CenTuri Course 2022

Supervised Classification

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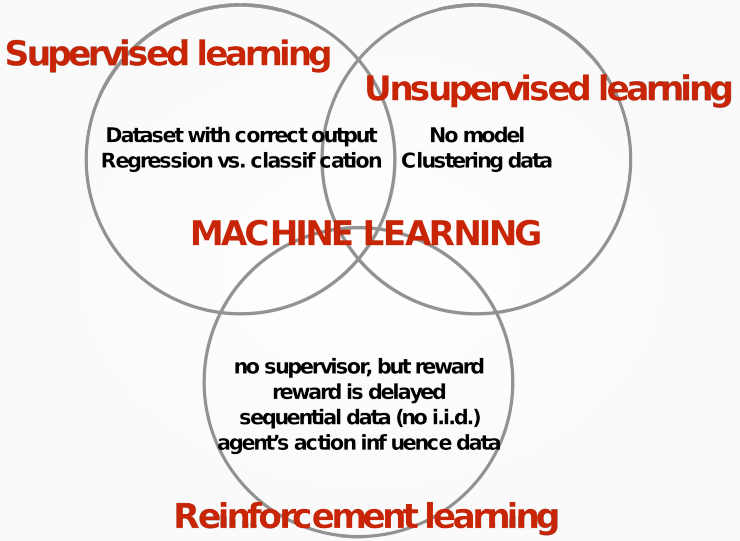
Branches of machine learning

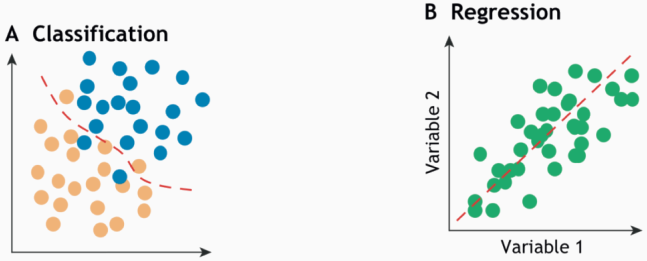


Some examples of machine learning problems

Classify emails as spam or not	Supervised Learning (Classification)
Predict the success of a movie	Supervised Learning (Regression)
Diagnose from list of symptoms	Supervised Learning (Classification)
Find groups in a social network	Unsupervised Learning
Drive a car autonomously	Reinforcement Learning
Defeat world champion of Go	Reinforcement Learning

Supervised learning

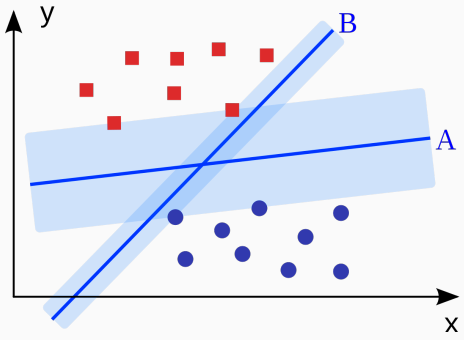
- Dataset with correct output
- Two main tasks: Regression and Classification



Classification

Support vector machine (SVM): intuition

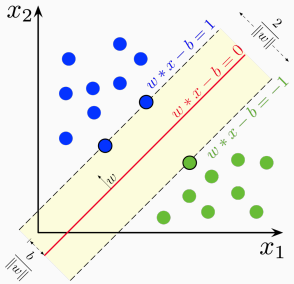
- Multiple hyperplanes could correctly classify binary data
- Can we find the hyperplane that best separates our two classes?



The SVM finds the hyperplane maximizing the margin between our classes

SVM: formal equations

- Our training data are $\{(\mathbf{x}^{(1)}, y^{(1)}), \cdots (\mathbf{x}^{(N)}, y^{(N)})\}$ with $\mathbf{x}^i \in \mathbb{R}^n$ and $y^i = \pm 1$



- We look for an hyperplane: $\mathbf{w}^T\mathbf{x} - b = 0$
- When $y^{(i)} = 1$ the points lie on or above the boundary and when $y^{(i)} = -1$ on or below it:

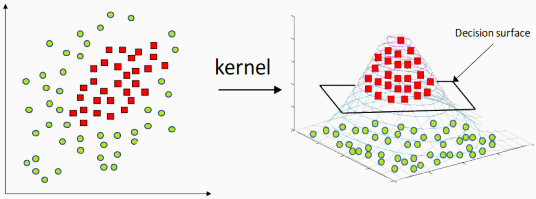
$$\begin{cases} \mathbf{w}^T\mathbf{x}^{(i)} - b \geq 1, & \text{if } y^{(i)} = 1 \\ \mathbf{w}^T\mathbf{x}^{(i)} - b \leq -1, & \text{if } y^{(i)} = -1 \end{cases}$$

- The margin's width is $2/\|w\|$

We want to minimize $\|w\|$ under the constraint $y^{(i)}\,(\mathbf{w}^T\mathbf{x}^{(i)} - b) \geq 1,\ \forall i$

SVM: the kernel trick

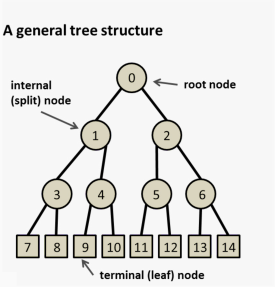
What happen when the data are not linearly separable?

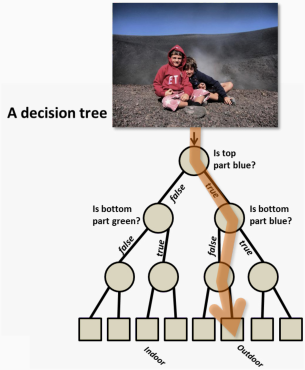


- Proper feature mapping can make non-linear to linear separable
- We do not need the feature space transformation, we only need the kernels
- Popular kernels:
  - Polynomial: $k(x, x') = (\mathbf{x}^T\mathbf{x}' + c)^d$
  - Gaussian: $k(x, x') = exp(-\left\|\mathbf{x} - \mathbf{x}'\right\|^2 / 2\sigma)$

Decision Trees

Image classification example





[Criminisi et al, 2011]

How do we build a tree

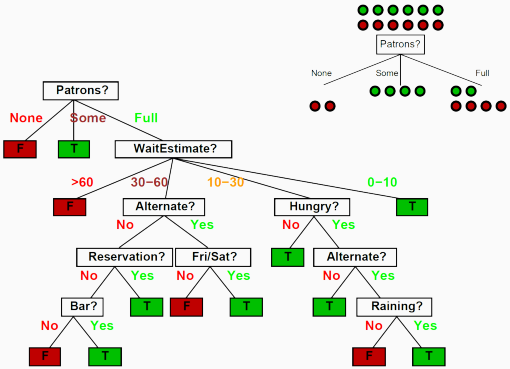
Building a node from data

Example	Input Attributes										Goal
	Alt	*Bar*	*Fri*	*Hun*	*Pat*	*Price*	*Rain*	*Res*	*Type*	*Est*	*WillWait*
$\mathbf{x}_1$	*Yes*	*No*	*No*	*Yes*	*Some*	*$$$*	*No*	*Yes*	*French*	*0–10*	$y_1 = Yes$
$\mathbf{x}_2$	*Yes*	*No*	*No*	*Yes*	*Full*	*$*	*No*	*No*	*Thai*	*30–60*	$y_2 = No$
$\mathbf{x}_3$	*No*	*Yes*	*No*	*No*	*Some*	*$*	*No*	*No*	*Burger*	*0–10*	$y_3 = Yes$
$\mathbf{x}_4$	*Yes*	*No*	*Yes*	*Yes*	*Full*	*$*	*Yes*	*No*	*Thai*	*10–30*	$y_4 = Yes$
$\mathbf{x}_5$	*Yes*	*No*	*Yes*	*No*	*Full*	*$$$*	*No*	*Yes*	*French*	*>60*	$y_5 = No$
$\mathbf{x}_6$	*No*	*Yes*	*No*	*Yes*	*Some*	*$$*	*Yes*	*Yes*	*Italian*	*0–10*	$y_6 = Yes$
$\mathbf{x}_7$	*No*	*Yes*	*No*	*No*	*None*	*$*	*Yes*	*No*	*Burger*	*0–10*	$y_7 = No$
$\mathbf{x}_8$	*No*	*No*	*No*	*Yes*	*Some*	*$$*	*Yes*	*Yes*	*Thai*	*0–10*	$y_8 = Yes$
$\mathbf{x}_9$	*No*	*Yes*	*Yes*	*No*	*Full*	*$*	*Yes*	*No*	*Burger*	*>60*	$y_9 = No$
$\mathbf{x}_{10}$	*Yes*	*Yes*	*Yes*	*Yes*	*Full*	*$$$*	*No*	*Yes*	*Italian*	*10–30*	$y_{10} = No$
$\mathbf{x}_{11}$	*No*	*No*	*No*	*No*	*None*	*$*	*No*	*No*	*Thai*	*0–10*	$y_{11} = No$
$\mathbf{x}_{12}$	*Yes*	*Yes*	*Yes*	*Yes*	*Full*	*$*	*No*	*No*	*Burger*	*30–60*	$y_{12} = Yes$

[AI book of of Stuart Russel and Peter Norvig]

How do we build a tree: A learned tree

A learned tree

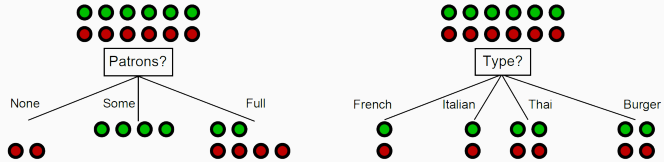


[AI book of of Stuart Russel and Peter Norvig]

How do we build a tree

Which split is better?

Ideally we want to separate negative and positive examples



[AI book of of Stuart Russel and Peter Norvig]

How do we build a tree

We use the information gain as criterion:

- Shannon Entropy

$$H = -\sum_i p_i log_2(p_i)$$

- Expected Entropy (for a feature F with K values)

$$EH(F) = -\sum_{i=1}^{K} \frac{n_i}{N} H_i$$

- Information Gain $I(F)$

$$I(F) = H(Data) - EH(F)$$

How do we build a tree

The patron vs type example

- Entropy data:

$$H(Data) = -2 \cdot \left[1/2 \cdot log_2(1/2)\right] = 1$$

- Entropy left split:

$$EH(L) = -\left[2/12 \cdot 1 \cdot log_2(1) + 4/12 \cdot 1 \cdot log_2(1) + \right.$$
$$\left. + 6/12 \cdot \left(2/6 \cdot log_2(2/6) + 4/6 \cdot log_2(4/6)\right)\right] \approx 0.46$$

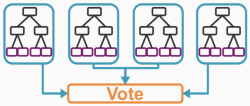
- Entropy right split:

$$EH(R) = -(2/12 + 2/12 + 4/12 + 4/12) \cdot \left[1/2 \cdot log_2(1/2)\right] = 1$$

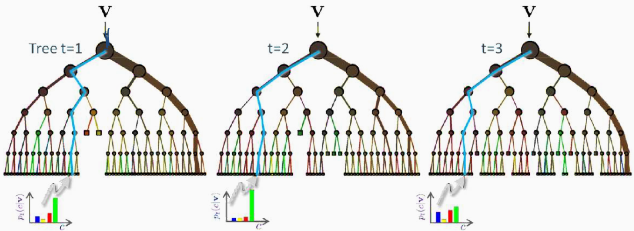
The information gain is clearly higher in the left split!

Random forest: intuition and example

A multitude of decision trees are generated at training time. The output of the random forest is the class selected by the forest (average or majority vote).



Example: We trained a forest of $T = 3$ trees and we want to classify a new point $\mathbf{v}$.



The new point is classified as green!

[Criminisi et al, 2011]

Random forest algorithm

Given a training set $(\mathbf{x}_1, \cdots, \mathbf{x}_N)$ with responses $(y_1, \cdots, y_N)$:

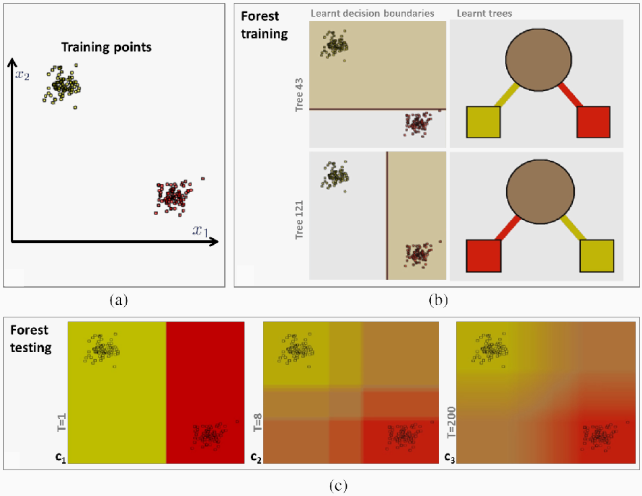
1. For b = 1 to B:
   (a) Draw a bootstrap sample (with replacement) Z of size N from the training data.
   (b) Grow a random-forest tree T_b to the bootstrapped data, by recursively repeating the following steps for each terminal node of the tree, until the minimum node size n min is reached.
      i. Select m variables at random from the p variables.
      ii. Pick the best variable/split-point among the m.
      iii. Split the node into two daughter nodes.
2. Output the ensemble of trees $\{T_b\}_1^B$.

To make a prediction at a new point $\mathbf{x}$:

- Let $\hat{C}_b(x)$ be the class prediction of the b-th random-forest tree.
- Then $\hat{C}_{rf}^B(x)$ = majority vote or average of $\{\hat{C}_b(x)\}_1^B$

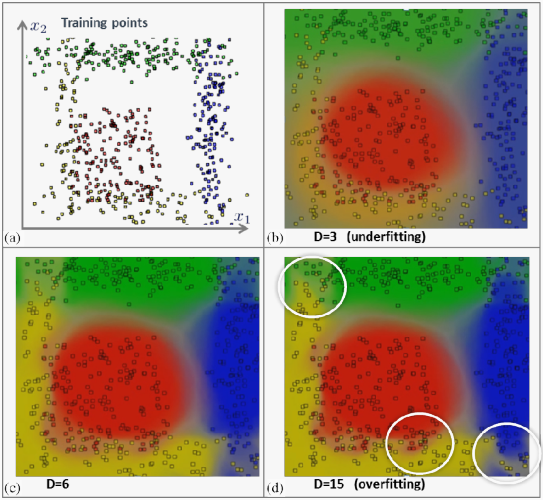
[From the book of Hastie, Friedman and Tibshirani]

Effects of size



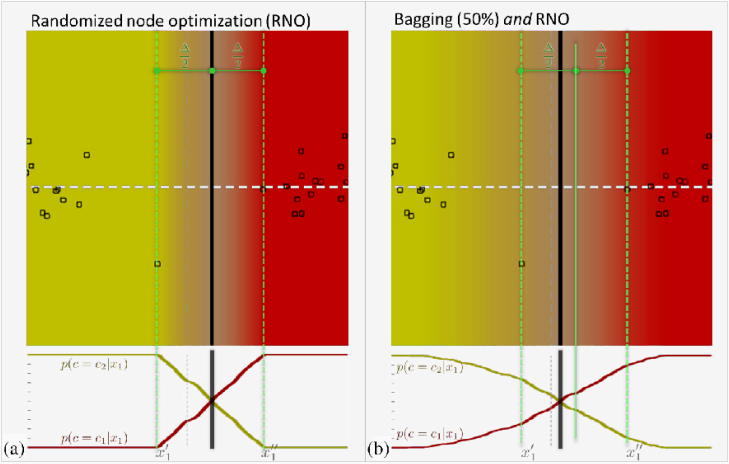
[Criminisi et al, 2011]

Effects of depth



[Criminisi et al, 2011]

Effects of bagging

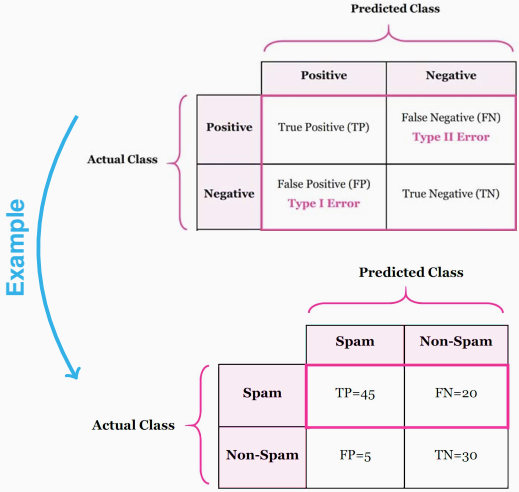


[Criminisi et al, 2011]

Model evaluation and selection

Measure of performance for a classification model

Confusion matrix



Sensitivity/True positive rate

$$TPR = \frac{TP}{TP + FN}$$

Precision/Positive predicted value

$$PPV = \frac{TP}{TP + FP}$$

Specificity/True negative rate

$$TNR = \frac{TN}{FP + TN}$$

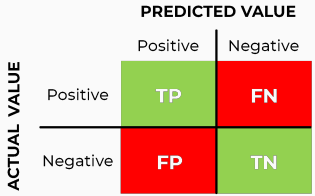
F_1-score

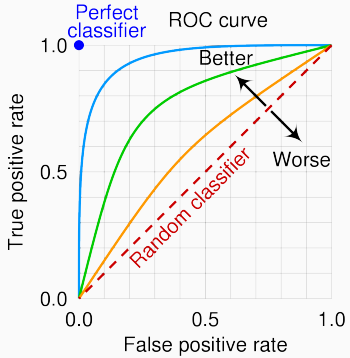
$$F_1 = 2\frac{PPV \cdot TPR}{PPV + TPR}$$

The receiver operating characteristic (ROC) curve

How to construct the ROC curve:

1. Getting model predictions.
2. Calculate the TPR and FPR.
3. Plot TPR and FPR for every cut-off.





$$TPR = \frac{TP}{TP + FN} \qquad TNR = \frac{TN}{FP + TN}$$

Maximizing the area under the curve allows to choose the best model

Model evaluation and selection: training/test sets

Model evaluation

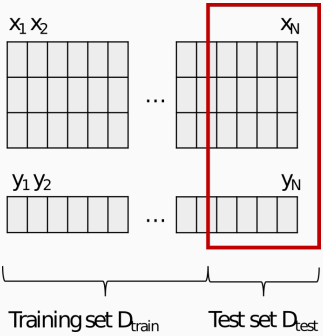
We evaluate a model h by computing the empirical risk ER over the training set D_{train} of size N_{train}

$$ER = \frac{1}{N_{\text{train}}} \sum_{i \in D_{\text{train}}} J(h(x_i), y_i)$$

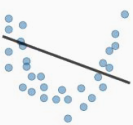
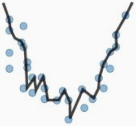
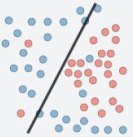
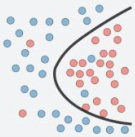
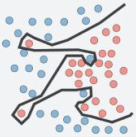
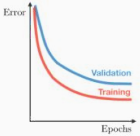
Model selection

For K models $h_1, h_2, \cdots h_K$ we select the best as:

$$h^* = \underset{k=1,\cdots,K}{\operatorname{argmin}} \frac{1}{N_{\text{test}}} \sum_{i \in D_{\text{test}}} J(h_k(x_i), y_i)$$



Training/test set error and appropriate fitting

	Underfitting	Just right	Overfitting
Symptoms	• High training error • Training error close to test error • High bias	• Training error slightly lower than test error	• Very low training error • Training error much lower than test error • High variance
Regression illustration			
Classification illustration			
Deep learning illustration			
Possible remedies	• Complexify model • Add more features • Train longer		• Perform regularization • Get more data

Parameters vs Hyperparameters

In machine learning models there are **two types of "parameters"**:

1. Model Parameters: learned from data automatically via the optimization procedure
2. Model Hyperparameters: set manually or tuned and used in processes to help estimate model parameters

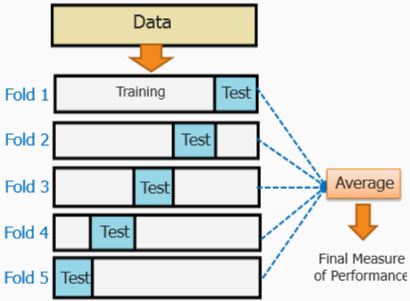
Example Hyperparameters of random forest:

- depth of the trees
- size of the forest

K-fold cross validation

K-fold cross validation:

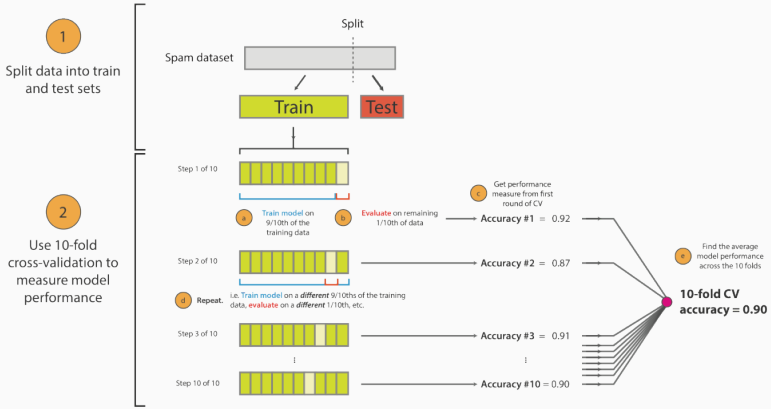
1. Partition the data into K subsets of similar sizes $D_1, \cdots, D_K$
2. For $i = 1, \cdots, K$: train on $D_1, \cdots, D_{i-1}, D_K$
3. At each iteration of the loop evaluate on D_i



(A) Way 1

- Apply k-fold validation on entire data set
- Calculate average of each validation score
- Using it as a final score

K-fold cross validation



(B) Way 2

- Split data into train set, test set
- Apply K-fold validation on train set
- Find best estimator from average of each validation score
- Calculate final score on test set with best estimator

Cross validation

Both ways can be correct depending on what the purpose of the procedure is.

- **(A)** uses cross validation for **validation** (or rather, verification), that is, to estimate generalization error.
- **(B)** uses cross validation for **optimizing some hyperparameters** (e.g. model complexity) and then tests the optimized model with the "test" data.

Other usefull remarks:

- The term **"cross validation"** refers only to this particular scheme of splitting data (drawing **without replacement** and calculating a pre-determined number of surrogate models so that each case is used for testing exactly once).
- The **K-fold** procedure is called **leave-one-out when K** $=$ **N**, with N indicating the number of data.
- **Bootstrap** can be alternatively used for validation: similar strategy, except than samples are randomly drawn **with replacement** from the dataset.