Basics of Machine Learning

TSIA-SD 210 - P3

Lecture 6 - Ensemble methods: bagging, random forests, boosting

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Outline

Ensemble methods for classification and regression

1. Remark:
   - Machine Learning not so "automatic": too many hyperparameters to tune
2. **meta-learning**: a procedure that learns to learn
3. **committee learning** or **wisdom of the crowd**: better results are obtained by combining the predictions of a set of **diverse** classifiers/regressors
4. **ensemble learning**: Improve upon a single base predictive model by building an ensemble of predictive model (with no hyperparameter)

Ensemble methods for regression

Let $f_t, t = 1, \dots, T$ be T different regressors.
Notations:

$$
\begin{aligned}
\epsilon_t(x) &= y - f_t(x) \\
MSE(f_t) &= \mathbb{E}[\epsilon_t(x)^2] \\
f_{ens}(x) &= \frac{1}{T}\sum_t f_t(x) \\
&= y - \frac{1}{T}\sum_t \epsilon_t(x).
\end{aligned}
$$

Encourage the diversity of base models

$$MSE(f_{ens}) = \mathbb{E}[(y - f_{ens}(x))^2]$$

If ϵ_t are mutually independent with zero mean, then we have:

$$MSE(f_{ens}) = \frac{1}{T^2}\mathbb{E}[\sum_t \epsilon_t(x)^2]$$

The more diverse are the models, the more we reduce the mean square error !

Ensemble methods for supervised classification

Binary classification

$$h_{ens}(x) = \text{sign}(\sum_t h_t(x))$$

Multiclass classification

$$h_{ens}(x) = \arg\max_c \text{vote}(c, h_1, \ldots, h_T)$$

with : $\text{vote}(c, h_1, \ldots, h_T) = \sum_t 1_{h_t(x)=c}(h_t(x))$

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

Outline

Motivation

Bagging

Random forests

Boosting

References

Reminder: Decomposition bias/variance in regression

Given x,

$$\mathbb{E}_S \mathbb{E}_{y|x}(y - f_S(x))^2 = \mathit{noise}(x) + \mathit{bias}^2(x) + \text{variance}(x) \qquad (1)$$

noise(x): $E_{y|x}[(y - E_{y|x}(y))^2]$:
quantifies the error made by the Bayes model ($E_{y|x}(y)$)
$\mathit{bias}^2(x) = (E_{y|x}(y) - E_S[f_S(x)])^2$
measures the difference between minimal error (Bayes error) and the average model
$\mathit{variance}(x) = E_S[(f_S(x) - E_S[f_S(x)])^2]$
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 $\mathcal{S}_1, \dots, \mathcal{S}_T$ from P(x,y).

A first algorithm:

- draw T training independent samples $\{\mathcal{S}_1, \dots, \mathcal{S}_T\}$
- learn a model $f_t \in \mathcal{F}$ from each training sample $\mathcal{S}_t; t = 1, \dots, T$
- compute the average model : $f_{ens}(x) = \frac{1}{T} \sum_{t=1}^{T} f_t(x)$

Introduction to bagging - 2

The bias ($E_{\mathcal{S}_1,\ldots,\mathcal{S}_T}[f_{ens}(x)] - f_{target}(x)$) remains the same because :
$E_{\mathcal{S}_1,\ldots,\mathcal{S}_T}[f_{ens}(x)] = \frac{1}{T}\sum_t E_{\mathcal{S}_t}[f_t(x)] = E_{\mathcal{S}}[f_{\mathcal{S}}(x)]$
But the variance is divided by T:
$E_{\mathcal{S}_1,\ldots,\mathcal{S}_T}[(f_{ens}(x) - E_{\mathcal{S}_1,\ldots,\mathcal{S}_T}[f_{ens}(x)])^2] = \frac{1}{T} E_{\mathcal{S}}[(f_{\mathcal{S}}(x) - E_{\mathcal{S}}[f_{\mathcal{S}}(x)])^2]$
When is it useful? When the learning algorithm is unstable, producing high variance estimators such as trees !

Bagging (Breiman 1996)

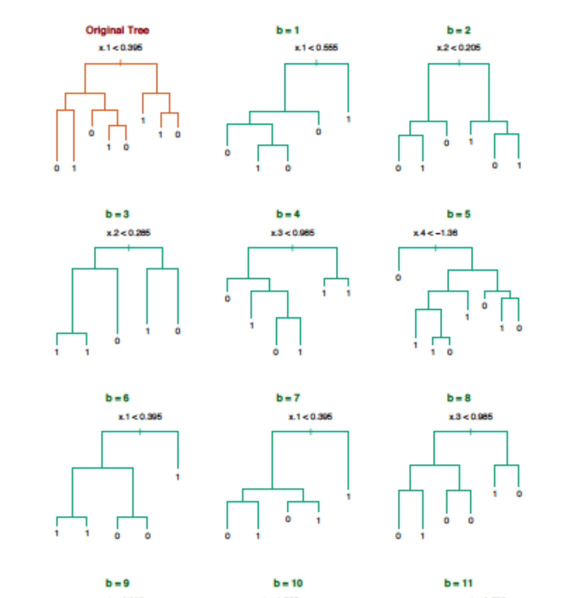
In practice, we do not know P(x,y) and we have only **one training sample** $\mathcal{S}$: we are going to use Bootstrap samples !

Bagging = Bootstrap Aggregating

- draw T bootstrap samples $\{_1 \ldots ,_T\}$ from $\mathcal{S}$ (bootstrap: uniform sampling with replacement)
- Learn a model f_t for each $_t$
- Build the average model: $f_{bag}(x) = \frac{1}{T} \sum_t f_t(x)$

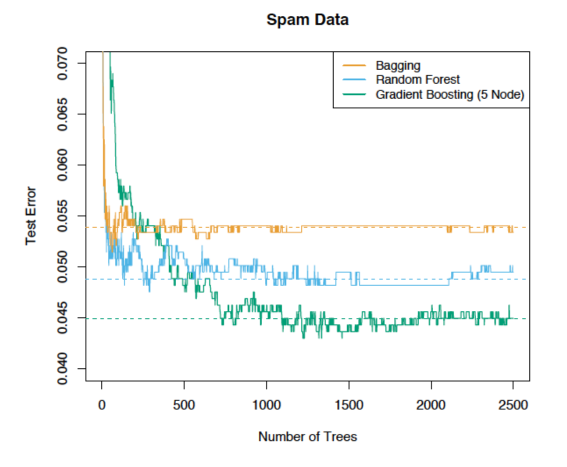
Example of bagged trees

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



Example of bagged trees

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



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

Outline

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

Random forests algorithm

- INPUT: F= p candidate feature splits, $\mathcal{S}_{train}$
- for t=1 to T
  - $\mathcal{S}_{train}^{(t)}$ m instance randomly drawn with replacement from $\mathcal{S}_{train}$
  - $h_{tree}^{(t)} \leftarrow$ randomized decision tree learned from $\mathcal{S}_{train}^{(t)}$
- OUTPUT: $H^T = \frac{1}{T}\sum_t h_{tree}^{(t)}$

Learning a single randomized tree

- To select a split at a node:
  - $R_f(F) \leftarrow$ randomly select (without replacement) f feature splits from F with $f << p$
  - Choose the best split in $R_f(F)$ (consider the different cut-points)
- Do not prune this tree

Extra-trees: Geurts et al. 2006

Extra-trees

- INPUT: candidate feature splits $F = \{1, \dots, p\}$, $\mathcal{S}_{train}$
- for t=1 to T
  - Always use $\mathcal{S}_{train}$
  - $h_{tree}^{(t)} \rightarrow$: randomized decision tree learned from $\mathcal{S}_{train}$
- OUTPUT: $H^T = \frac{1}{T} h_{tree}^{(t)}$

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

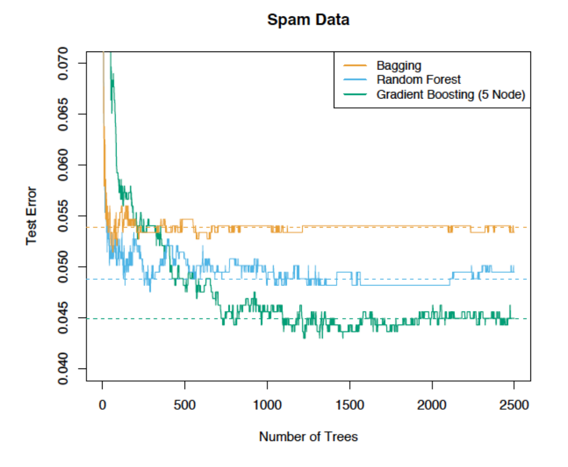
To select a split at a node:

- randomly select (without replacement) K feature splits from F with $K << |F|$
- Draw K splits using the procedure Pick-a-random-split($\mathcal{S}$,i):
  - 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 a_c in $[a^i_{max}, a^i_{min}]$
- Choose the best split among the K previous splits

Do not prune this tree

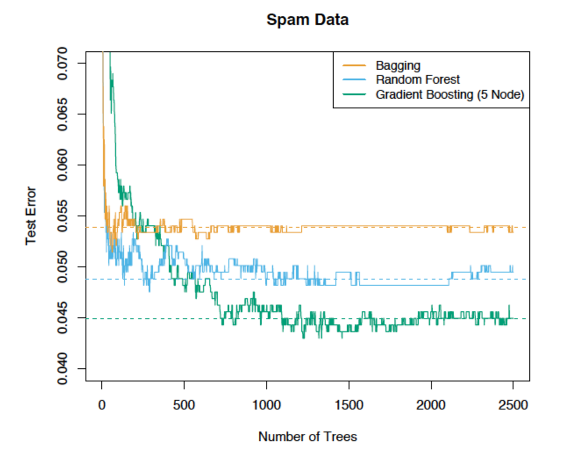
Random forest

Example of decision frontier:



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)

Variable importance

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

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

Variable importance

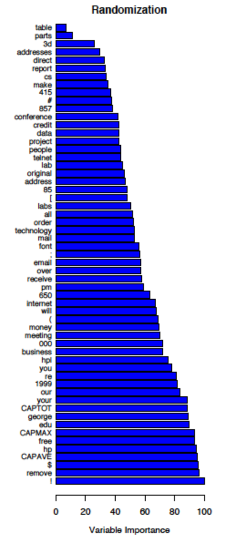
Let $\{\bar{\mathcal{S}}_n^t = \mathcal{S}_n - \mathcal{S}_n^t, t = 1, \ldots, n_{tree}\}$ **out-of-bag samples**
Let $\{\bar{\mathcal{S}}_n^{t,j}, t = 1, \ldots, n_{tree}\}$: permuted out-of-bag-samples (the values of the jth variable have been randomly permuted).

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

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

Variable importance: spam data

Spam dataset :



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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 Godel prize in 2003 for their work on AdaBoost.

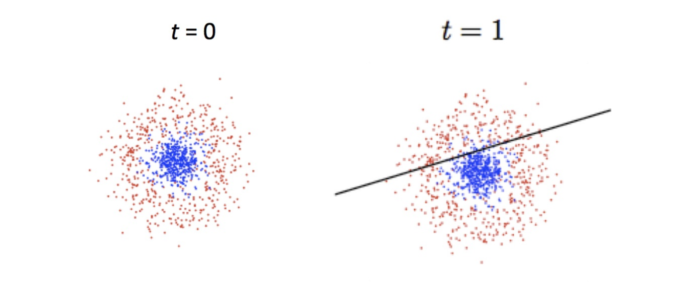
Boosting a linear classifier

$H_1(x) = h_1(x)$

Binary Classifier: $F_1(x) = \text{sign}(H_1(x))$

Here: h_1: linear classifier

Training error$= R_n$

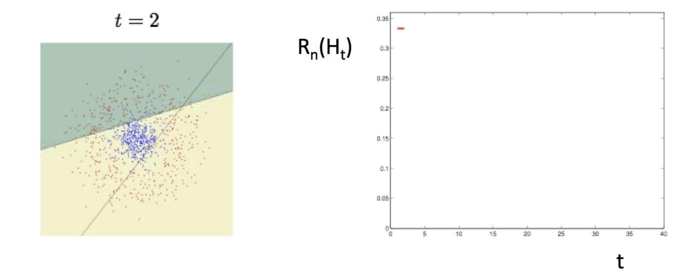


Source Jiri Matas (Oxford U.)

Boosting a linear classifier

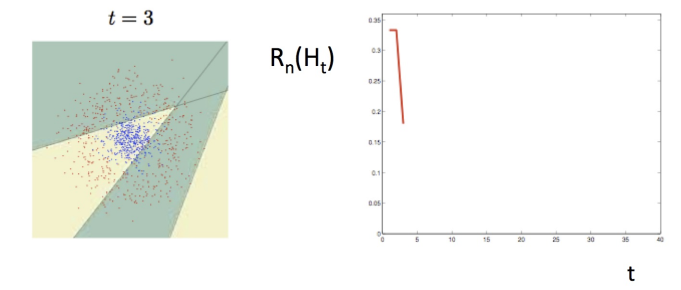
$H_2(x) = \alpha_1 h_1(x) + \alpha_2 h_2(x)$

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



Source Jiri Matas (Oxford U.)

Boosting a linear classifier



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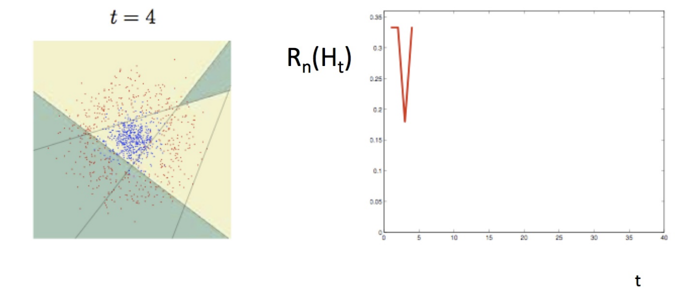
Boosting a linear classifier



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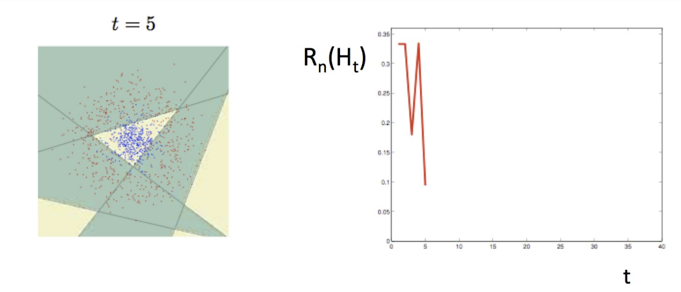
Boosting a linear classifier



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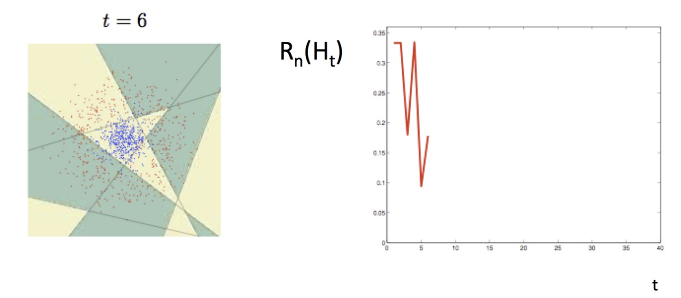

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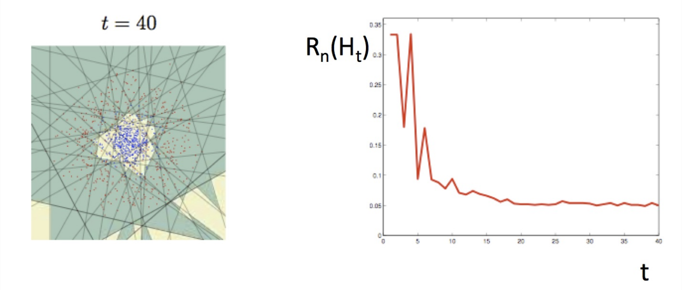
Boosting a linear classifier



Source Jiri Matas (Oxford U.)

Weak classifier

Definition: weak classifier
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...)

Adaboost idea

1. $\mathcal{H}$: a chosen class of "weak" binary classifiers, $\mathcal{A}$: a learning algorithm for $\mathcal{H}$

- Set $w_1(i) = 1/n$; $H_0 = 0$
- For $t = 1$ to T
    - $h_t = \arg\min_{h \in \mathcal{H}} \epsilon_t(h)$
    - with $\epsilon_t(h) = \mathbb{P}_{i \sim \mathbf{w}_t}[h(x_i) \neq y_i]$
    - Choose α_t
    - Choose w_{t+1}
    - $H_t = H_{t-1} + \alpha_t h_t$
- Output $F_T = \text{sign}(H_t)$

$\mathcal{H}$: a chosen class of "weak" binary classifiers

- Set $w_1(i) = 1/n$; $H_0 = 0$
- For $t = 1$ to T
  - $h_t = \arg\min_{h \in \mathcal{H}} \sum_{i=1}^{n} \epsilon_t(h)$
  - With $\epsilon_t(h) = \mathbb{P}_{i \sim \mathbf{w}_t}[h(x_i) \neq y_i]$
  - $\epsilon_t = \epsilon_t(h_t)$
  - $\alpha_t = \frac{1}{2} \log \frac{1-\epsilon_t}{\epsilon_t}$
  - let $w_{t+1,i} = \frac{w_t(i) e^{-\alpha_t y_i h_t(x_i)}}{Z_{t+1}}$ where Z_{t+1} is a renormalization constant such that $\sum_{i=1}^{n} w_{t+1,i} = 1$
- $H_t = H_{t-1} + \alpha_t h_t$

Output $F_T = \mathrm{sign}(H_t)$

What weight to choose ?

With the chosen definition, we have:

$$\begin{aligned} w_{t+1,i} &= \frac{w_{t,i} e^{-\alpha_t y_i h_t(x_i)}}{Z_t} \\ &= \frac{w_{t-1,i} e^{-\alpha_{t-1} y_i h_{t-1}(x_i)} e^{-\alpha_t y_i h_t(x_i)}}{Z_{t-1} Z_t} \\ &= \frac{e^{-y_i \sum_{s=1}^{t} \alpha_s h_s(x_i)}}{n \prod_{s=1}^{t} Z_s} \\ &= \frac{e^{-y_i H_t(x_i)}}{n \prod_{s=1}^{t} Z_s} \end{aligned}$$

You see the weights encourage to correct examples badly classified by the whole combination H_t

First of all let us study Z_t

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

Bounding the training error

The training error theorem for boosting
The training error of the classifier returned by Adaboost at time T verifies:

$$R_n(F_T) \leq e^{-2\sum_{t=1}^{T}(\frac{1}{2}-\epsilon_t)^2}.$$

Furthermore, if for all $t \in [1, T]$, $\gamma \leq (\frac{1}{2} - \epsilon_t)$, then

$$R_n(F_T) \leq e^{-2\gamma^2 T}.$$

Adaboost: Bound on the training error: proof

For all $u \in \mathbb{R}$, we have $1_{u \leq 0} \leq \exp(-u)$.
Then

$$
\begin{aligned}
, R_n(F_T) &= \frac{1}{n} \sum_{i=1}^{n} 1_{y_i F_T(x_i) \leq 0} \\
&\leq \frac{1}{n} \sum_{i=1}^{n} \exp(-y_i F_T(x_i)) = \frac{1}{n} \sum_{i=1}^{n} [n \prod_{t=1}^{T} Z_t] w_{t+1,i} = \prod_{t=1}^{T} Z_t
\end{aligned}
$$

Bound on the training error: proof ctd'

We can now express $\prod Z_t$ in terms of ϵ_t:

$$
\begin{aligned}
\prod_{t=1}^{T} Z_t &= \prod_{t=1}^{T} 2\sqrt{\epsilon_t(1-\epsilon_t)} \\
&= \text{by remarkable identity} \\
&= \prod_{t=1}^{T} \sqrt{1-4(1/2-\epsilon_t)^2} \\
&\leq \prod_{t} e^{-2(1/2-\epsilon_t)^2} = e^{-2\sum_{t=1}^{T}(1/2-\epsilon_t)^2}
\end{aligned}
$$

using the identity $1-u \leq \exp(-u)$.

Choice of α_t

The proof reveals several interesting properties:

1. α_t is chosen to minimize $\prod_t Z_t = g(\alpha)$ with $g(\alpha) = (1-\epsilon_t)e^{-\alpha} + \epsilon_t e^{\alpha}$
   - $g'(\alpha) = -(1-\epsilon_t)e^{-\alpha} + \epsilon_t e^{\alpha}$
   - $g'(\alpha) = 0$ iff $(1-\epsilon_t)e^{-\alpha} = \epsilon_t e^{\alpha}$ iff $\alpha = 1/2 \log \frac{1-\epsilon_t}{\epsilon_t}$
2. The equality $(1-\epsilon_t)e^{-\alpha} = \epsilon_t e^{\alpha}$ means that Adaboost assigns at each time t the same distribution mass to correctly classified examples and incorrectly classified ones. However there is no contradiction because the number of incorrectly examples decreases.

Adaboost with scikitlearn

http://scikit-learn.org/stable/modules/ensemble.htmladaboost

\>>> from sklearn.crossvalidation import crossva$l$score

\>>> from sklearn.datasets import loadiris

\>>> from sklearn.ensemble import AdaBoostClassifier

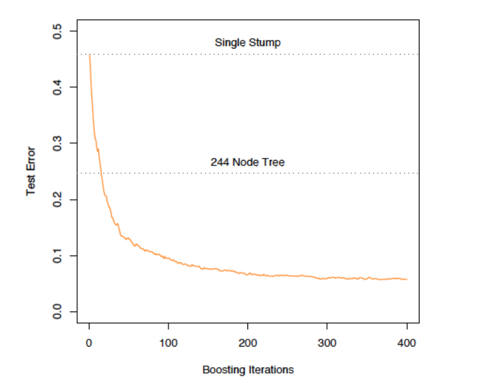
\>>> iris = loadiris()

\>>> clf = AdaBoostClassifier(nestimators=100)

\>>> scores = crossvalscore(clf, iris.data, iris.target)

\>>> scores.mean() 0.9...

Typical behavior of boosting



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

Outline

Boosting as a coordinate descent

At the same time, different groups proved that Adaboost writes as a coordinate descent in the convex hull of $\mathcal{H}$.

- Greedy function approximation, Friedman, 1999.
- MarginBoost and AnyBoost : Mason et al. 1999.

Gradient Boosting: the idea

- At each boosting step, one need to solve

$$(h_t, \alpha_t) = \arg\min_{h,\alpha} \sum_{i=1}^{n} \ell(y_i, H_{t-1}(x_i) + \alpha h) = L(y, H_{t-1} + \alpha h)$$

- Gradient approximation $L(y, H_{t-1} + \alpha h) \sim L(y, H_{t-1}) + \alpha \langle \nabla L(H_{t-1}), h \rangle$.
- Gradient boosting: replace the minimization step by a *gradient descent* type step:
    - Choose h_t as the best possible descent direction in $\mathcal{H}$
    - Choose α_t that minimizes $L(y, H + \alpha h_t)$
- Easy if finding the best descent direction is easy!

Gradient boosting and Adaboost

Those two algorithms are equivalent!

- Denoting $H_t = \sum_{t'=1}^{t} \alpha_{t'} h_{t'}$,

$$\begin{aligned}\sum_{i=1}^{n} e^{-y_i(H_{t-1}(x_i)+\alpha h(x_i))} &= \sum_{i=1}^{n} e^{-y_i H_{t-1}(x_i)} e^{-\alpha y_i h(x_i)} \\ &= \sum_{i=1}^{n} w_i'(t) e^{-\alpha y_i h(x_i)} \\ &= (e^{\alpha} - e^{-\alpha}) \sum_{i=1}^{n} w_i'(t) \ell^{0/1}(y_i, h(x_i)) \\ &\quad + e^{-\alpha} \sum_{i=1}^{n} w_i'(t)\end{aligned}$$

Gradient boosting and adaboost (ctd)

Those two algorithms are equivalent!

- The minimizer h_t in h is independent of α and is also the minimizer of

$$\sum_{i=1}^{n} w_i'(t)\ell^{0/1}(y_i, h(x_i))$$

Gradient boosting and Adaboost

- The optimal α_t is then given by

$$\alpha_t = \frac{1}{2}\log\frac{1-\epsilon'_t}{\epsilon'_t}$$

with $\epsilon'_t = (\sum_{i=1}^n w'_i(t)\ell^{0/1}(y_i, h_t(x_i)))/(\sum_{i=1}^n w'_i(t))$

- One verify then by recursion that

$$w_i(t) = w'_i(t)/(\sum_{i=1}^n w'_i(t))$$

and thus the two procedures are equivalent!

AnyBoost or Foward Stagewise Additive model

- General greedy optimization strategy to obtain a linear combination of *weak* predictor
    - Set $t = 0$ and $H_0 = 0$.
    - For $t = 1$ to T,
        - $(h_t, \alpha_t) = \arg\min_{h,\alpha} \sum_{i=1}^{n} \ell(y_i, H_{t-1}(x_i) + \alpha h(x_i))$
        - $H_t = H_{t-1} + \alpha_t h_t$
    - Output $H_T = \sum_{t=1}^{T} \alpha_t h_t$

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...

Continuous loss functions and gradient boosting

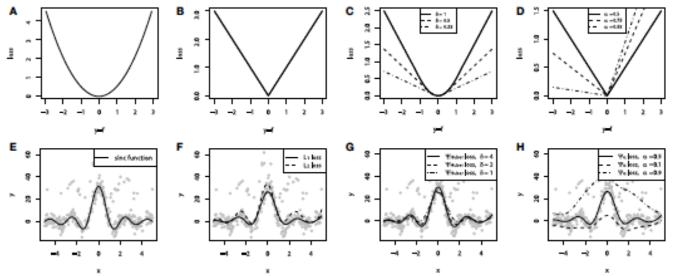


FIGURE 1 | Continuous loss functions: (A) L_2 squared loss function; (B) L_1 absolute loss function; (C) Huber loss function; (D) Quantile loss function. Demonstration of fitting a smooth GBM to a noisy sinc(x) data: **(E)** original sinc(x) function; **(F)** smooth GBM fitted with L_2 and L_1 loss; **(G)** smooth GBM fitted with Huber loss with $\delta = \{4, 2, 1\}$; **(H)** smooth GBM fitted with Quantile loss with $\alpha = \{0.5, 0.1, 0.9\}$.

L_2 Boosting

- Loss function for regression: $\ell(y, h) = (y - h)^2$
- $(h_t, \alpha_t) = \arg\min_{h,\alpha} \sum_{i=1}^{n} (y_i - H_t(x_i) + \alpha h)^2$

  Fitting the residuals.

Outline

References

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