Classification

Tiphaine Viard

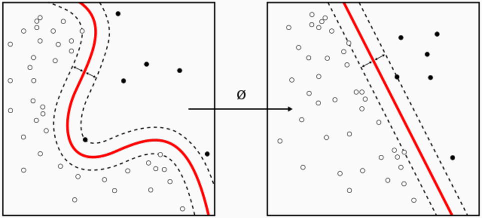
What is classification?

Wikipedia definition

Classification *is the problem of identifying to which of a set of categories (sub-populations) a new observation belongs, on the basis of a training set of data containing observations (or instances) whose category membership is known.*

Classification

Generalize known structures to apply to new data.



An e-mail program might attempt to classify an e-mail as "legitimate" or as "spam".

Spam example

Data set that describes e-mail features for deciding if it is spam.

Example

Contains “Money”	Domain type	Has attach.	Time received	spam
yes	com	yes	night	yes
yes	edu	no	night	yes
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Assume we have to classify the following new instance:

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Definition

Given a set of classes $C_1 \ldots C_N$, a classifier algorithm builds a model that predicts for every unlabelled instance I the class C_i to which it belongs with accuracy.

Example
Spam filter

Example
Twitter Sentiment analysis: analyze tweets with positive or negative feelings

Example
Cat or Dog?

A note about classification

Finding a defining feature for classification can cause unjust consequences; **redlining** can be exacerbated by machine learning models.

Dutch welfare ordered to stop using SyRI (2020)

Find the balance between **technical** and **social** aspects

Privacy
Discrimination
Opacity
...

Symbolic AI
Baked-in fairness
"White-box" models
...

Basic Classifiers

Majority vote

Training

Compute the majority class in the dataset

Prediction

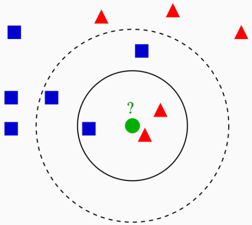
Output the majority class

Training

Store all instance (+ eventual index)

Prediction

Find the k closest point in the input and output the majority over those k points.



k-Nearest Neighbors (k-NN)

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Closest according to what metric?

L_1 vs L_2 vs L_∞ vs cos

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Rule of thumb: $k = \sqrt{n}$

Better k-NN

Problem. Finding distance from all points to all others is costly : $\mathcal{O}(n^2)$ time

We only care about close data points

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We only care about close data points

Solution : use **locality-sensitive hashing** (LSH)

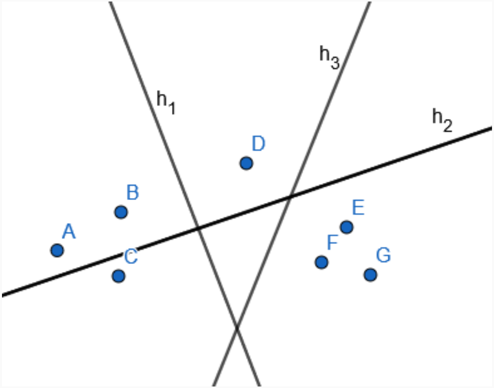
- Close points in the same bucket with high probability,
- Distant points are in different buckets with high probability.

Random hyperplanes for LSH

```
Generate K hyperplanes h_1, ..., h_K;
H_{i,k} ← −1, ∀i, ∀k;
for every datapoint x_i do
    if x_i · h_k ≥ 0 then
        H_{i,k} ← 0;
    end
    else
        H_{i,k} ← 1;
    end
end
```

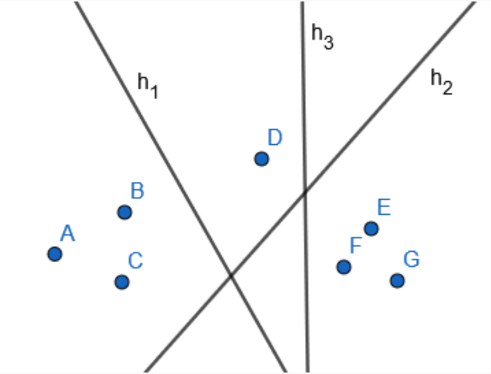
Repeat multiple times $\rightarrow$ more robust

LSH : an example



Hash	Data points
000	A, B
001	
010	C
011	
100	D
101	
110	
111	E, F, G

LSH : an example



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Bayes theorem

Formula

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

Proof.

$$P(A \cap B) = P(A) \times P(B|A)$$

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$\square$

Bayes theorem

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Interpretation

$$\text{prior} \times \frac{\text{likelihood}}{\text{evidence}} = \text{posterior}$$

Grouping attributes

$$P(C_i) \times \frac{P(\bar{x}|C_i)}{P(\bar{x})} = P(C_i|\bar{x})$$

Multiple attributes

$$P(C_i) \times \frac{\prod_j P(x_j|C_i)}{P(\bar{x})} = P(C_i|\bar{x})$$

Naive Bayes Classifier

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With independence hypothesis!

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With independence hypothesis!
$P(\bar{x})$ does not change with the class

Tree Methods

Classification

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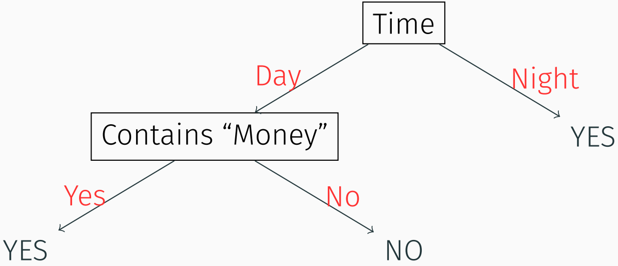
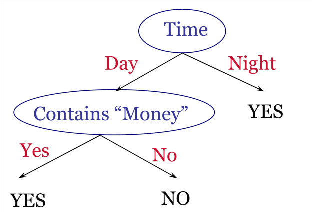
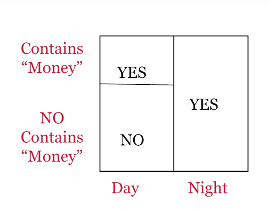






Recursive construction technique

- $A \leftarrow$ the *best* decision attribute for next *node*
- Assign A as decision attribute for *node*
- For each value of A, create new descendant of *node*
- Sort training examples to leaf nodes
- If training examples perfectly classified, Then STOP, Else iterate over new leaf nodes

Decision Trees

- Interpretable: the DT is easy to understand
- Training is fast (greedy algorithm)
- Expressive: can approximate complex non-linear functions
- Complex function = large tree
- Large tree = more variance = overfitting

In practice, decision trees underperform compared with other methods

Bagging (Breiman, 1996)

Example

Dataset of 4 Instances : A, B, C, D

Classifier 1: B, A, C, B
Classifier 2: D, B, A, D
Classifier 3: B, A, C, B
Classifier 4: B, C, B, B
Classifier 5: D, C, A, C

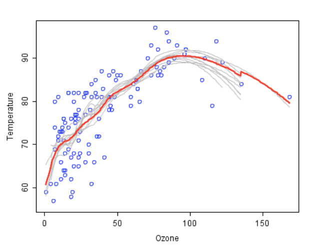
Bagging:

1. Bootstrap: generate multiple samples of data, train decision tree
2. Aggregate: output the average output of all models

Bagging

Bagging builds a set of M base models, with a bootstrap sample created by drawing random samples with replacement.

- Highly expressive: each model can estimate complex functions/boundaries
- a low-variance method: averaging the prediction of all models reduces variance (if M large enough)



Bagging implies **multiple models**, running on **different, overlapping** datasets

How can we evaluate its performance?

Evaluating bagging: out-of-bag error

Bagging implies **multiple models**, running on **different, overlapping** datasets

How can we evaluate its performance?

The **out-of-bag error**

1. for each data point x, average predicted output over models that do **not** contain x in bootstrap $\Rightarrow$ **point-wise out-of-bag error**;
2. **Average** point-wise out-of-bag error over training set.

Problems with bagging

In practice, trees are **strongly correlated**.

- Suppose that x_j is a strong predictor. Then most models will split on x_j;
- Then, each tree is essentially the same, and the averaged output is irrelevant.

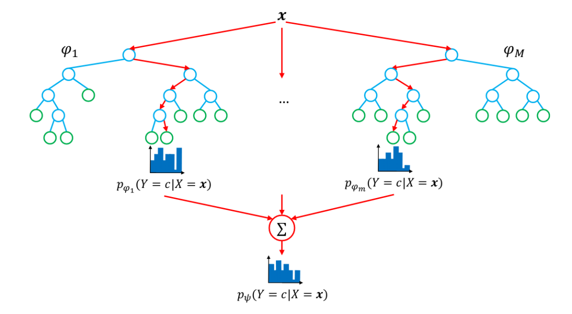
For F identically, dependently distributed variables with pairwise correlation ρ and variance σ^2, variance of mean:

$$\rho\sigma^2 + \frac{1-\rho}{F}\sigma^2$$

Variance reduction of bagging is **limited**.

Random Forests

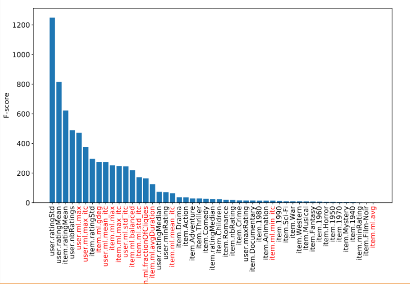
- Bagging
- Random Trees: trees that in each node only uses a random subset of k of the attributes



$\Rightarrow$ one of the most popular methods in machine learning.

Feature importance with random forests

- Record prediction accuracy on the oob samples for each tree;
- Randomly permute the data for column *j* in the oob samples;
- Record the accuracy again;
- Average the decrease in accuracy over all trees, and use as a measure of the importance of variable *j*.



Final thoughts on Random Forest

- Ensemble methods: **not easily interpretable**
- One of the best "off-the-shelf" methods, near to 0 tuning necessary
- **Averaging** and **randomization** offer fine control of the bias-variance trade-off
- Reasonably efficient: $\Omega(mk\hat{n}log^2\hat{n})$, with $\hat{n} \approx 0.63n$
- use `n_jobs` to make parallel
- `sklearn` implementation (Python + Cython) is by far the fastest available

Gradient Boosting

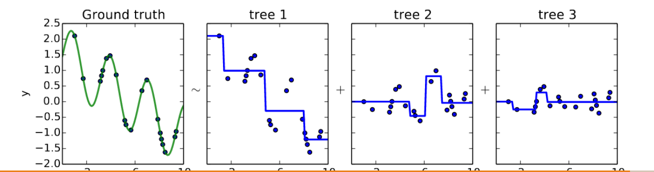
Train each of the M trees on the error of the precedent trees

$$\phi(x) = \sum_{m=0}^{M} \phi_m(x)$$

with each step being staged:

$$\phi_m(x) = \phi_{m-1}(x) + \hat{\phi}_m(x)$$

and $\hat{\phi}_m$ is a tree that approximates the gradient step.



Last thoughts on gradient boosting

- Usually more accurate than Random Forests
- Can adapt to most loss functions
- Under- and overfitting are adressed through regularization (learning rate, subsampling, term in loss function...)
- Tuning is harder than for random forests
- Slow to train (no parallelism!), fast predictions
- Still, blazing-fast implementation (Python and C++): XGBoost
- Easy to get *feature importance*

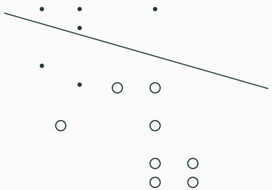
Gradient-based Methods

Training

Learn an hyperplan $\mathcal{P}$ separating well the two classes.

Prediction

What side of the hyperplan $\mathcal{P}$ is the point?



Based on the gradient of the logit function.

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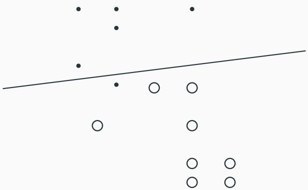

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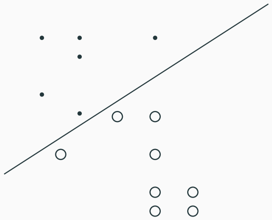
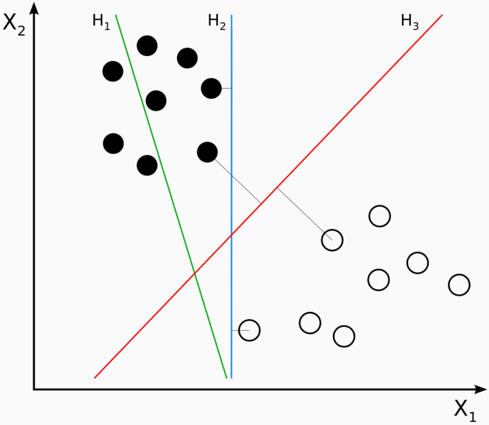


Based on the gradient of the logit function.

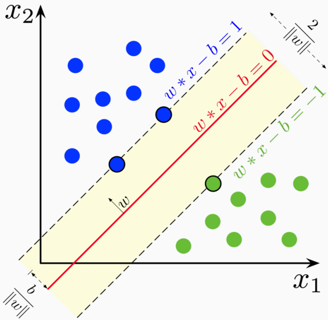
Similarly to logistic regression, we want to find the **best separating hyperplane**



SVM: under the hood

Suppose a **linear separation** exists

$$w^T x + b = 1, w^T x + b = -1$$

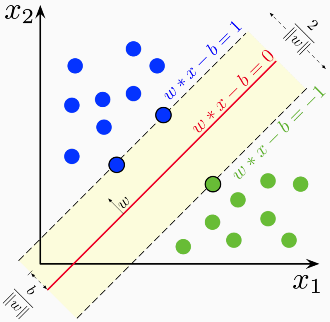


x_i near the margin determine the solution →**support vectors**

SVM: under the hood

Suppose a **linear separation** exists

$$w^T x_i + b \geq 1, \text{ if } y_i = 1, w^T x_i + b \leq -1, \text{ if } y_i = -1$$



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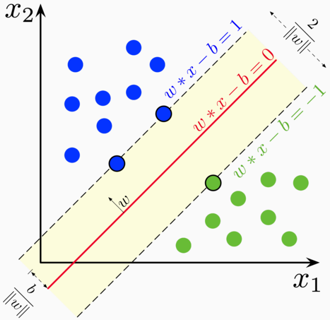
$$y_i(w^T x + y) \geq 1$$



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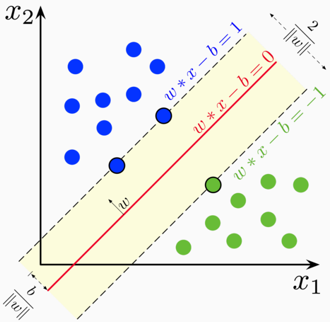
SVM: under the hood

Suppose a **linear separation** exists

$$\text{minimize } ||w|| \text{ subject to } y_i(w^T x_i + b) \geq 1, \text{ for } i = 1..n$$



x_i near the margin determine the solution →**support vectors**

Solving SVM

$$\text{minimize } ||w|| \text{ subject to } y_i(w^T x_i + b) \geq 1, \text{ for } i = 1..n$$

$||w||$ is the L_1 norm

The gradient of $||w||$ is $\frac{w}{||w||}$

Let's switch instead to L_2 norm

The gradient of $||w||^2$ is $2w$

$$\text{minimize } \frac{1}{2}||w||^2 \text{ subject to } y_i(w^T x_i + b) \geq 1, \text{ for } i = 1..n$$

This is a **quadratic optimization problem**.

Final thoughts on SVM

- What about non linearly separable data?

  Add misclassification term (number or distance)

- Use hinge function as regularization:
  $\min ||w||^2 + \lambda \left[\frac{1}{n} \sum_i^n \max(0, 1 - y_i(w^T x - b)\right]$
- λ trade-off between increasing margin and ensuring x_i outside of margin
- Only adapted to binary classification
- But you can do ”one-versus-all” classification