Machine Learning

SD-TSIA210

Decision and regression trees - Ensemble methods

Ekhine Irurozki

irurozki@telecom-paris.fr,
Télécom Paris, IP Paris, France

Supervised learning

X a random vector that takes its value in $\mathcal{X} = \mathbb{R}^p$

Y a random variable that takes its value in $\mathcal{Y}$

$\mathcal{D}$ is the joint probability distribution of (X, Y)

$\mathcal{Y} = \mathbb{R}$ in case of regression

$\mathcal{Y} = \{1, -1\}$ in case of supervised binary classification

$\mathcal{Y} = \{1, \ldots, C\}$ in case of supervised multiclass classification

Minimizing the true risk

Denote $\mathcal{H}$ the hypothesis class: e.g. the set of models we consider

Define a local loss function $\ell : \mathbb{R} \times \mathbb{R} \to \mathbb{R}^+$,

One wishes to solve this problem:

$$\arg\min_{f \in \mathcal{H}} \mathbb{E}_{(X,Y)\sim\mathcal{D}}[\ell(Y, f(X))]$$

from the knowledge of $\{(x_i, y_i), i = 1, \dots n\}$.

Minimizing the empirical risk Since we do not access to the true distribution $\mathcal{S} = \{(x_i, y_i), i = 1, \dots, n\}$, i.i.d. sample

$$\arg\min_{f \in \mathcal{H}} \frac{1}{n} \sum_{i=1}^{n} \ell(y_i, f(x_i))$$

Target functions for a given loss

Classification: For $\ell(y, f(x))$: (0/1) prediction loss, the best classifier is the **Bayes classifier**:

$$f_{Bayes}(x) = \arg\max_c \mathbb{P}(Y = c|x)$$

Regression: For $\ell(y, f(x))) = (y - f(x))^2$: ℓ_2 loss, the best solution in regression is the regression function:

$$f_{reg}(x) = \mathbb{E}[Y|x]$$

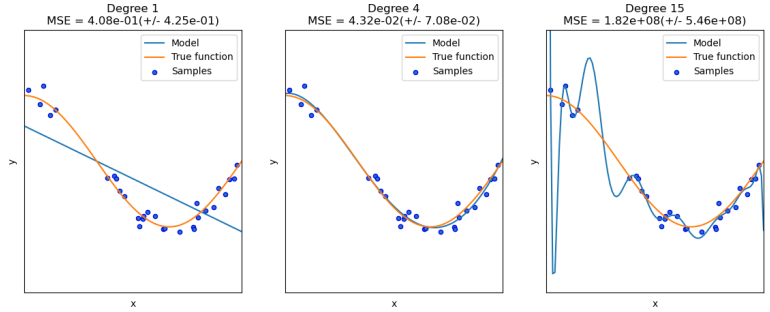
Minimizing the (regularized) empirical risk

$\mathcal{S} = \{(x_i, y_i), i = 1, \ldots, n\}$, i.i.d. sample; Ω: regularization term

$$\arg\min_{f \in \mathcal{H}} \frac{1}{n} \sum_{i=1}^{n} \ell(y_i, f(x_i))$$

$$s.c. \Omega(f) \leq C$$

Or equivalently: with $\lambda > 0$, a hyperparameter term, $\arg\min_{f \in \mathcal{H}} \frac{1}{n} \sum_{i=1}^{n} \ell(y_i, f(x_i)) + \lambda \Omega(f)$



Source: SKlearn

Statistical Learning in a nutshell

The most important slide of the whole course

Learning: given $\mathcal{H}$,ℓ, Ω, $\mathcal{S}_n$, define a learning algorithm $\mathcal{A}$ allowing to build $f_n = \mathcal{A}(\mathcal{S}_n, \mathcal{H}, \ell, \Omega)$ with

- $\mathcal{A}$: learning algorithm
- $\mathcal{S}_n$: training data
- $\mathcal{H}$: class of functions
- Ω: some complexity/capacity measure on $f \in \mathcal{H}$
- ℓ : local loss function

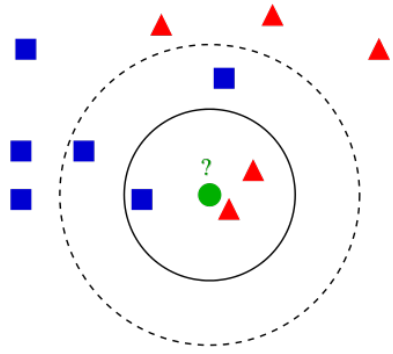
Prediction: given a new x, and compute $f_n(x)$

Statistical Learning with local average models and trees

- Nonparametric approach to machine learning
- Training data are the main parameters !
- Motivations: Local average / Majority vote: prediction is made locally, looking at the neighbors, like k-nearest neighbors (KNN) algorithm

Locallity

Exercise Which is the complexity?



Source: Wikipedia

Problem: **the curse of dimensionality**, as the number of dimensions grows, the amount of data we need to generalize accurately grows exponentially

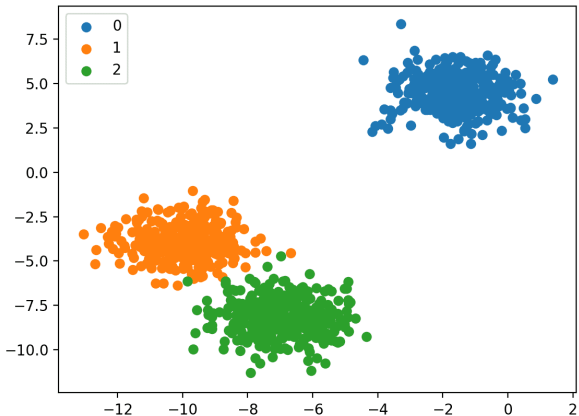
Statistical Learning with local average models and trees

- **Why is it important ?** Simple way to handle a learning problem, very general, can be extended to many kinds of outputs/ many ML tasks
- Limited number of hyperparameters
- **Drawback:** heavily depends on the number of data
- **Advantage**: the model itself contains the training data on which it is based (transparency, pre-training), interpretability

Decision trees: learning and prediction

Learning: construct the regions

Prediction: find the region



Decision trees

Trees belong to the family of models of the following form:

$$f(x) = \sum_{\ell=1}^{m} \mathbb{I}(x \in \mathcal{R}_\ell) f_\ell,$$

In practise, the $\mathcal{R}_\ell$'s form a partition and are estimated/learned using the training dataset as well as the f_ℓ's.

f_ℓ only depends on regions $\mathcal{R}_\ell \subset \mathcal{X}$ in the input space and on training data in this region.

Classification into C classes (multiclass and binary) is done by majority voting

$$f_\ell = \arg \max_{c=1,\ldots,C} \hat{p}_{\ell c}, \tag{1}$$

with $\hat{p}_{\ell c} = \frac{1}{N_\ell} \sum_{x_i \in \mathcal{R}_\ell} \mathbb{I}(y_i = c)$, and N_ℓ is the number of training data falling into region $\mathcal{R}_\ell$.

Regression trees

Similarly, regression trees belong to the family of models of the following form:

$$f(x) = \sum_{\ell=1}^{m} \mathbb{I}(x \in \mathcal{R}_\ell) f_\ell,$$

with

$$f_\ell = \frac{1}{N_\ell} \sum_{x_i \in \mathcal{R}_\ell} y_i,$$

N_ℓ is the number of training data falling into region $\mathcal{R}_\ell$.

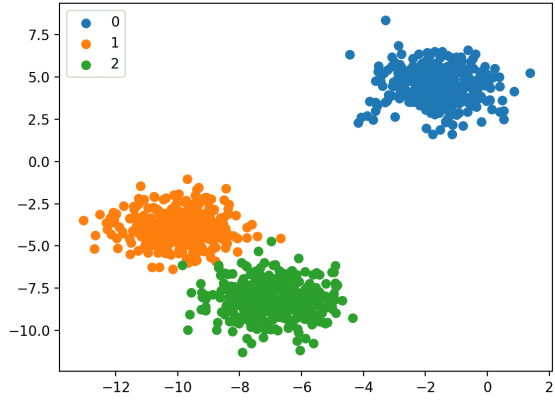
Decision and regression trees: issues

- How to build automatically these regions ? Loss function ? Learning Algorithm ?
- How to control the complexity of the model ? How to choose m the size of the partition ?
- Why is this model ubiquitous in bank/marketing/medecine fields ?
- Why trees are so important in Machine Learning ?

Decision trees

Invented simultaneously between 1979 and 1983 par L. Breiman et al. (CART, Berkeley, USA) et R. Quinlan (ID3, Sydney, Australia) in two different communities: applied statistics and computer science. Decision and regression trees have been proposed to build automatically the partition $\mathcal{R}_1 \cup \ldots \mathcal{R}_m$ from the training set.

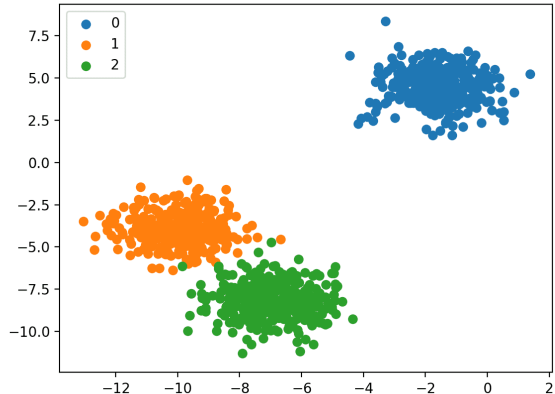
- Local criterion and Constructive algorithm
- Build a binary tree by choosing at each node, a splitting rule that splits the current dataset in two, minimizing a local criterion
- Greedy algorithm



Source: SKlearn

Decision trees

- Use several linear separators to build nonlinear decision frontiers
- These linear separators are chosen to be orthogonal to each basis vector, e.g. defining hyperplane of equation: $x^j = \theta$ to allow an interpretability of the decision function
- At the end of training, we know the features that take part to the decision.



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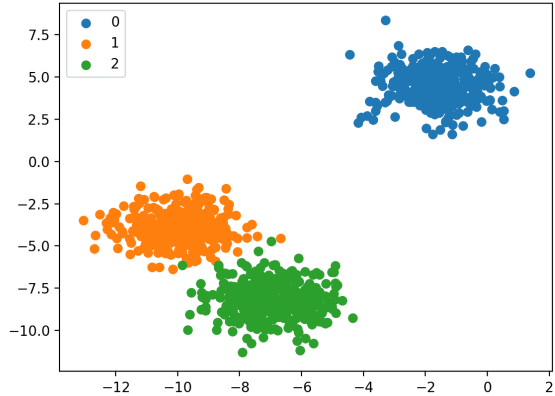
Decision trees

The decision function can be represented by a tree (binary tree) whose each intermediary node is associated to a separating hyperplane $x^j = c$ and each leaf is associated to a majority vote (classification) or a local average (regression).



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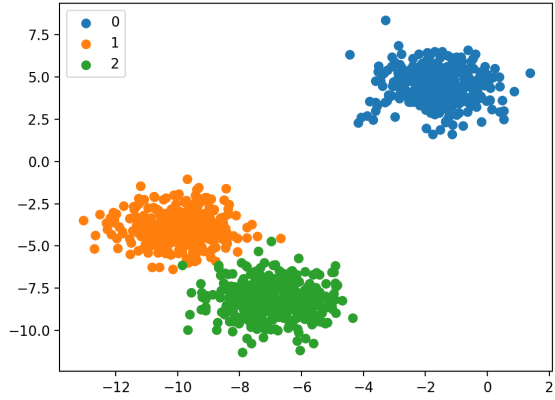
Decision trees

The tree codes for a set of logical rules (symbolic logic of order zero+): each leaf is associated to a logical rule if $(x^1 - 4)$ and $(x^2 < -6)$ then x is predicted to belong to the green class.



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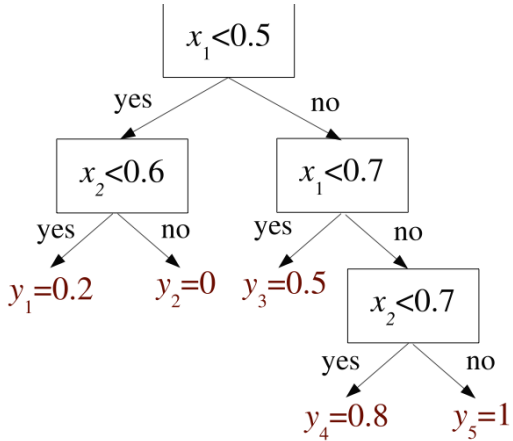
Regression tree



Separator or split t

Huge combinatorial problem

Continuous Variable x^j:

$$t_{j,s}(\mathbf{x}) = \text{sign}(x^j - s) \tag{2}$$

Categorical variable x^j with K values $\{v_1^j, \ldots, v_K^j\}$:

$$t_{j,\mathbf{v},k}(\mathbf{x}) = 1(x^j = v_k^j) \tag{3}$$

To keep the tree binary, every K-value categorical variable is converted into K binary variables.

Recursive building algorithm for trees

1. Let $\mathcal{S}$ the training data set
2. Build a root node
3. At the current node, find the best binary separation defined by the split t to be applied to $\mathcal{S}$ such that $L(t, \mathcal{S})$ be minimal
4. Associate the chosen separator $t(\hat{j}, \hat{s})$ to the current node and split the current training dataset into two datasets at right and left side, $\mathcal{S}_r$ et $\mathcal{S}_l$.
5. Build two child nodes: a node at right, a node at left, the right (resp. left) node is now associated with $\mathcal{S}_r$ (resp. $\mathcal{S}_l$)
6. Compute a stopping criterion on the right node: if it is satisfied, this node becomes a leaf, otherwise, go to 3.
7. Compute a stopping criterion on the left node: if it is satisfied, this node becomes a leaf, otherwise, go to 3.

How to find the best separation/split in a classification task ?

We seek the splitting feature j and the split threshold s that minimizes an **impurity criterion**.
We want to have children nodes as "pure" or "homogeneous" as possible in terms of classes.

$$\min_{j,s}[\frac{N_r}{N}H(\mathcal{S} \cap \mathcal{R}_r(j,s)) + \frac{N_l}{N}H(\mathcal{S} \cap \mathcal{R}_l(j,s))].$$

where H is an impurity criterion.

Impurity criteria

For a given $\mathcal{S}$ with n labeled data:$p_k(\mathcal{S}) = \frac{1}{n}\sum_{i=1}^{n} \mathbb{I}(y_i = k)$ with $k(\mathcal{S})$: majority class in $\mathcal{S}$.

Misclassification

$$H(\mathcal{S}) = 1 - p_{k(\mathcal{S})},$$

Cross-entropy:

$$H(\mathcal{S}) = -\sum_{k=1}^{C} p_k(\mathcal{S}) \log p_k(\mathcal{S})$$

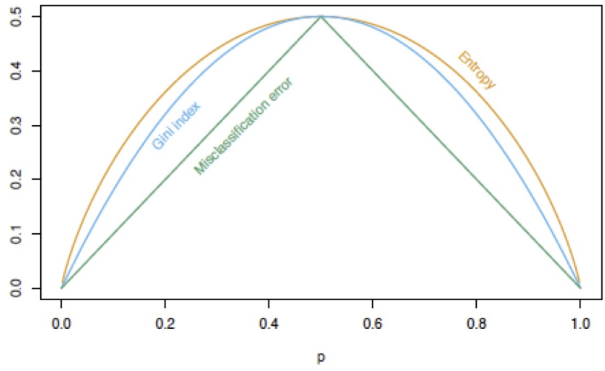
Gini index

$$H(\mathcal{S}) = 1 - \sum_{k=1}^{C} p_k(\mathcal{S})^2$$

Exercise (300,100),(100,300) vs (400,200),(200,0)

Exercise Relate the cross entropy with the Kullback-Leibler divergence, $KL(p, q) = \sum p_i \log \frac{p_i}{q_i}$

Impurity criteria



Are we maximizing or minimizing?

Impurity criteria: computational aspects

All impurity measures depend on $\mathbb{I}(y_i = k)$ via the probability

$$p_k(\mathcal{S}) = \frac{1}{n} \sum_{i=1}^{n} \mathbb{I}(y_i = k)$$

Exercise Finding the best split (naively) has complexity $O(dn^2c)$ for a sample of n points on d dimensions and c clases. Propose an incremental version and give the complexity.

Exercise Propose the extension of Gini and the combination of nodes for weighted samples.

How to find the best separation/split in a regression task ?

Let us define the pair of half-planes defined by the sign of $t_{j,s}$: $\mathcal{R}_l(j,s) = \{x, x^j \leq s\}$ and $\mathcal{R}_r(j,s) = \{x, x^j > s\}$.
We seek the splitting feature j and the split threshold s that solve $\min_{j,s} L((j,s), \mathcal{S})$:

$$\min_{j,s}[\min_{f_r} \sum_{x_i \in \mathcal{S} \cap \mathcal{R}_r(j,s)} (y_i - f_r)^2 + \min_{f_l} \sum_{x_i \in \mathcal{S} \cap \mathcal{R}_l(j,s)} (y_i - f_l)^2].$$

You can see that for any choice of j and s that the inner minimization problem can be solved for:

$$\hat{f}_r = \frac{1}{N_r} \sum_{x_i \in \mathcal{S} \cap \mathcal{R}_r} y_i$$

and

$$\hat{f}_l = \frac{1}{N_r} \sum_{x_i \in \mathcal{S} \cap \mathcal{R}_l} y_i$$

How to find the best separation/split in a regression task ?

In practise, it is thus sufficient to find the splitting feature j and the split threshold s that solve:

$$\min_{j,s}[\sum_{x_i,x_j \in \mathcal{S}\cap\mathcal{R}_r}(y_i - y_j)^2 + \sum_{x_i \in \mathcal{S}\cap\mathcal{R}_l}(y_i - y_j)^2].$$

e.g., we want to find the split that minimizes the sum of the empirical variances on the two parts of the splitted dataset.

N.B. As for s candidates we will take a finite number of candidates in the interval of values of X^j.

Stopping criterion

- A maximal depth is reached
- All the leaves are pure
- No improvement
- A number of minimal number of data is reached at a node
- ...

Cross-validation can be used to select that hyperparameter.
Otherwise, the tree is built until the training dataset is perfectly predicted (possible in classification) : **overfitting** !
In the past, people were building deep trees and then used a pruning procedure to erase some branches.

Exercise why is XOR not adequate for "No improvement" rule?

Exercise Which is the predicted function by a regression tree for the given (see board) function and splits?

Exercise See the given code. Which are the **main disadvantages and advantages of trees**?

Ensemble methods

Encourage the diversity of base predictors by:

- using bootstrap samples (Bagging and Random forests)
- using randomized predictors (ex: Random forests)
- using weighted version of the current sample (Boosting) with weights dependent on the previous predictor (adaptive sampling)

Ensemble methods at a glance

- 1995: Boosting, Freund and Schapire
- 1996: Bagging, Breiman
- 2001: Random forests, Breiman
- 2006: Extra-trees, Geurts, Ernst, Wehenkel

Reminder: Decomposition bias/variance in regression

Given x,

$$\mathbb{E}_S \mathbb{E}_{y|x}(y - f_S(x))^2 = noise(x) + bias^2(x) + \text{variance}(x) \tag{4}$$

$noise(x)$: $\mathbb{E}_{y|x}[(y - \mathbb{E}_{y|x}(y))^2]$: quantifies the error made by the Bayes model ($\mathbb{E}_{y|x}(y)$)

$bias^2(x) = (\mathbb{E}_{y|x}(y) - \mathbb{E}_S[f_S(x)])^2$ measures the difference between minimal error (Bayes error) and the average model

$variance(x) = \mathbb{E}_S[(f_S(x) - \mathbb{E}_S[f_S(x)])^2]$ measures how much $h_S(x)$ varies from one training set to another

Introduction to bagging (regression) - 1

Assume we can generate several training independent samples $\mathcal{S}_1, \ldots, \mathcal{S}_T$ from P(x,y).

A first algorithm:

Algorithme : Reducing variance

Données : T training independent samples $\{\mathcal{S}_1, \ldots, \mathcal{S}_T\}$
Résultat : An ensemble model f_{ens}
pour *sample* $\mathcal{S}_t$ *in* $\{\mathcal{S}_1, \ldots, \mathcal{S}_T\}$ **faire**
  $f_t \leftarrow$ learn a model with $\mathcal{S}_t$
retourner $f_{ens}(x) = \frac{1}{T} \sum_{t=1}^{T} f_t(x)$

Introduction to bagging - 2

The bias $(\mathbb{E}_{\mathcal{S}_1,\ldots,\mathcal{S}_T}[f_{ens}(x)] - f_{target}(x))$ remains the same because :

$$E_{\mathcal{S}_1,\ldots,\mathcal{S}_T}[f_{ens}(x)] = \frac{1}{T}\sum_t \mathbb{E}_{\mathcal{S}_t}[f_t(x)] = \mathbb{E}_{\mathcal{S}}[f_{\mathcal{S}}(x)]$$

But the variance is divided by T:

$$\mathbb{E}_{\mathcal{S}_1,\ldots,\mathcal{S}_T}[(f_{ens}(x) - \mathbb{E}_{\mathcal{S}_1,\ldots,\mathcal{S}_T}[f_{ens}(x)])^2] = \frac{1}{T}\mathbb{E}_{\mathcal{S}}[(f_{\mathcal{S}}(x) - \mathbb{E}_{\mathcal{S}}[f_{\mathcal{S}}(x)])^2]$$

When is it useful? When the learning algorithm is unstable, producing high variance estimators such as trees !

Bagging (Breiman 1996)

In practice, we do not know P(x,y) and we have only **one training sample** $\mathcal{S}$: we are going to use Bootstrap samples, i.e., random samples with replacement of the original dataset.

Bagging (or Bootstrap aggregating) is a machine learning ensemble meta-algorithm based on resampling the dataset used here to reduce variance

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Algorithme : Bagging = Bootstrap Aggregating

Données : Sample $\mathcal{S}$
Résultat : An (bootstrap) ensemble model f_{bag}
pour t *in* $\{1, \ldots, T\}$ **faire**
  $\mathcal{B} \leftarrow$ bootstrap sample from $\mathcal{S}$
  $f_t \leftarrow$ learn a model (a tree) with $\mathcal{B}$
retourner $f_{bag}(x) = \frac{1}{T} \sum_{t=1}^{T} f_t(x)$

Exercises

- Define sampling with and without replacement.
- How do we average discrete labels? See Equation (1).
- Give the pseudocode for bagging
- (Effective sample) Show that each bootstrap sample (or bagged tree) will contain $1 - e^{-1} \approx 0.632$ of the original sample $\mathcal{S}$.
- Is $\mathcal{B}_i$ drawn from the same distribution as $\mathcal{S}$?
- Are the samples i.i.d.?

Bagging in practise

- Variance is reduced but the bias can increase a bit (the effective size of a bootstrap sample is 30% smaller than the original training set $\mathcal{S}$
- The obtained model is however more complex than a single model
- Bagging works for unstable predictors (neural nets, trees)
- In supervised classification, bagging a good classifier usually makes it better but bagging a bad classifier can make it worse

What if there is a feature with large predictive power? Correlated trees

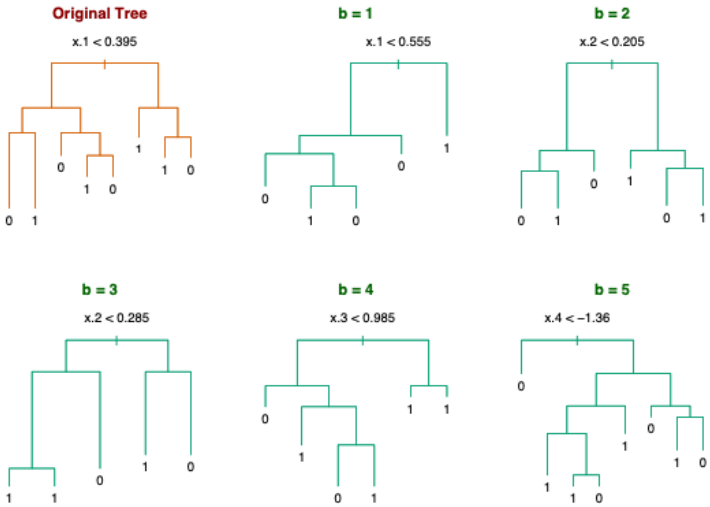


Figure: [Book: The elements of statistical learning, Hastie, Tibshirani, Friedman, 2001]

Other ensemble methods

- Perturbe and combine algorithms
  - Perturbe the base predictive model
  - Combine the perturbed predictive model

REFS: Random forests: Breiman 2001
Geurts, Ernst, Wehenkel, Extra-trees, 2006

Random forests: Breiman 2001

Algorithme : Random forest

Données : Sample $\mathcal{S}$
Résultat : ...
pour t *in* $\{1, \dots, T\}$ **faire**
  $\mathcal{B} \leftarrow$ bootstrap sample from $\mathcal{S}$
  $f_t \leftarrow$ learn a **randomized** tree with $\mathcal{B}$
retourner $f_{bag}(x) = \frac{1}{T} \sum_{t=1}^{T} f_t(x)$

Algorithme : Randomized tree

Données : Sample $\mathcal{S}$
Résultat : Randomized tree
tant que *not halting condition* **faire**
  $\mathcal{F} \leftarrow$ randomly keep $k = \sqrt{p}$ features
  find best split in $\mathcal{F}$
  $\vdots$
retourner randomized tree

Extra-trees: learning a single randomized tree in extra-trees

To select a split at a node:

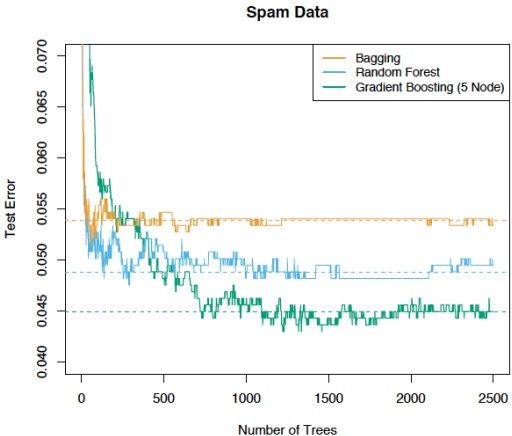
Algorithme : Randomized extra-tree

Données : Sample $\mathcal{S}$
Résultat : Extra-tree
tant que *not halting condition* **faire**
randomly select (without replacement) K feature with $K << p$
let a^i_{max} and a^i_{min} denote the maximal and minimal value of x_i in $\mathcal{S}$
Draw uniformly a cut-point s_c in $[s^i_{max}, s^i_{min}]$
Choose the best split among the K previous splits associated to the K cut-points.
$\vdots$
retourner randomized tree

Do not prune this tree
K is a hyperparameter, usually 10 to 20% of the number p of features.

Comparison (just an example)

[Book: The elements of statistical learning, Hastie, Tibshirani, Friedman, 2001]



Random forest

Pros

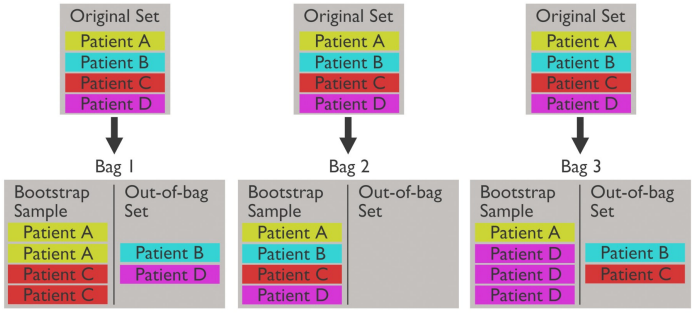
- Fast, parallelizable and appropriate for a large number of features
- Relatively easy to tune
- Frequently the winner in challenges

Cons

- Overfitting if the size of the trees is too large
- Interpretability is lost (however importance of feature can be measured)

Out-of-bag samples

$\{\bar{\mathcal{S}}_n^t = \mathcal{S}_n - \mathcal{S}_n^t, t = 1, \ldots, n_{tree}\}$ **out-of-bag samples**: contains the samples not selected by bootstrap



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Used for

- Out-of-bag error: evaluating at training time
- Variable importance

Variable importance

A variable X^j is important to predict Y if breaking the link between X^j and Y increase the prediction error

Let $\{\bar{\mathcal{S}}_n^t = \mathcal{S}_n - \mathcal{S}_n^t, t = 1, \ldots, n_{tree}\}$ **out-of-bag samples**

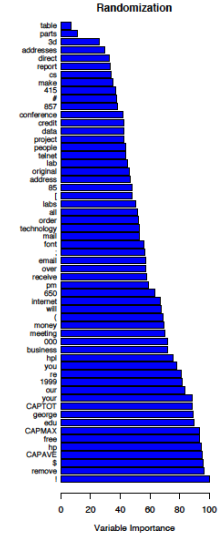
Let $\{\bar{\mathcal{S}}_n^{t,j}, t = 1, \ldots, n_{tree}\}$: permuted out-of-bag-samples (the values of the jth variable have been randomly permuted).

$$\hat{I}(X^j) = \frac{1}{n_{tree}} \sum_{t=1}^{n_{tree}} R_n(h_t, \bar{\mathcal{S}}_n^{t,j}) - R_n(h_t, \bar{\mathcal{S}}_n^t)$$

with $R_n(h, \mathcal{S})$: empirical loss of h measured on $\mathcal{S}$

Variable importance: spam data

Spam dataset :



Boosting: A preliminary question

Is it possible to "boost" a weak learner into a strong learner ? Michael Kearns Yoav Freund and Rob Schapire proposed an iterative scheme, called, Adaboost to solve this problem

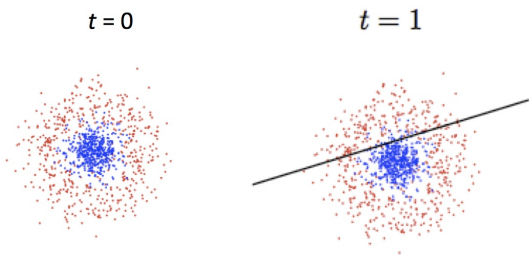
Idea: train a sequence of learners on weighted datasets with weights depending on the loss obtained so far.

Freund and Schapire received the Gödel prize in 2003 for their work on AdaBoost.

A **weak classifier** is a classifier whose average training error is no more than 0.5, nb., it means that we do not need to have a deep architecture as the base classifier (a "short" tree will fit for instance, a linear classifier will be perfect and so on...)

Boosting a linear classifier

$H_1(x) = h_1(x)$
Binary Classifier: $F_1(x) = \text{sign}(H_1(x))$
Here: h_1: linear classifier
Training error= R_n

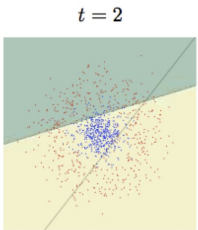


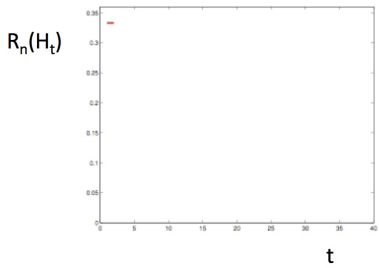
Source Jiri Matas (Oxford U.)

Boosting a linear classifier

$H_2(x) = \alpha_1 h_1(x) + \alpha_2 h_2(x)$

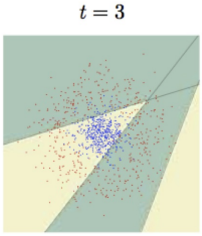
Binary Classifier: $F_2(x) = \text{sign}(H_2(x))$



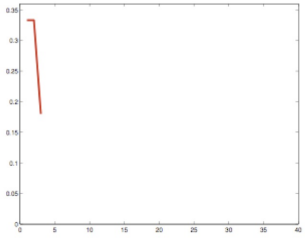


Source Jiri Matas (Oxford U.)

Boosting a linear classifier



$R_n(H_t)$



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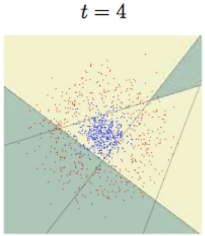
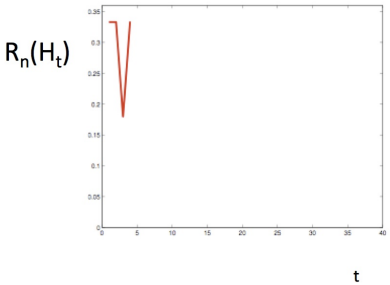
Boosting a linear classifier





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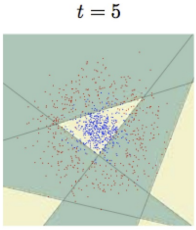
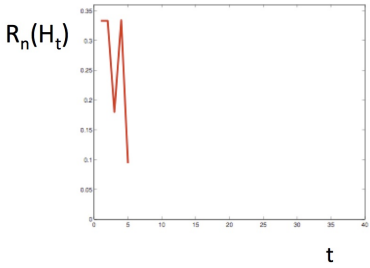
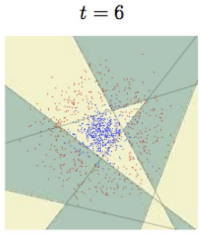
Boosting a linear classifier



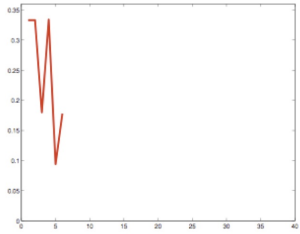


Source Jiri Matas (Oxford U.)

Boosting a linear classifier

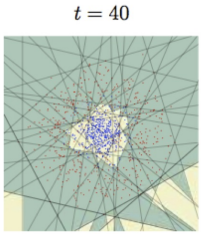


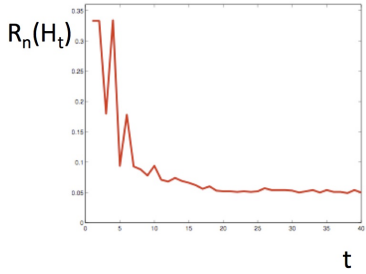
$R_n(H_t)$



Source Jiri Matas (Oxford U.)

Boosting a linear classifier





Source Jiri Matas (Oxford U.)

$H_T(x) = \sum_{t=1}^{T} \alpha_t h_t(x)$

Greedy version

AdaBoost (Freund and Schapire 1996)

$\mathcal{H}$: a chosen class of "weak" binary classifiers. Learn a sequence of classifiers for weighted samples

---

Données : $l, \alpha, \{(x_i, y_i)\}$
Résultat : AdaBoost model
$H_0 = 0$
$w_i = 1/n \quad \forall i$
pour t *in* $\{1, \ldots, T\}$ **faire**

- $h = \arg\min_{h \in \mathcal{H}} \sum_{i:h(x_i) \neq y_i} w_i$ `/* which algorithm? */`
- $\epsilon \leftarrow \sum_{i:h(x_i) \neq y_i} w_i$ `/* Training error, for a weak learner` $\epsilon > .5$ `*/`
- $\alpha = \frac{1}{2} \log \frac{1-\epsilon}{\epsilon}$
- $H_t = H_{t-1} + \alpha h$
- $w_i \leftarrow \frac{w_i \exp(-\alpha h(x_i) y_i)}{2\sqrt{\epsilon(1-\epsilon)}}$

retourner H_{t-1}

Can we use trees here?

Give the prediction rule

AdaBoost is a forward stage-wise additive model

An additive model can be written as $H(x) = \sum_t \alpha_t h_t(x)$

Typically, these models are learnt by sequentially adding new models without updating those already learnt. Each new model minimizes a loss L, for $t = 1..T$ as

$$(\alpha_t, h_t) = \arg\min_{\alpha,h} L(y_i, H_{t-1}(x) + \alpha h(x))$$

and set $H_t = H_{t-1}(x_i) + \alpha_t h_t(x_i)$.

This is a greedy approach

Theorem: AdaBoost is a forward stage-wise additive model for the exponential loss $L(y, h(x)) = \exp(-yh(x))$.

A general theory: gradient boosting

Iterative strategy. Given a training set $\{(x_1, y_1), \ldots, (x_n, y_n)\}$ minimizes the empirical risk.

$H_0(x) = \arg\min_\gamma \sum_{i=1}^n L(y_i, \gamma)$, as initialization, asn then at each iteration,

$H_t(x) = H_{t-1}(x) + (\arg\min_{h_t \in \mathcal{H}} [\sum_{i=1}^n L(y_i, H_{t-1}(x_i) + h_t(x_i))])(x)$, for $t \geq 1$, where $h_t \in \mathcal{H}$ is a base learner function.

Steepest descent step to this minimization problem (functional gradient descent) is equivalent to choosing

$H_t(x) = H_{t-1}(x) - \gamma \sum_{i=1}^n \nabla_{H_{t-1}} L(y_i, H_{t-1}(x_i))$

where $\gamma > 0$. For small γ, this implies that $L(y_i, H_t(x_i)) \leq L(y_i, H_{t-1}(x_i))$.

A general theory: gradient boosting

To prove the following, consider the objective

$$\sum_{i=1}^{n} L(y_i, H_{t-1}(x_i) + h_t(x_i))$$

Doing a Taylor expansion around the fixed point $H_{t-1}(x_i)$ up to first order:

$$\sum_{i=1}^{n} \left(L(y_i, H_{t-1}(x_i)) + h_t(x_i) \nabla_{H_{t-1}} L(y_i, H_{t-1}(x_i)) + \ldots \right)$$

Differentiating with respect to $h_t(x_i)$, only the derivative of the second term remains $\nabla_{H_{t-1}} L(y_i, H_{t-1}(x_i))$.

A general theory: gradient boosting

We can optimize γ by finding the γ value for which the loss function has a minimum:

$$\gamma_t = \arg\min_{\gamma} \sum_{i=1}^{n} L(y_i, H_t(x_i)) = \arg\min_{\gamma} \sum_{i=1}^{n} L\left(y_i, H_{t-1}(x_i) - \gamma \nabla_{H_{t-1}} L(y_i, H_{t-1}(x_i))\right).$$

If we considered the continuous case, i.e., where $\mathcal{H}$ is the set of arbitrary differentiable functions on $\mathbb{R}$, we would update the model in accordance with the following equations:

$$H_t(x) = H_{t-1}(x) - \gamma_t \sum_{i=1}^{n} \nabla_{H_{t-1}} L(y_i, H_{t-1}(x_i))$$

where γ_t is the step length, defined as:

$$\gamma_t = \arg\min_{\gamma} \sum_{i=1}^{n} L\left(y_i, H_{t-1}(x_i) - \gamma \nabla_{H_{t-1}} L(y_i, H_{t-1}(x_i))\right).$$

A general theory: gradient boosting

Algorithme : AnyBoost Gradient Boosting Algorithm

Données : Training set $\{(x_i, y_i)\}$, a differentiable loss function $L(y, H(x))$, number of iterations M

Résultat : AnyBoost model

Initialize model with a constant value: $H_0(x) = \arg\min_\gamma \sum_{i=1}^n L(y_i, \gamma)$

pour $t = 1$ *to* T **faire**

$$r_{it} = -\left[\frac{\partial L(y_i, H(x_i))}{\partial H(x_i)}\right]_{H(x)=H_{t-1}(x)} \text{ for } i = 1, \ldots, n$$

$$h_t(x) = \arg\min \sum_i r_i h(x_i)$$

$$\gamma_t = \arg\min_\gamma \sum_{i=1}^n L\left(y_i, H_{t-1}(x_i) + \gamma h_t(x_i)\right)$$

$$H_t(x) = H_{t-1}(x) + \gamma_t h_t(x)$$

retourner H_M

Prop 1: AdaBoost is a gradient descent algorithm in the functional space

Theorem: AdaBoost is a gradient descent algorithm in the functional space where the exponential loss $l(H) = \sum_{i=1}^{n} \exp(-y_i H(x_i))$ and α is obtained via line search

Part 1: What is the next classifier $h_{t+1} = \arg\min_{h \in \mathcal{H}} \sum_{i=1}^{n} r_i * h(x_i)$?

Let

$w_i = Z^{-1} \exp(-y_i H(x_i))$ be relative contribution of the point i to the loss,

$Z = \sum_{i=1}^{n} \exp(-y_i H(x_i))$ a normalizing constant,

$r_i = -y_i \exp(-y_i H(x_i))$ the gradient of the loss

Note that Z is the loss!

AdaBoost is a gradient descent algorithm in the functional space

Theorem: AdaBoost is a gradient descent algorithm in the functional space

$$
\begin{aligned}
h_{t+1} &= \arg\min_h \sum_{i=1}^{n} r_i h(x_i) = \arg\min_h \sum_{i=1}^{n} y_i \exp(-y_i H(x_i)) h(x_i) \\
&= \arg\min_h \sum_{i=1}^{n} y_i w_i h(x_i) = \arg\min_h \sum_{i:y_i \neq h(x_i)} w_i - \sum_{i:y_i = h(x_i)} w_i \qquad (5) \\
&= \arg\min_h \sum_{i:y_i \neq h(x_i)} w_i = \arg\min_h \epsilon
\end{aligned}
$$

Conclusion: the next classifier h_{t+1} is the one that minimizes the weighted classification error.

AdaBoost is a gradient descent algorithm in the functional space

Part 2: What is the step size (via line search)?

$$\alpha = \arg\min_{\alpha} \ell(H + \alpha h) = \arg\min_{\alpha} \sum_{i=1}^{n} e^{-y_i[H(x_i)+\alpha h(x_i)]}$$

We differentiate w.r.t. α and equate with zero:

AdaBoost, updates

At each step, the weights are updated to the weighted classification error:

$$w_i \leftarrow \frac{w_i \exp(-\alpha h(x_i) y_i)}{2\sqrt{\epsilon(1-\epsilon)}}$$

The normalizitaion constant $Z \leftarrow Z 2\sqrt{\epsilon(i-\epsilon)}$ since

$$\begin{aligned} Z_s =& \sum_{i=1}^{n} w_t(i) e^{-\alpha_t y_i h_t(x_i)} \\ =& \sum_{i:y_i h_t(x_i)=+1} w_t(i) e^{-\alpha_t} + \sum_{i:y_i h_t(x_i)=-1} w_t(i) e^{\alpha_t} \\ =& (1-\epsilon_t) e^{-\alpha_t} + \epsilon_t e^{\alpha_t} \\ =& 2\sqrt{\epsilon_t(1-\epsilon_t)} \end{aligned} \tag{6}$$

AdaBoost, convergence

Rem: The loss equals the normalization constant, $l(H) = Z$. We use this observation to bound the loss.

$$l(H) = n \prod_{i=1}^{T} 2\sqrt{\epsilon_t(1-\epsilon_t)}$$

Let $c = \max t\epsilon_t$, then

$$l(H) \leq n(2\sqrt{c(1-c)})^T$$

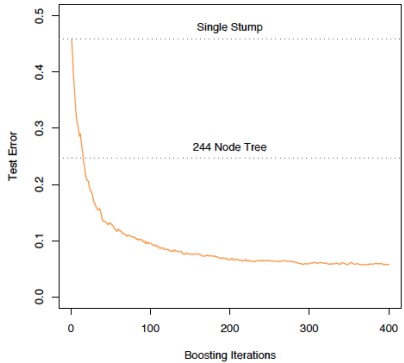
Since $\epsilon_t < .5$ for weak classifiers then $c(1-c) < .25$ or equivalently, $c(1-c) = .25 - \gamma^2$ and thus,

$$l(H) \leq n(1 - 4\gamma^2)^{T/2})$$

.

Typical behavior of boosting

Stump: a two terminal node classification tree



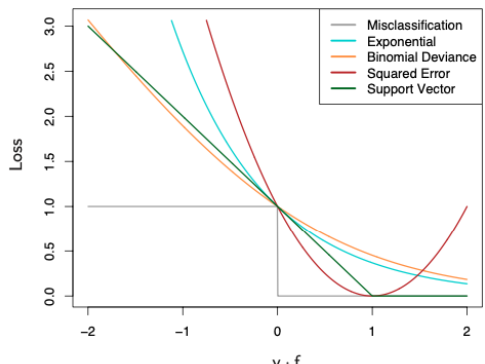
Boosting and regularization

- You have to wait a long time to see Boosting overfit. However contrary to first assertions, Adaboost does overfit
- Early stopping: an answer
- or... bound with ℓ_1 norm the magnitude of the weights

Losses in Forward Stagewise Additive Modeling

- AdaBoost with $\ell(y,h) = e^{-yh}$
- LogitBoost with $\ell(y,h) = \log(1+e^{-yh})$
- L_2Boost with $\ell(y,h) = (y-h)^2$ (Matching pursuit)
- L_1Boost with $\ell(y,h) = |y-h|$
- HuberBoost with $\ell(y,h) = |y-h|^2 \mathbf{1}_{|y-h|<\epsilon} + (2\epsilon|y-h| - \epsilon^2)\mathbf{1}_{|y-h|\geq\epsilon}$

Simple principle but no easy numerical scheme except for AdaBoost and L_2Boost...



Advantages and drawbacks of Decision trees

Advantages

- Produces an interpretable nonlinear decision function,
- Consistency of decision trees (not all the discrimination rules imply consistency, see Scott, Nowak, IEEE Trans. Information Theory 2006 - for a review)
- Works for multiple classes without any pre-processing
- Efficient prediction stage : $O(\log L)$, L: number of leaves
- Works for continuous and categorial features
- Support many extensions to many other ML tasks

Advantages and drawbacks of Decision trees

Drawbacks

- Large variance estimator, instability : a small variation in the training set produces a very different tree $\rightarrow$ so, ensemble of trees are therefore very attractive
- No global optimization

Exercises

- Write a detailed pseudocode for the regression trees for a maximum depth of d
- Code the k-fold cross validation for decision trees for obtaining the best *maximum tree depth* among the values 5,10,15 20
- Define a regularization function for trees.
- Give pros and cons of all algithms
- Describe all algorithms seen today

References

- CART : Classification and Regression Trees, Breiman, , Olshen, Friedman and Stone, Wadsworth Statistics, 1984.
- Induction and Decision trees, Quinlan, Machine Learning Journal 1, 1986.
- **Chapter Additive models and trees : The elements of statistical learning, Hastie, Tibshirani, Friedman, Springer.**

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