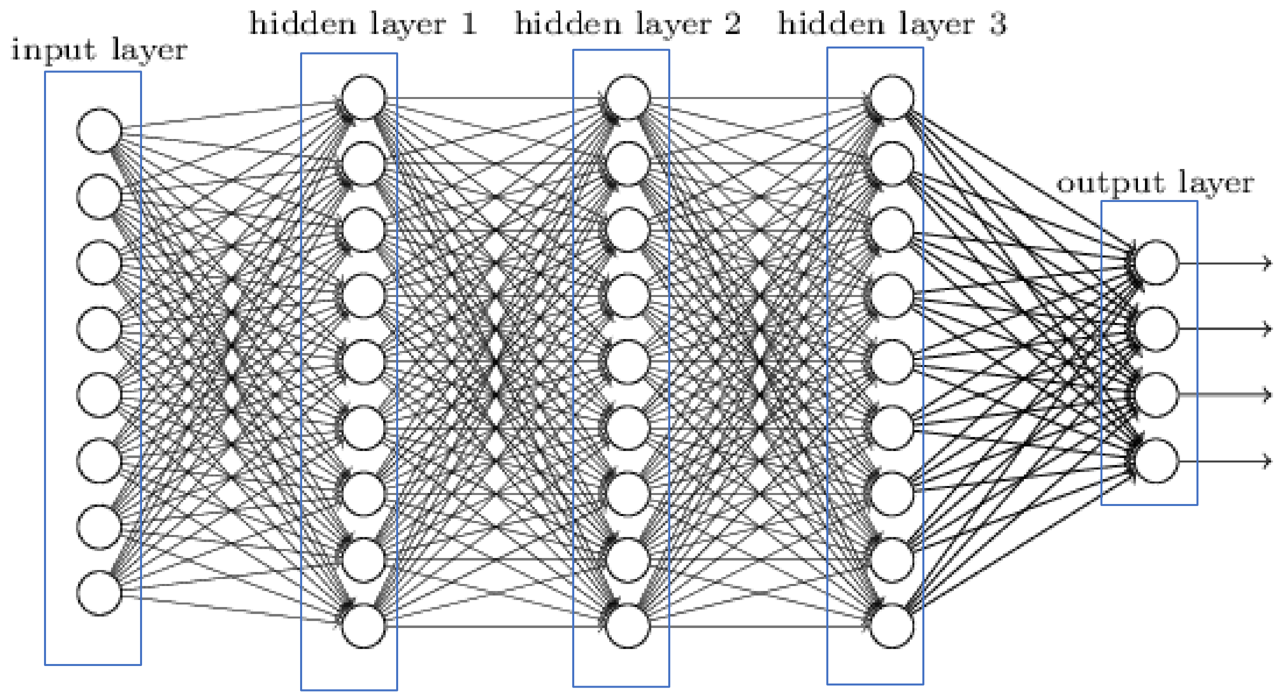
General Structure of an ANN



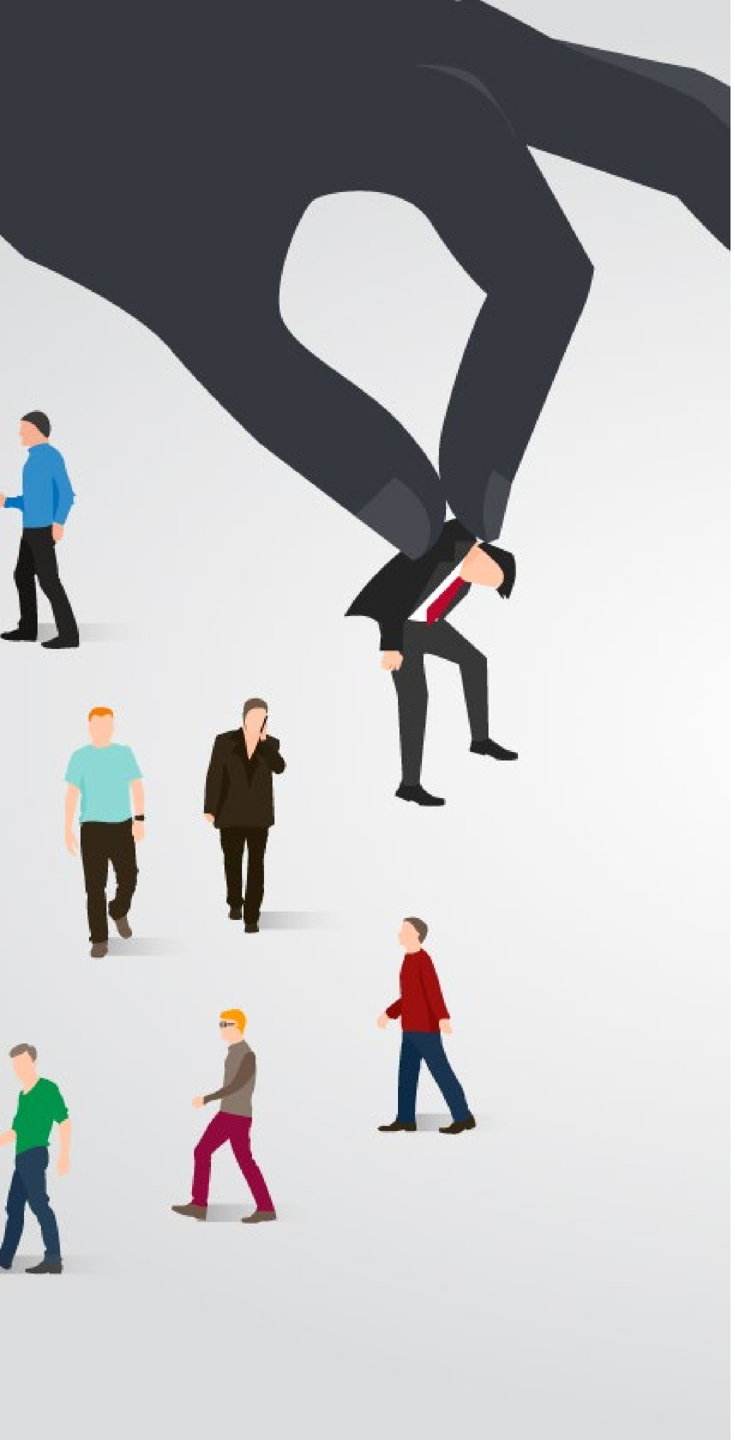


- Collect the weights of all neurons in a layer into a matrix:
$$\boldsymbol{W}^{[l]} = \left[\boldsymbol{w}_1^{[l]}, \boldsymbol{w}_2^{[l]}, \dots\right]$$
- $\hat{y} = \sigma^{[2]}\left(\boldsymbol{W}^{[2]}\sigma^{[1]}\left(\boldsymbol{W}^{[1]}\boldsymbol{x}\right)\right)$
- **Training**: learn weights that minimize $L(\hat{y}, y)$ using gradient descent with backpropagation.
- ANNs with a single hidden layer are **universal approximators**, i.e., can approximate any function $y = f(x)$.

Deep Learning / Deep Neural Networks



- Can make training more efficient. Pretrained layers may be used (i.e., transfer learning).
- Needs lots of data + computation (GPU).
- Applications: computer vision, speech recognition, natural language processing, audio recognition, machine translation, bioinformatics, …
- Tools: Keras, Tensorflow and many others.
- Related: Deep belief networks, recurrent neural networks (RNN), convolutional neural network (CNN), …



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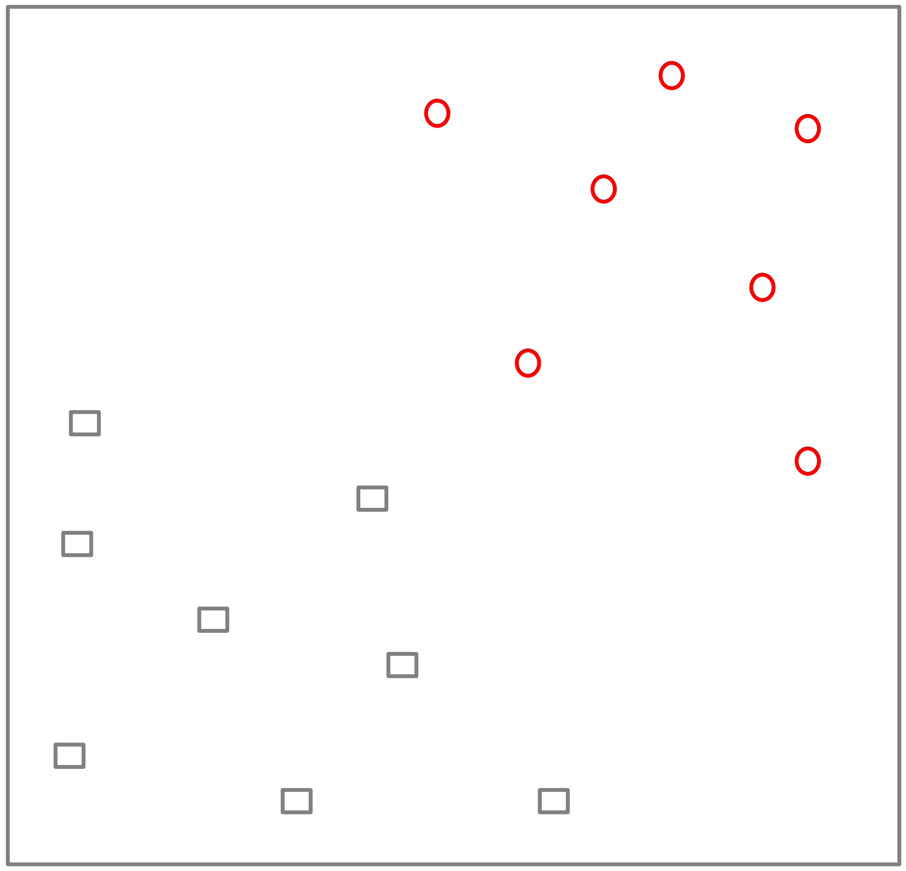
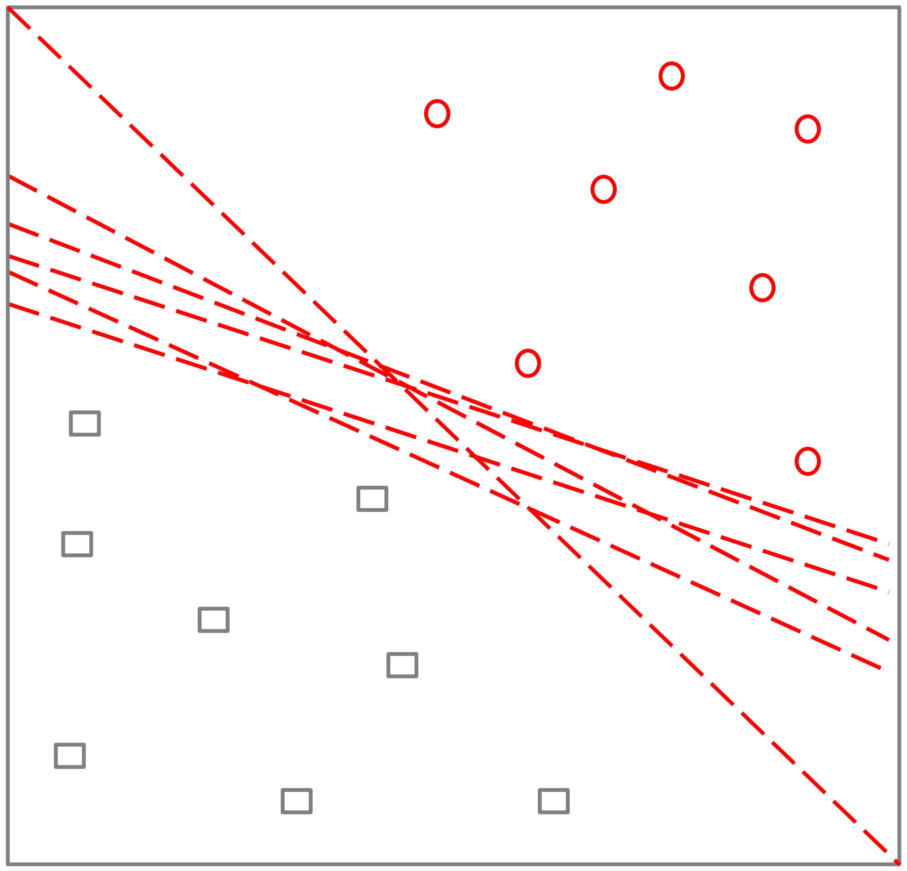
Support Vector Machines



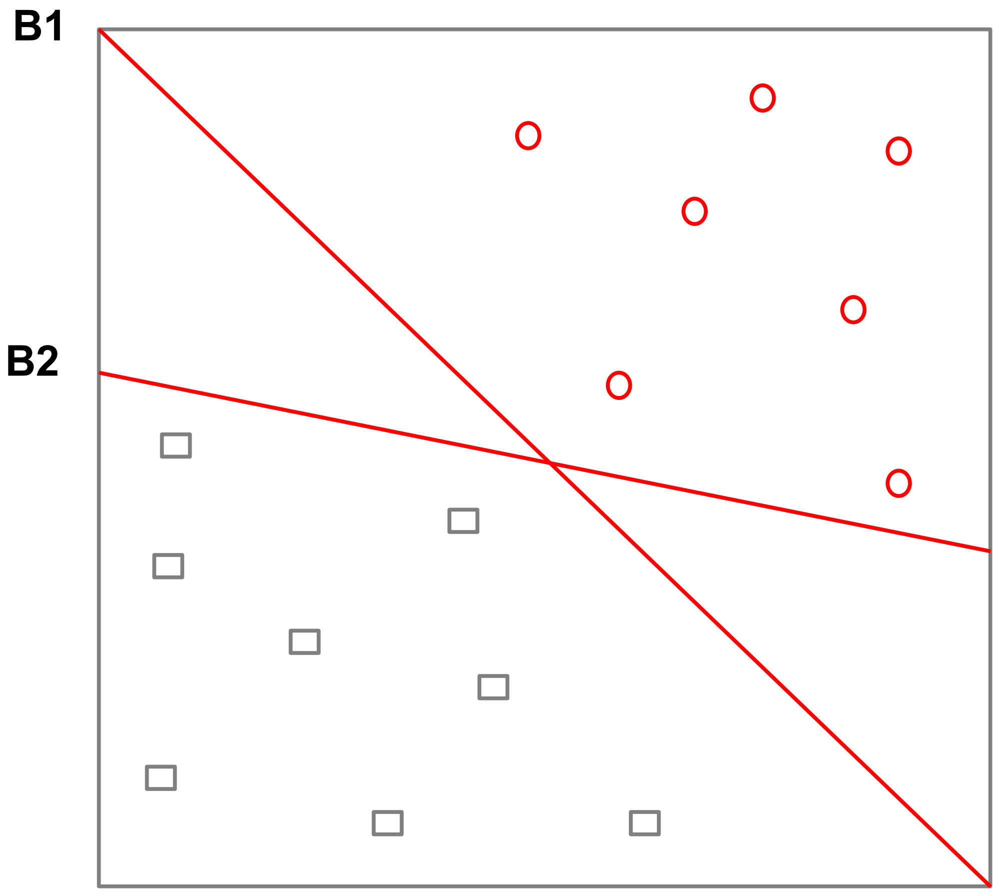
Goal: Find a linear hyperplane (decision boundary) that will separate the data.

Support Vector Machines



Many possible solutions

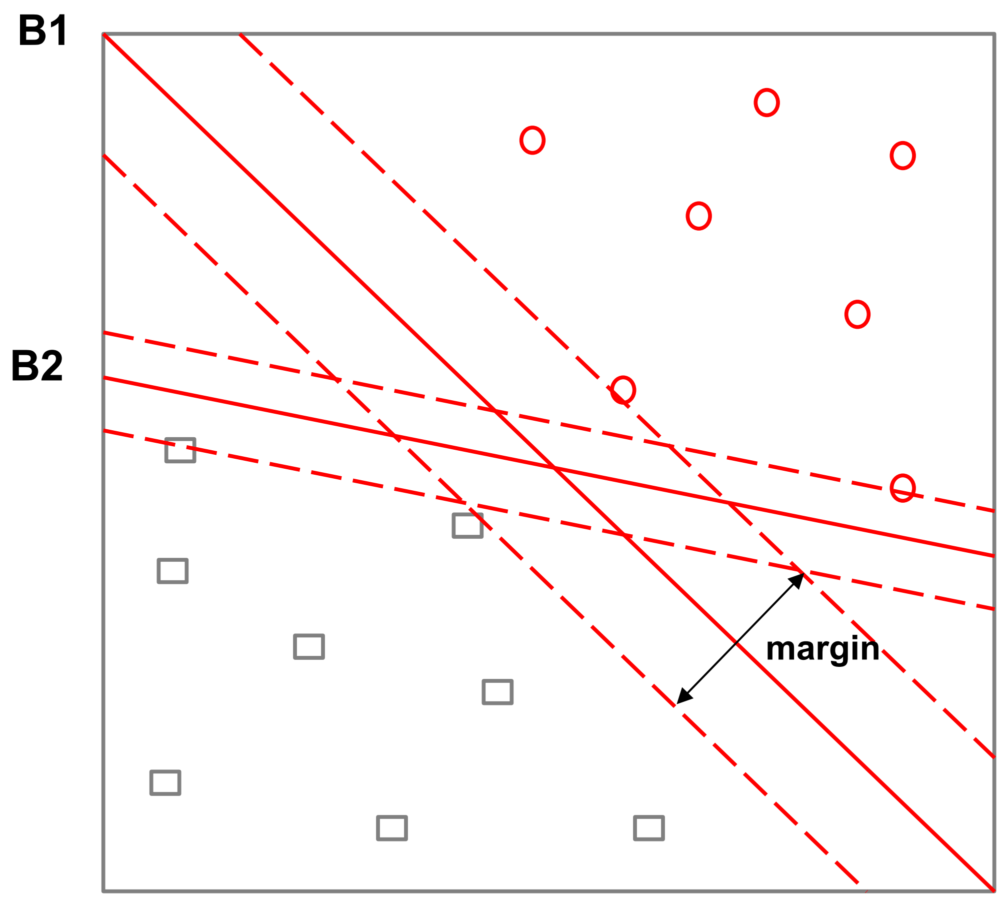
Support Vector Machines



Which one is better? B1 or B2?

How do you define better?

Support Vector Machines



Find the hyperplane with the maximal margin => B1 is better than B2

Larger margin = more robust = less expected generalization error

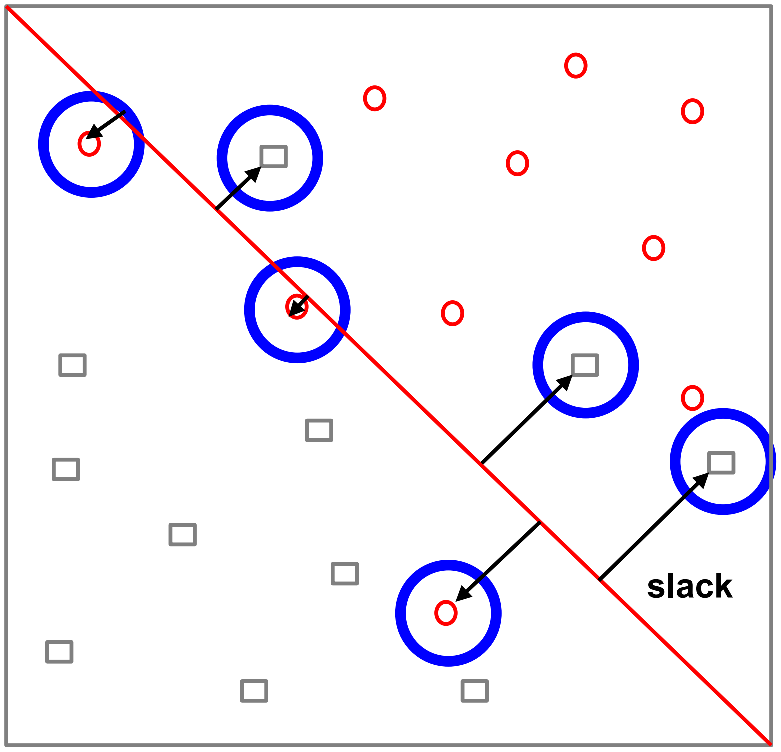
Support Vector Machines

What if the problem is not linearly separable?

- Use slack variables to account for violations.
- Use hyperplane that minimizes the total slack.

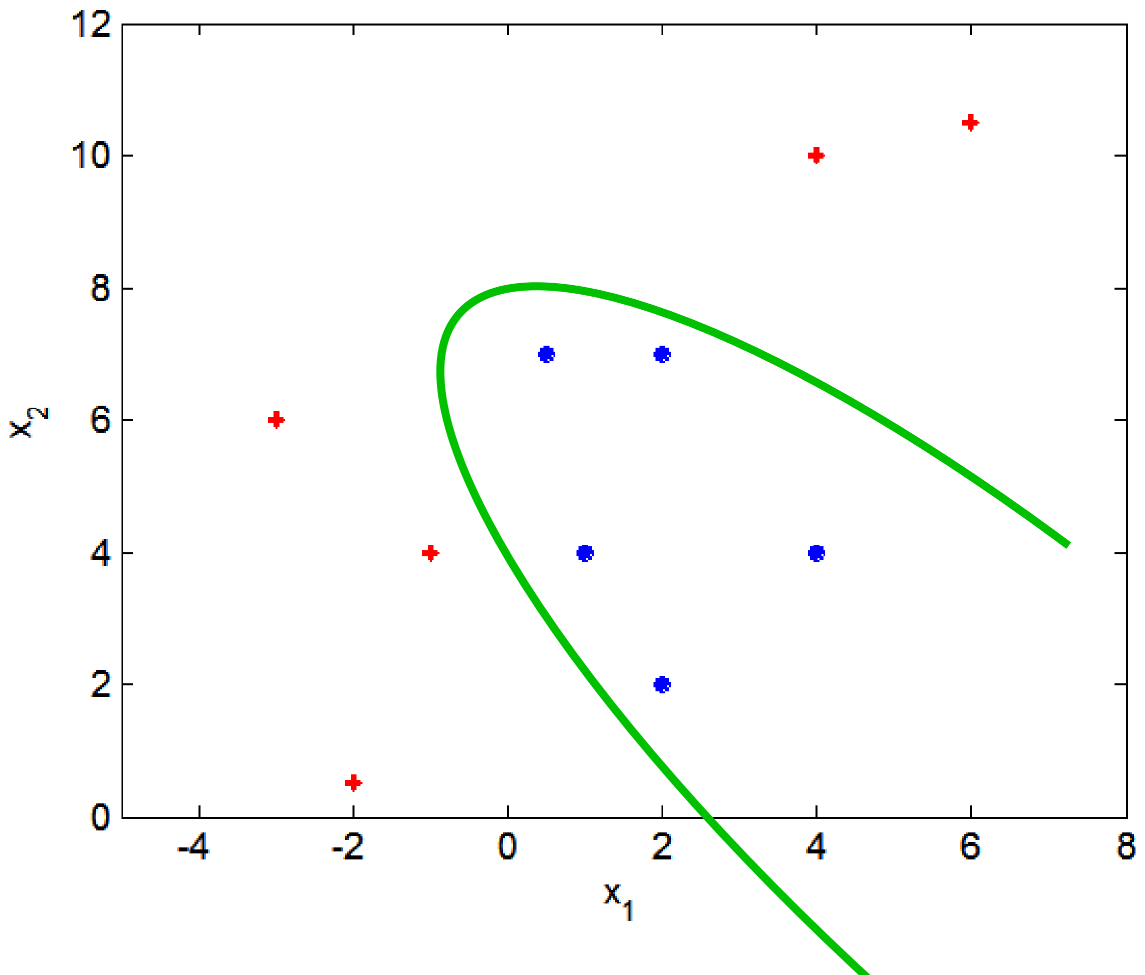
Solution:

- The optimization problem can be written as a **quadratic optimization problem** with linear constraints that **only depends on a few close data points** called the support vectors.

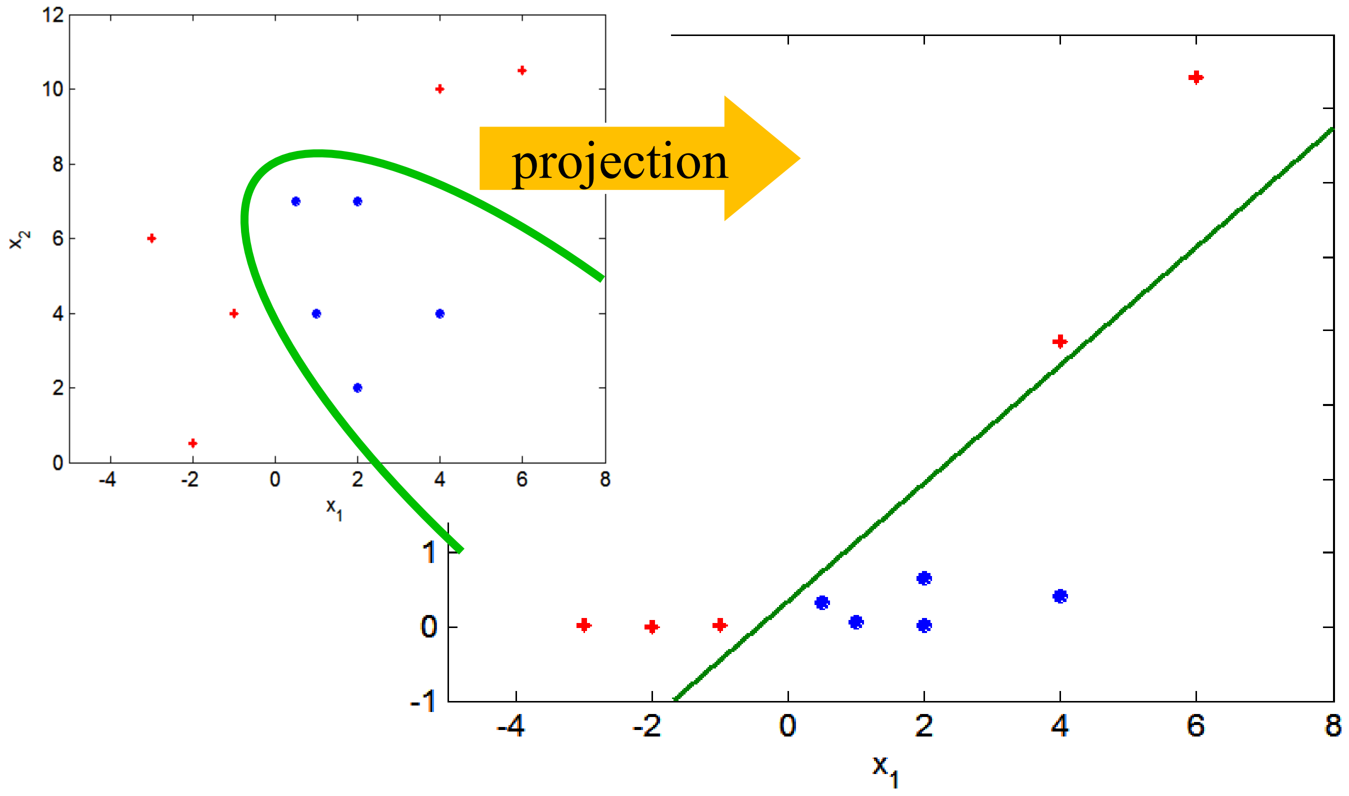


Nonlinear Support Vector Machines

SVMs look for linear decision boundaries. What if decision boundary is not linear?

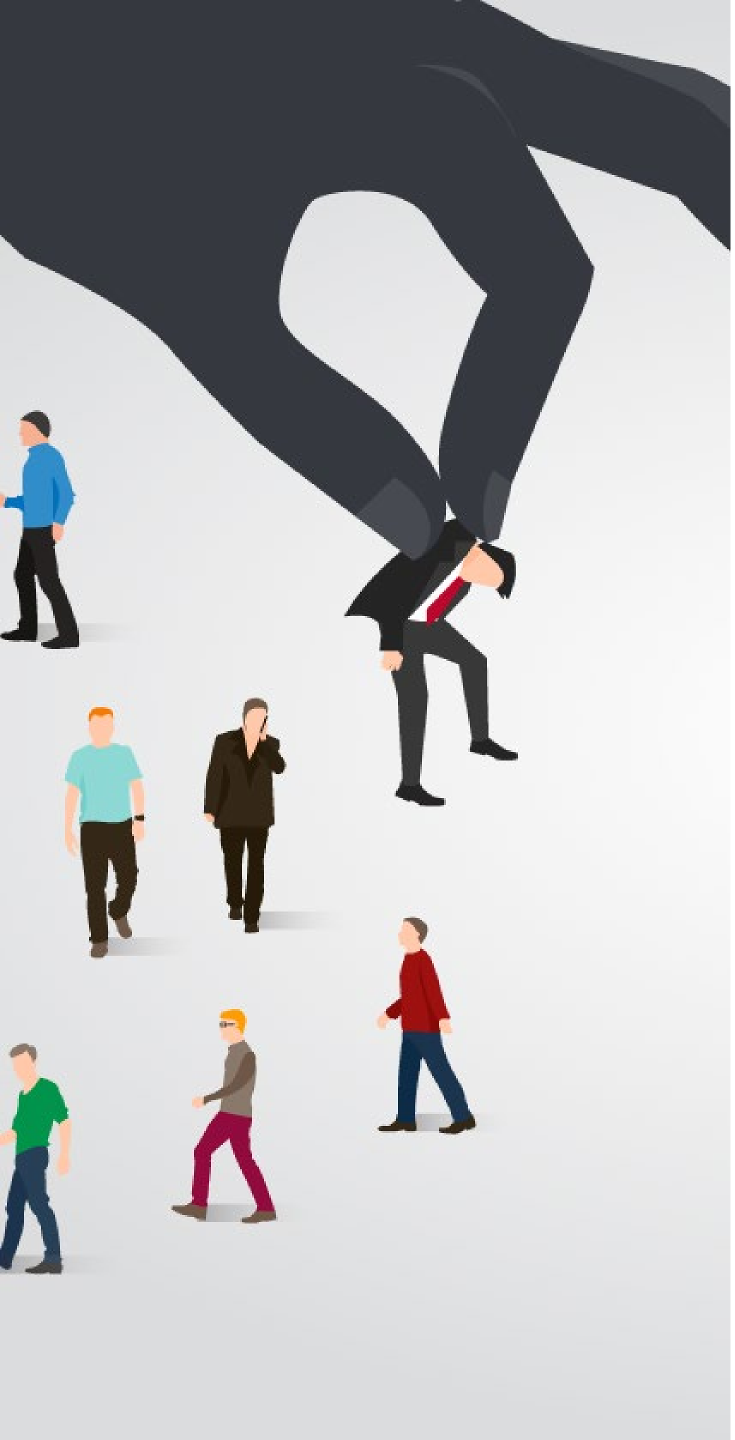


Nonlinear Support Vector Machines



- Project data into a higher dimensional space where the classes are linearly separable.

- Projection is expensive!
  Kernel trick: Compute the similarity (inner product) in the projected space directly from the original data. This trick can be used with other method like clustering as well.



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Ensemble Methods

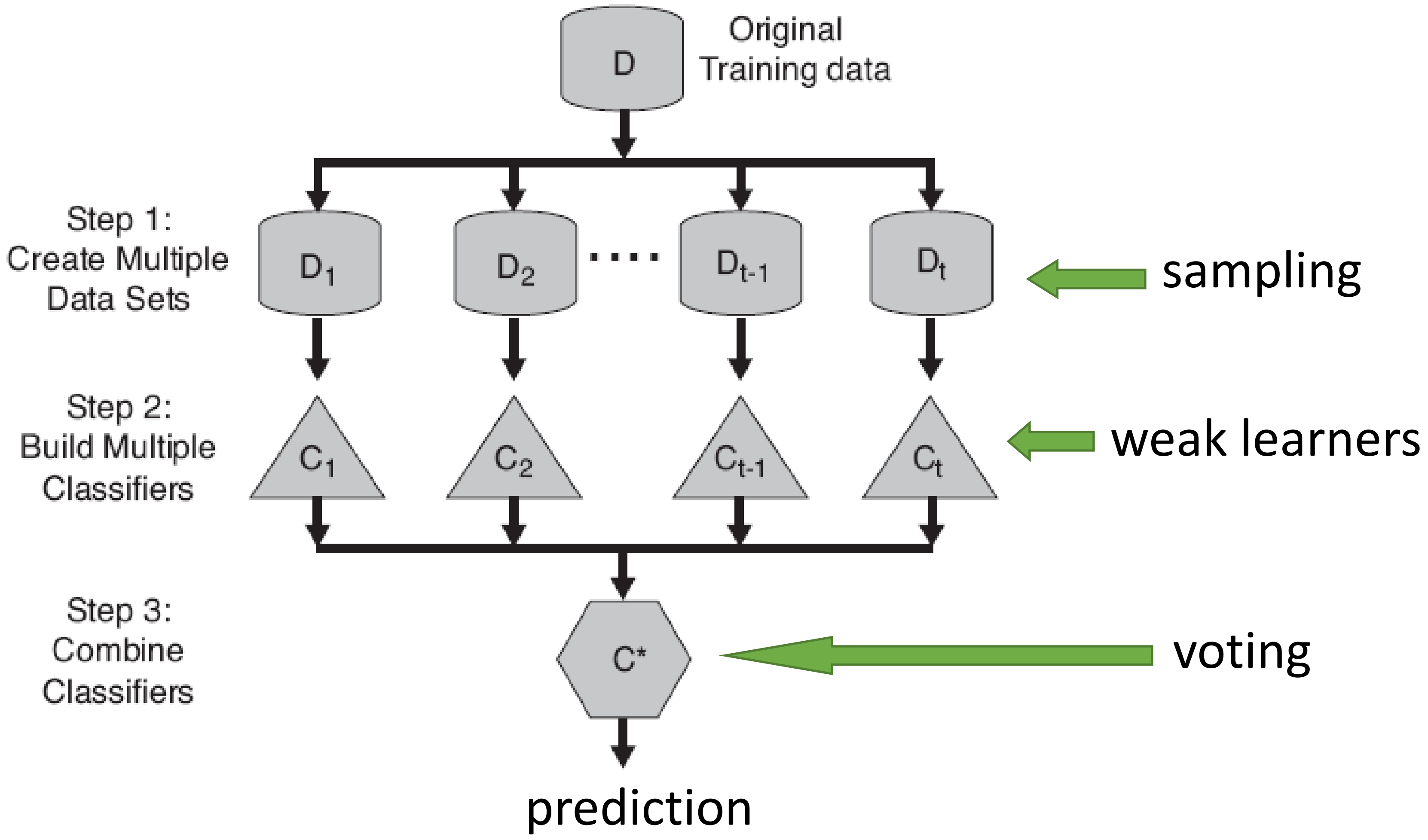
Method

1. Construct a set of (possibly weak) classifiers from the training data.
2. Predict class label of previously unseen records by aggregating predictions made by multiple classifiers.

Advantages

- Improve the stability and often also the accuracy of classifiers.
- Reduces variance in the prediction.
- Reduces overfitting.

General Idea



Why does it work?

- Suppose there are 25 base classifiers.
  - Each classifier has error rate $\epsilon = 0.35$
  - Assume classifiers are independent (different features and/or training data).
- Probability that the ensemble classifier makes a wrong prediction:

$$\sum_{i=13}^{25} \binom{25}{i} \epsilon^i (1-\epsilon)^{25-i} = 0.06$$

= Probability that the majority (13 or more classifiers) make the wrong decision.

Note

- The binomial coefficient gives the number of ways you can choose i out of 25.

Examples of Ensemble Methods

- How to generate an ensemble of independent classifiers?

Bagging	Boosting	Random Features
• Use several samples	• Increase the weight for misclassified data points	• Use different features

Bagging (Bootstrap Aggregation)

1. **Sampling** with replacement (bootstrap sampling)

Original Data	1	2	3	4	5	6	7	8	9	10
Bagging (Round 1)	7	8	10	8	2	5	10	10	5	9
Bagging (Round 2)	1	4	9	1	2	3	2	7	3	2
Bagging (Round 3)	1	8	5	10	5	5	9	6	3	7

Note: some objects are chosen multiple times in a bootstrap sample while others are not chosen! A typical bootstrap sample contains about 63% of the objects in the original data.

2. **Build classifiers,** one for each bootstrap sample (classifiers are hopefully independent since they are learned from different subsets of the data)

3. **Aggregate** the classifiers' results by averaging or voting

Boosting

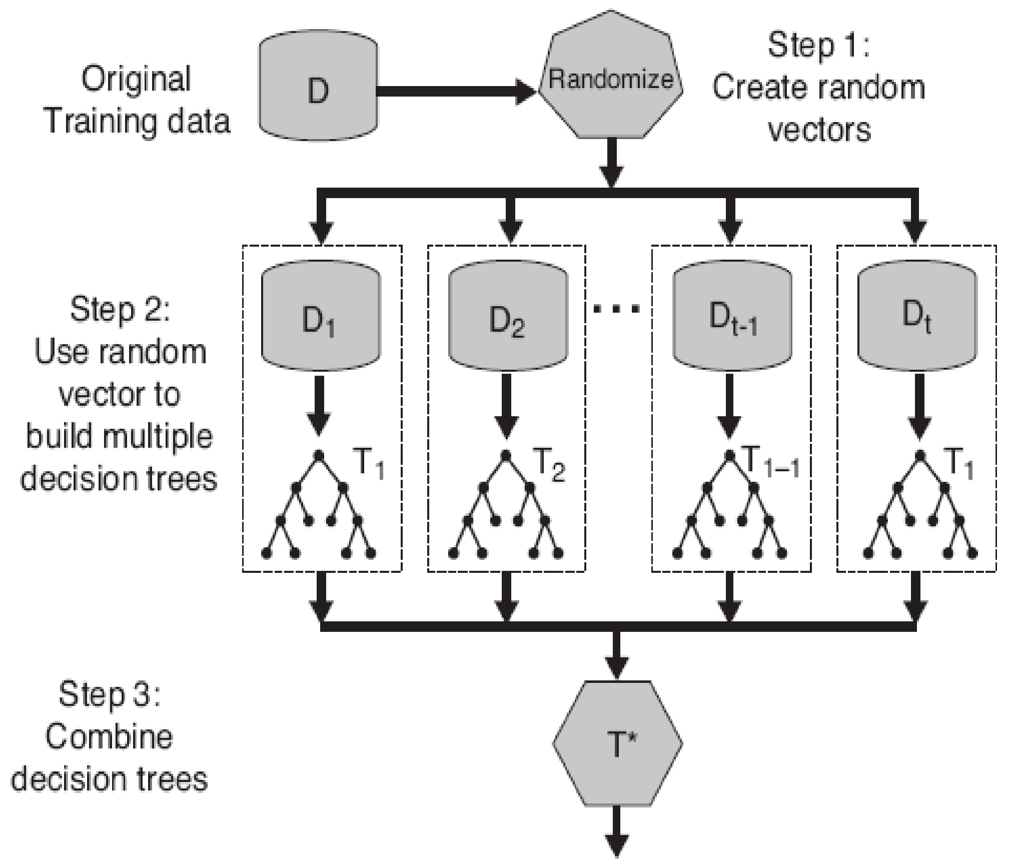
- Records that are incorrectly classified in one round will have their weights increased in the next

Original Data	1	2	3	4	5	6	7	8	9	10
Boosting (Round 1)	7	3	2	8	7	9	4	10	6	3
Boosting (Round 2)	5	4	9	4	2	5	1	7	4	2
Boosting (Round 3)	4	4	8	10	4	5	4	6	3	4

- Example 4 is hard to classify. Its weight is increased so it is more likely to be chosen again in subsequent rounds. This creates a larger error, and the classifier will try harder to predict it correctly.

- **Popular algorithm**: AdaBoost (Adaptive Boosting) typically uses decision trees as the weak learner.

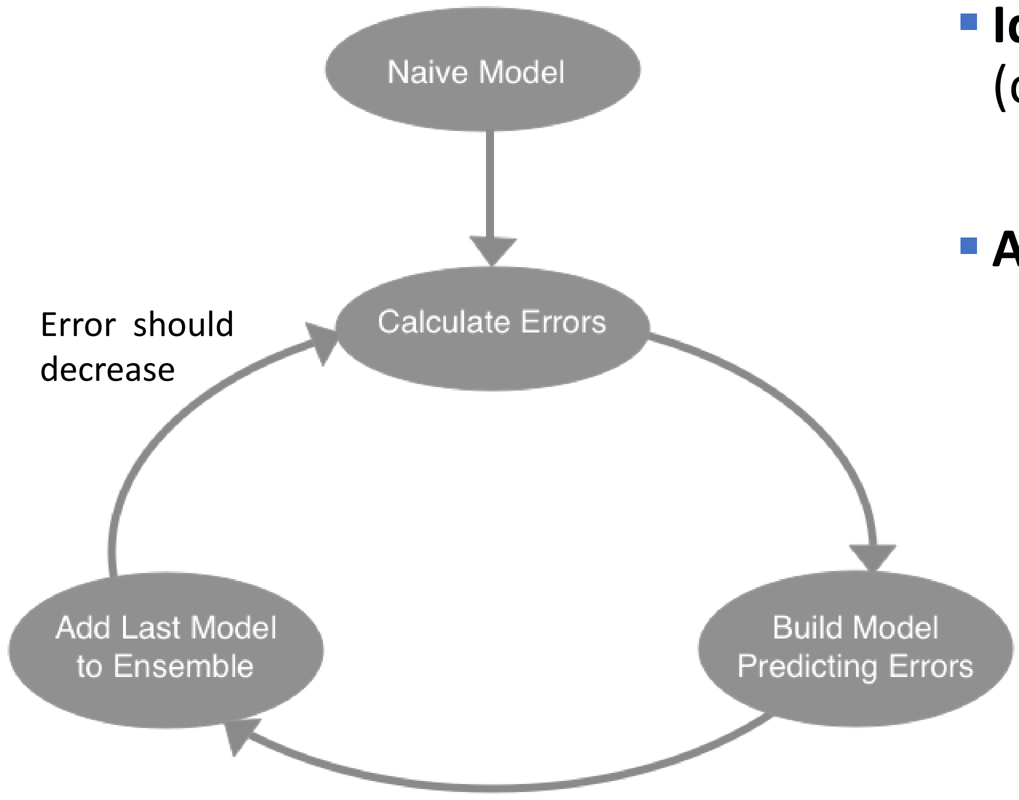
Random Forests



Original Training data
D
Randomize
Step 1: Create random vectors
Step 2: Use random vector to build multiple decision trees
D1
D2
...
Dt-1
Dt
T1
T2
T1–1
T1
Step 3: Combine decision trees
T*

- Introduce two sources of randomness: “Bagging” and “Random input vectors”
- **Bagging method**: each tree is grown using a bootstrap sample of training data
- **Random vector method**: At each node, the best split is chosen only from a random sample of the m possible attributes.

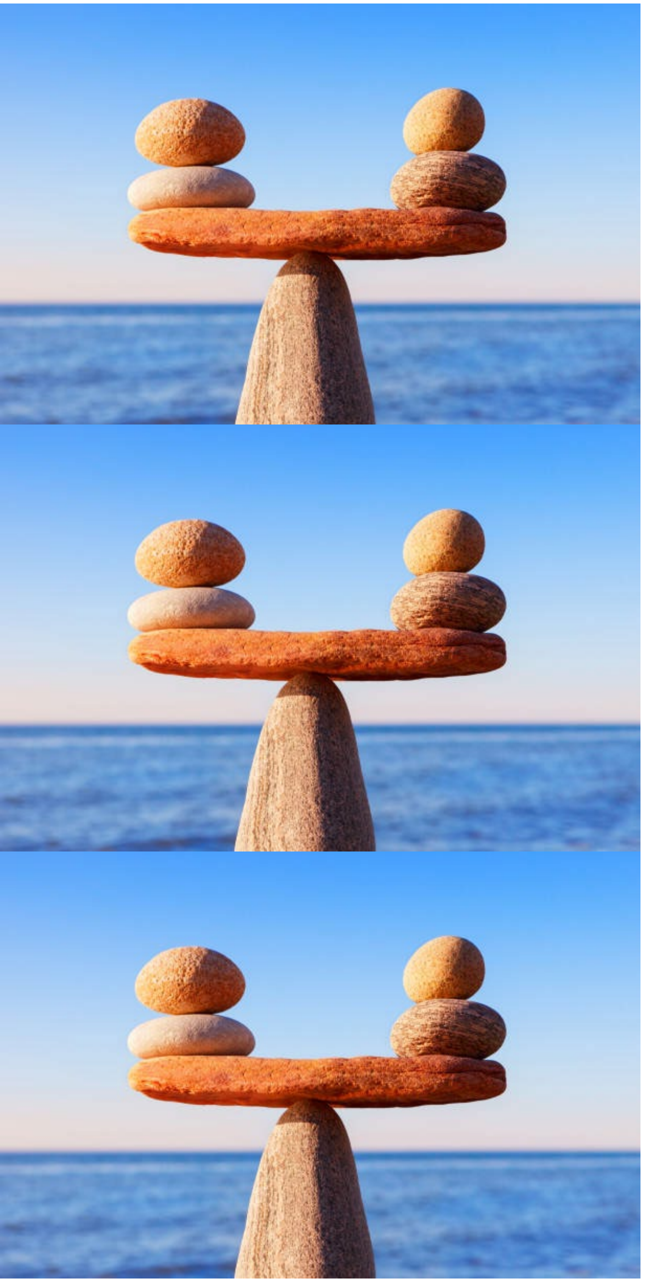
Gradient Boosted Decision Trees (XGBoost)



- **Idea**: build models to predict (correct) errors (= boosting).
- **Approach**:
  1. Start with a naive (weak) model
  2. Calculate errors for each observation in the dataset.
  3. Build a new model to predict these errors and add to the ensemble.
  4. Go to 2.

Other Popular Approaches

- Logistic Regression (Generalized linear models).
- Linear Discriminant Analysis (LDA).
- Regularized Models (Shrinkage).
- Stacking.



Topics

- Other Classification Methods
  - Rule-Based Classifier
  - Nearest Neighbor Classifier
  - Naive Bayes Classifier
  - Artificial Neural Networks
  - Support Vector Machines
  - Ensemble Methods
- **Class Imbalance Problem**

Class Imbalance Problem

Consider a 2-class problem

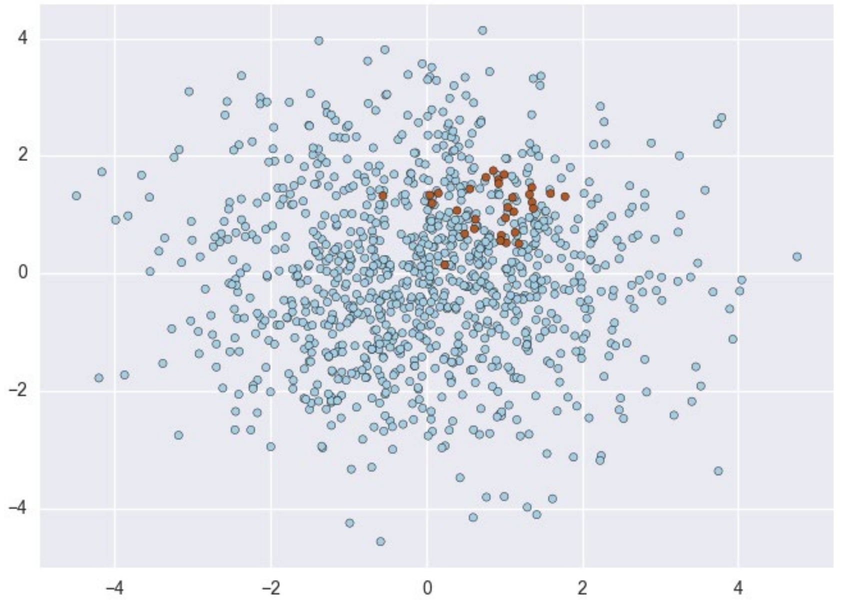
- Number of Class 0 examples = 9990
- Number of Class 1 examples = 10

A simple model:

- Always predict Class 0
- accuracy = 9990/10000 = 99.9 %
- error = 0.1%

Issues:

1. Evaluation: accuracy is misleading.
2. Learning: Most classifiers try to optimize accuracy/error. **These classifiers will not learn how to find examples of Class 1!**



Class Imbalance Problem: Evaluation

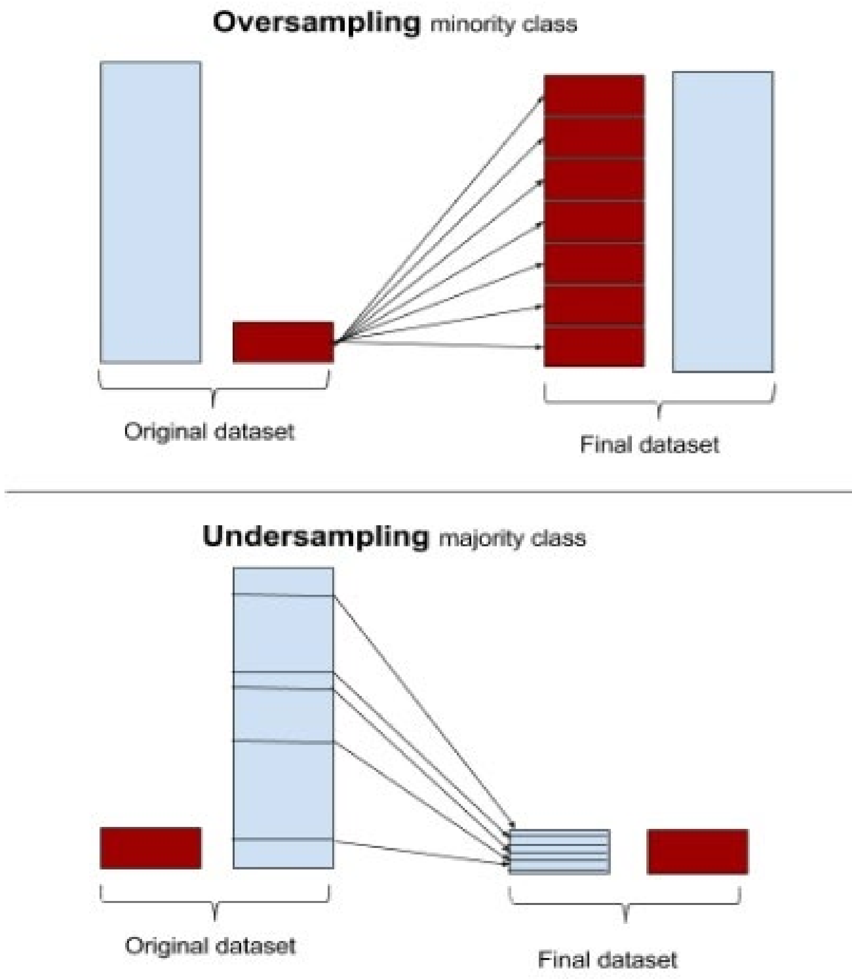
Do not use accuracy to evaluate problems with strong class imbalance!

Use instead:

- ROC curves and AUC (area under the curve) for binary classifiers.
- Cohen's Kappa which corrects for random accuracy.
- Misclassification cost.
- Precision/Recall plots or the F1 Score.

Class Imbalance Problem: Learning

- **Do nothing**. Sometimes you get lucky!
- **Balance the data set**: Down-sample the majority class and/or up-sample the minority class (use sampling with replacement). Synthesize new examples with SMOTE.
  This will artificially increase the error for a mistake in the minority class.
- Use **algorithms** that can deal with class imbalance (see next slide).
- Throw away minority examples and switch to an **anomaly detection** framework.


Oversampling minority class
Original dataset
Final dataset
Undersampling majority class
Original dataset
Final dataset

Class Imbalance Problem: Learning

Some algorithms that can deal with class imbalance:

- Use a **cost-sensitive classifier** that considers a cost matrix (not too many are available).
- Use boosting techniques like **AdaBoost**.
- Use a classifier that **predict a probability** $P(y \mid x)$ and instead of choosing $\mathrm{argmax}_y P(y \mid x)$, choose the minority class if

  $$\mathrm{P}\left(y_{\mathrm{minority}} \mid x\right) > \theta,$$

  where θ is the decision threshold that is made smaller to account for the imbalance. Probabilities are produced by many classifiers and for decision trees they can be estimated using the positive and negative training examples in each leaf node.

Conclusion

- **Bias**: There are many ways to implement the classification function. Each of them has a different inductive bias.
- Feature extraction and feature creation is important (e.g., interaction effects in linear models). Deep learning can also learn to create features.
- **Overfitting and model variability** are issues. Appropriate validation and test data needs to be used to produce and evaluate models that generalize well.
- Accuracy is problematic for **imbalanced data sets**. Rebalancing the data may be necessity.
- **Model explainability** is often important. Rules and trees may be easier to explain than other models.
- **(Deep) artificial neural networks** are a very powerful method but other methods may be preferable since ANNs:
  - Have no or very low bias and need lots of training data.
  - Have many hyperparameters which need to be tuned experimentally.
  - Model represents a black box and it is hard to explain why it makes decisions.