Introduction to Statistical Learning

Nicolas Vayatis

Lecture # 6 - Statistical analysis of mainstream ML algorithms

Part II - Analysis of Ensemble Methods and Boosting

Reminder on Part I

Kernel methods applied to classification
(*aka* Support Vector Machines)

Algorithmic Principles of SVM

- Search space : soft classifiers in an RKHS (kernel k)

$$\mathcal{H}(X) \doteq \left\{ h = \sum_{i=1}^{n} \alpha_i k(X_i, \cdot) \ : \ \alpha_1, \ldots, \alpha_n \in \mathbb{R} \right\}$$

- Regularized optimization problem : set $\lambda > 0$

$$\hat{h}_\lambda = \arg\min_{\mathcal{H}_k} \left\{ \sum_{i=1}^{n} (1 - Y_i h(X_i))_+ + \lambda \|h\|_k \right\}$$

- Resolution of the dual formulation thanks to quadratic optimization solvers

Theoretical analysis of SVM

- First ingredient : Complexity control
  When RKHS norm bounded by M and kernel bounded by R^2, we have the bound on Rademacher complexity of kernel classes :
  $$\widehat{R}_n(\mathcal{F}_M) \leq \frac{MR}{\sqrt{n}}$$
- Second ingredient : key inequalities (concentration and contraction or Zhang's Lemma)
- Two theorems can be derived : margin bound *or* classification error bound based on CRM

Margin bounds for SVM classification

Theorem. (Fixed margin)

Let $\mathcal{H}_k$ the RKHS with kernel k.

Fix $\rho \in (0,1)$, and $\delta > 0$. Then with probability at least $1-\delta$, we have, for any SVM classifier g :

$$L(g) \leq \widehat{L}_{n,\rho}(g) + 2\left(\frac{MR}{\rho\sqrt{n}}\right) + \sqrt{\frac{\log(1/\delta)}{2n}}$$

and

$$L(g) \leq \widehat{L}_{n,\rho}(g) + 2\left(\frac{M\sqrt{\mathrm{trace}\,(K)}}{\rho n}\right) + 3\sqrt{\frac{\log(2/\delta)}{2n}}$$

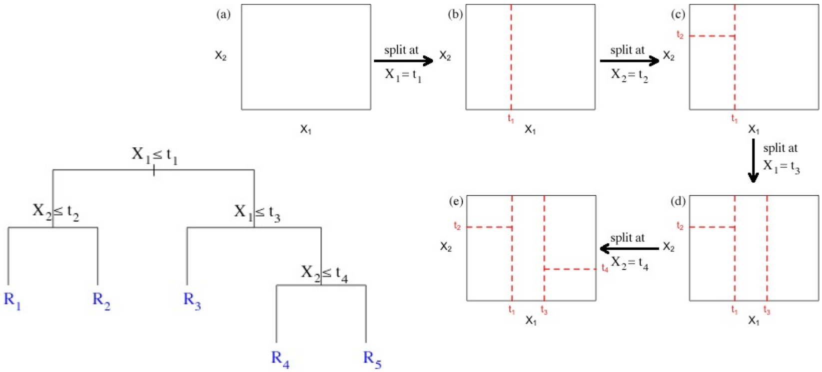
Interlude - The (al)most perfect algorithm

Decision trees

Algorithmic principles of Decision Trees

- Belongs to the family of *local* methods using (a) recursive partitioning, and (b) label averaging (or majority voting)
- Main inputs : (1) Geometry/number of splits (perpendicular, linear, binary or more, ...), (2) Local cost function (impurity) : entropy, Gini, classification error, (3) Stopping criterion, (4) with/out pruning
- Historical references : Hyafil, Rivest (1976), Breiman, Friedman, Olshen, Stone (1984), Quinlan (1986

Construction through recursive partitioning



Stopping crirteria and tree balancing

- Hyperparameters : type/number of splits, cost function, minimal number of points per partition cell, maximal depth of the tree (number of layers)

- Pruning the tree : amounts to exploring the class of all subpartitions (subtrees) and optimize a penalized criterion of the form
$$\arg\min_c \hat{L}_n(h_c) + \lambda|c|$$
where $c \subset \hat{c}$ is the collection of subpartitions obtained from the learned partition by pruning from bottom to top

Theory for partition-based classifiers

- Case of fixed and regular partitions with cells which are hypercubes of $\mathbb{R}^d$ with edges of length δ_n :

$$\mathbb{E}L(\hat{h}(\cdot, \delta_n)) \to L^*$$

  under the condition : $n\delta_n^d \to \infty$ and $\delta_n \to 0$ when $n \to \infty$ (need enough data points in every cell and cell diameter go to zero as sample size grows)

- Case of empirical data-driven partitions : Vapnik-Chervonenkis and Rademacher theory do apply...

Take-home message on decision trees

Major limitations :

- Prediction performance below state-of-the-art methods since the mid-90s (SVM, boosting, neural networks)
- Decision trees are extremely unstable - see Bertsimas, Digalakis (2023) for recent improvements
- Numerical cost for the pruning step is high - as $\mathcal{O}(2^L)$ for binary trees where L is the number of layers of the master tree

Virtues of decision trees :

- Can handle missing/categorical data, scale change
- Can be expressed in terms of logical rule $\longrightarrow$ explainable machine learning

Part II. Ensemble methods

What can be saved from decision trees ?

The concept of weak classifier

- Intuition : a weak classifier performs at least slightly better than random guessing (probability $\frac{1}{2} + \gamma$ for some $\gamma > 0$ to predict the true label).
- Formalization : weakly PAC-learnable algorithm - see Kearns and Valiant (1989), Freund (1990), Schapire (1990)
- Typical example : decision trees with single-variable splits (aka decision stumps) and fixed number of layers (say 3 to 7)

Definition of ensemble methods

- Consider a weak learning algorithm over a base class $\mathcal{H}$ of predictors
- An ensemble method has a search space which is either

$$\mathcal{F}_\alpha = \left\{ \sum_{t \geq 1} \alpha_t h_t \ : \ \forall t \geq 1, \alpha_t \in \mathbb{R}, h_t \in \mathcal{H}) \right\}$$

or

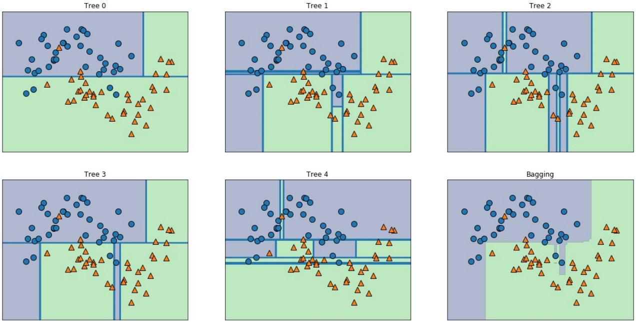
$$\mathcal{F}_1 = \left\{ \sum_{t \geq 1} h_t \ : \ \forall t \geq 1, h_t \in \mathcal{H}) \right\}$$

- Popular ensemble methods : Bagging (Breiman (1996)), Random forests (Amit, Geman (1997), Breiman (2000)), Boosting (Freund, Schapire (1995))

Complexity of ensembles

- Vapnik-Chervonenkis dimension of $\mathcal{F}_\alpha$ is $+\infty$ even for base class with finite VC dimension V
- For truncated sums (with T terms), the VC dimension is upper bounded by $2(V+1)(T+1)\log_2(e(T+1))$
- the Rademacher average of ensembles is in $\mathcal{O}\left(\sqrt{\frac{V}{n}}\right)$

Ensemble of decision trees with stumps



Ensemble methods

Bagging and Random Forests

How to generate the ensemble ? Bootstrap and aggregation

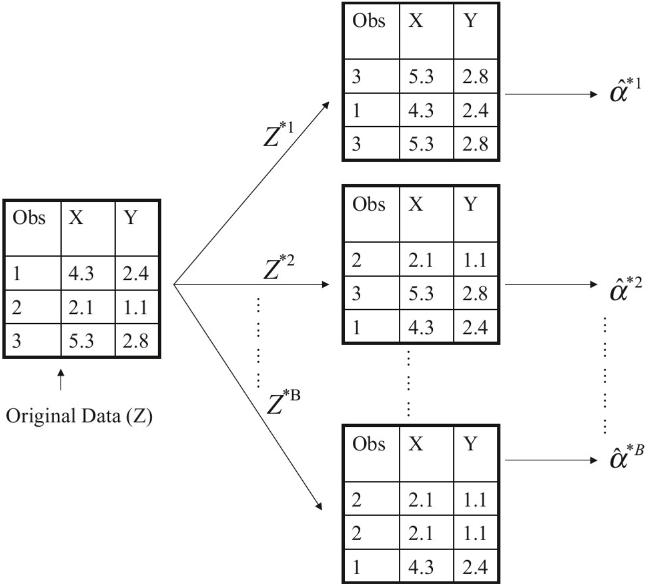
- Bagging and random forests operate on the search space

$$\mathcal{F}_1 = \left\{ \sum_{t \geq 1} h_t \; : \; \forall t \geq 1, h_t \in \mathcal{H}) \right\}$$

- Bagging and random forests rely on bootstrap samples of the training data, meaning if we denote by D_n the training data, we assume that we can sample functions $\hat{h}_1, \ldots, \hat{h}_t$ (the ensemble) from $\mathcal{H}$ conditionnally to D_n

- They differ by some different specifications of the recursive partitioning procedure to build each tree (no pruning involved)

What is bootstrap in general ?



Randomized rules (1/2)

- For a given sample $D_n = \{(X_i, Y_i) \ : \ i = 1, \dots, n\}$
- Introduce $\mathcal{Z}$ a measurable space and Z a random variable over $\mathcal{Z}$
- Conditionally on the sample D_n and on (X, Y), draw independent sequences $Z_1, \dots, Z_B$ of B copies of Z
- Design a pool of decision rules $\widehat{g}_{n,b}(x) = \widehat{g}_{n,b}(x, Z_b, D_n)$ for $b = 1, \dots, B$

Randomized rules (2/2)

- *Voting classifier* :

$$\widehat{g}_n^B(x) = \mathbb{I}\left\{\sum_{b=1}^{B} \widehat{g}_{n,b}(x) > B/2\right\} \ ,$$

- *Averaging classifier* (which is not a randomized classifier) :

$$\overline{g}_n^B(x) = \mathbb{I}\left\{\mathbb{E}_Z \widehat{g}_n(x, Z) > 1/2\right\} \ .$$

Bagging - Breiman, 1996

- Randomization through bootstrap replicates of D_n
- Randomized rule through bagging :

$$g_n(x, Z, D_n) = g_n(x, D_n(Z))$$

- ... and $D_n(Z) = \{(X_i^*, Y_i^*) \ : \ i = 1, \ldots, n\}$ where the points are drawn through random sampling from D_n
- Typical sampling is sampling with replacement and $|D_n(Z)| = n$

Bagging - a consistency result

- Special case with subsampling and without replicates in the bootstrap sample
- $|D_n(Z)| = N \leq n$ and ...
- ... we assume $N \sim \mathrm{Bin}(n, q_n)$ and $q_n = \mathbb{P}((X_i, Y_i) \in D_n(Z))$
- Consistency of both voting classifier and averaging classifier under assumptions :
  - $\{g_n\}$ sequence of classifiers that is consistent for P
  - $nq_n \to \infty$ when $n \to \infty$

Bagging can render consistent rules that are inconsistent

- Biau, Devroye and Lugosi (2008) have considered bagging 1-NN
- 1-NN is consistent if and only if $L^* \in \{0, 1/2\}$
- Bagging averaged 1-NN classifier is consistent for any P if and only if $q_n \to 0$ and $nq_n \to \infty$ when $n \to \infty$
- Proof follows the lines of Stone theorem (cf. Devroye, Györfi, Lugosi (1996))

Random Forest consistency

- Simplified model : the *purely random forest* in Biau, Devroye, Lugosi (2008) (further work in Scornet, Biau, Vert (2015))
- Start with a tree classifier with rectangular cells with orthogonal splits over $[0,1]^d$ and build randomized versions as follows :
  - Draw a leave according to a uniform distribution over the set of leaves of the tree
  - Draw one split variable among the d dimensions of input space with a uniform
  - Position the split at random (uniform distribution again)
  - Repeat k times splitting of terminal cells of the tree
- Result : The averaged classifier is consistent if $k_n \to \infty$ and $k_n/n \to 0$ when $n \to \infty$

Ensemble methods

Boosting

Historical perspective on Boosting

- Original paper : Freund and Schapire (ECML, 1995).
- Interpretation of the optimization problem solved as stochastic gradient descent : Friedman (CSDA, 2002).
- Wald Memorial lecture (IMS, 2000) : Leo Breiman declares that *"understanding Boosting is the most important problem in Machine Learning"*
- Proofs of boosting consistency : Jiang (2004), Lugosi, G. and Vayatis, N. (2004), Zhang (2004), Bartlett and Traskin (2007)
- Xgboost, a scalable implementation : Chen, T. and Guestrin, C. (ACM SIGKDD, 2016).

Algorithmic principle for Boosting

- **Input**
  - Data sample $D_n = \{(X_i, Y_i) \ : \ i = 1, \ldots, n\}$ with classification data $\{-1, +1\}$
  - Base hypothesis class $\mathcal{H}$ of *weak* classifiers such as decision trees (assumed to be symmetric, i.e. $h \in \mathcal{H}$ iff $-h \in \mathcal{H}$)
- **Iterations** $t = 1, \ldots, T$**.**
  - Compute weights $\widehat{\alpha}_t > 0$ and weak classifiers $\widehat{h}_t \in \mathcal{H}$
- **Output.**
  - The Boosting classifier takes the sign of the following linear combination of weak classifiers : $\widehat{f}_n(x) = \sum_{t=1}^{T} \widehat{\alpha}_t \widehat{h}_t(x)$

Weighting the data

- Boosting distributions on the data : sequence of discrete probability distributions over $\{1, \ldots, n\}$ denoted by Π_t, $t \geq 1$
- Weighted training error : for any weak classifier $h \in \mathcal{H}$ and for $t \geq 1$

$$\widehat{\varepsilon}_t(h) = \sum_{i=1}^{n} \Pi_t(i) \mathbb{I}\{h(X_i) \neq Y_i\}$$

The AdaBoost algorithm

1. **Initialization.** Π_1 is the uniform distribution on $\{1, \ldots, n\}$
2. **Boosting iterations.** For $t = 1, \ldots, T$, find the weak classifier such that :

$$\widehat{h}_t = \arg\min_{h \in \mathcal{H}} \widehat{\varepsilon}_t(h)$$

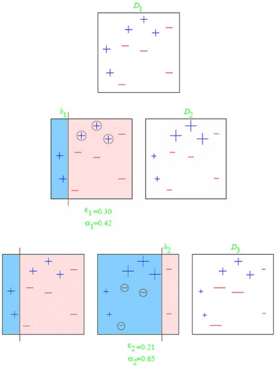
then set $e_t = \widehat{\varepsilon}_t(\widehat{h}_t)$ and take the weight to be

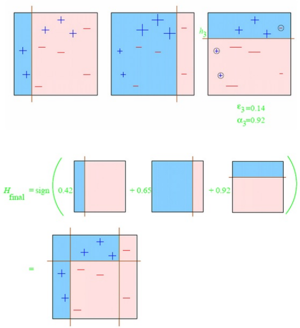
$$\widehat{\alpha}_t = \frac{1}{2} \log\left(\frac{1 - e_t}{e_t}\right)$$

3. **Boosting distribution update.** For any $i = 1, \ldots, n$,

$$\Pi_{t+1}(i) \propto \Pi_t(i) \exp\left(-\widehat{\alpha}_t Y_i \cdot \widehat{h}_t(X_i)\right)$$

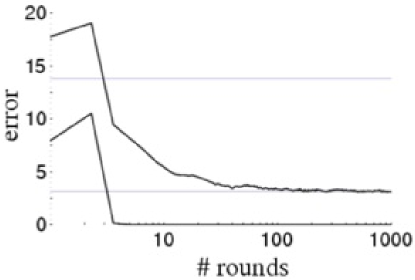
Illustration of Boosting on a toy example





Mysterious behavior of Boosting

The test error continues to drop along the iterations even though the training error is zero $\longrightarrow$ Regularization effect thanks to averaging ? ?



Boosting as a CRM principle

- Boosting can be interpreted as a functional gradient descent on the following functional :

$$\hat{A}_n(f) = \frac{1}{n}\sum_{i=1}^{n} \exp\left(-Y_i f(X_i)\right)$$

  where f is taken in a hypothesis space which is the linear span of 'simple' set $\mathcal{H}$ of classifiers.

- Exercise : why ?

  Refer to : J. Friedman, "Greedy Function Approximation : A Gradient Boosting Machine", The Annals of Statistics, Vol. 29, No. 5, 2001.

Which directions for the analysis of boosting ?