STK-IN4300
Statistical Learning Methods in Data Science

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Outline of the lecture

- AdaBoost
  - Introduction
  - algorithm
- Statistical Boosting
  - Boosting as a forward stagewise additive modelling
  - Why exponential loss?
  - Gradient boosting

AdaBoost: introduction

L. Breiman: *"[Boosting is] the best off-shelf classifier in the world"*.

- originally developed for classification;
- as a pure machine learning black-box;
- translated into the statistical world (Friedman et al., 2000);
- extended to every statistical problem (Mayr et al., 2014),
  - regression;
  - survival analysis;
  - ...
- interpretable models, thanks to the statistical view;
- extended to work in high-dimensional settings (Bühlmann, 2006).

AdaBoost: introduction

Starting challenge:
"Can [a committee of blockheads] somehow arrive at highly reasoned decisions, despite the weak judgement of the individual members?" (Schapire & Freund, 2014)

Goal: create a good classifier by combining several weak classifiers,

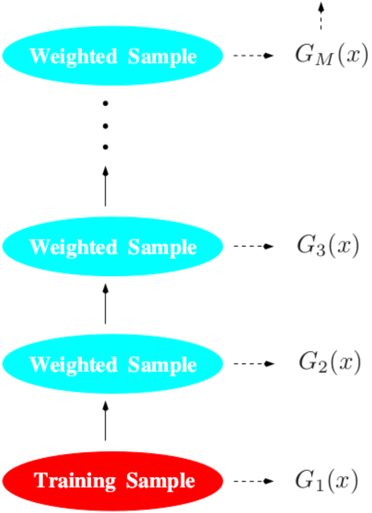
- in classification, a "weak classifier" is a classifier which is able to produce results only slightly better than a random guess;

Idea: apply repeatedly (iteratively) a weak classifier to modifications of the data,

- at each iteration, give more weight to the misclassified observations.

AdaBoost: introduction

$$G(x) = \text{sign}\left[\sum_{m=1}^{M} \alpha_m G_m(x)\right]$$



AdaBoost: algorithm

Consider a two-class classification problem, $y_i \in \{-1, 1\}$, $x_i \in \mathbb{R}^p$.

AdaBoost algorithm:

1. initialize the weights, $w^{[0]} = (1/N, \dots, 1/N)$;
2. for m from 1 to m_{stop},
   (a) fit the weak estimator $G(\cdot)$ to the weighted data;
   (b) compute the weighted in-sample missclassification rate,
   $$\text{err}^{[m]} = \sum_{i=1}^{N} w_i^{[m-1]} \mathbb{1}(y_i \neq \hat{G}^{[m]}(x_i));$$
   (c) compute the voting weights, $\alpha^{[m]} = \log((1 - \text{err}^{[m]})/\text{err}^{[m]})$;
   (d) update the weights
      - $\tilde{w}_i = w_i^{[m-1]} \exp\{\alpha^{[m]} \mathbb{1}(y_i \neq \hat{G}^{[m]}(x_1))\}$;
      - $w_i^{[m]} = \tilde{w}_i / \sum_{i=1}^{N} \tilde{w}_i$;
3. compute the final result,

$$\hat{G}_{\text{AdaBoost}} = \text{sign}(\sum_{m=1}^{m_{\text{stop}}} \alpha^{[m]} \hat{G}^{[m]}(x_1))$$

AdaBoost: example

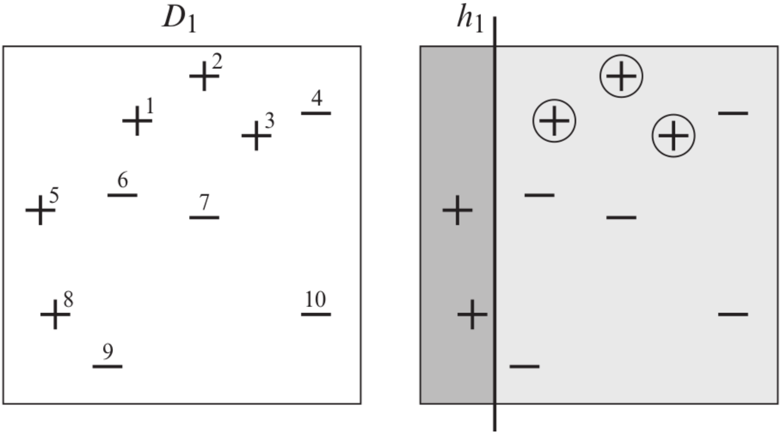


figure from Schapire & Freund (2014)

AdaBoost: example

First iteration:

- apply the classier $G(\cdot)$ on observations with weights:

	1	2	3	4	5	6	7	8	9	10
w_i	$\mathbf{0.10}$	$\mathbf{0.10}$	$\mathbf{0.10}$	0.10	0.10	0.10	0.10	0.10	0.10	0.10

- observations 1, 2 and 3 are misclassified $\Rightarrow$ err$^{[1]} = 0.3$;
- compute $\alpha^{[1]} = 0.5 \log((1 - \text{err}^{[1]})/\text{err}^{[1]}) \approx 0.42$;
- set $w_i = w_i \exp\{\alpha^{[1]} \mathbb{1}(y_i \neq \hat{G}^{[1]}(x_i))\}$:

	1	2	3	4	5	6	7	8	9	10
w_i	0.15	0.15	0.15	0.07	0.07	0.07	0.07	0.07	0.07	0.07

AdaBoost: example

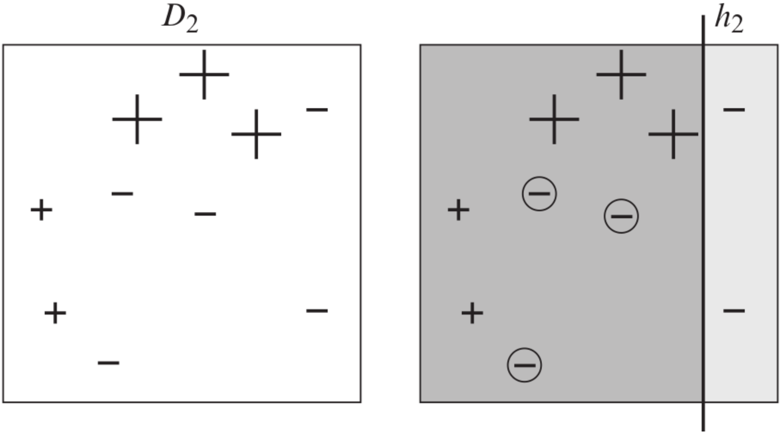


figure from Schapire & Freund (2014)

AdaBoost: example

Second iteration:

- apply classifier $G(\cdot)$ on re-weighted observations $(w_i/\sum_i w_i)$:

	1	2	3	4	5	6	7	8	9	10
w_i	0.17	0.17	0.17	0.07	0.07	**0.07**	**0.07**	0.07	**0.07**	0.07

- observations 6, 7 and 9 are misclassified $\Rightarrow$ $\text{err}^{[2]} \approx 0.21$;
- compute $\alpha^{[2]} = 0.5 \log((1 - \text{err}^{[2]})/\text{err}^{[2]}) \approx 0.65$;
- set $w_i = w_i \exp\{\alpha^{[2]} \mathbb{1}(y_i \neq \hat{G}^{[2]}(x_i))\}$:

	1	2	3	4	5	6	7	8	9	10
w_i	0.09	0.09	0.09	0.04	0.04	0.14	0.14	0.04	0.14	0.04

AdaBoost: example

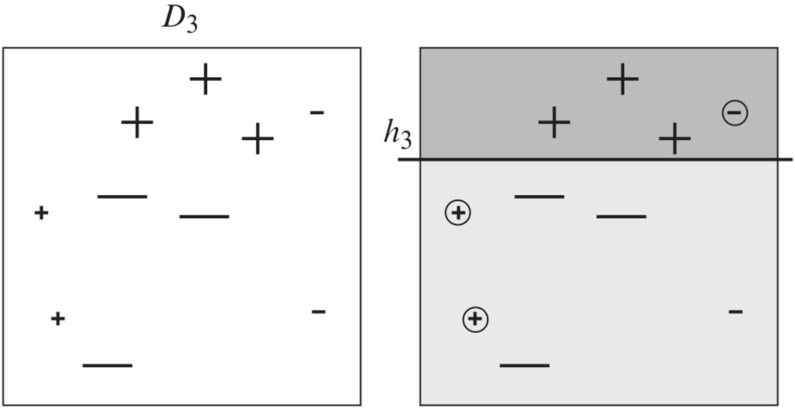


figure from Schapire & Freund (2014)

AdaBoost: example

Third iteration:

- apply classifier $G(\cdot)$ on re-weighted observations $(w_i / \sum_i w_i)$:

	1	2	3	4	5	6	7	8	9	10
w_i	0.11	0.11	0.11	**0.05**	**0.05**	0.17	0.17	**0.05**	0.17	0.05

- observations 4, 5 and 8 are misclassified $\Rightarrow$ err$^{[3]} \approx 0.14$;
- compute $\alpha^{[3]} = 0.5 \log((1 - \text{err}^{[3]})/\text{err}^{[3]}) \approx 0.92$;
- set $w_i = w_i \exp\{\alpha^{[3]} \mathbb{1}(y_i \neq \hat{G}^{[3]}(x_i))\}$:

	1	2	3	4	5	6	7	8	9	10
w_i	0.04	0.04	0.04	0.11	0.11	0.07	0.07	0.11	0.07	0.02

AdaBoost: example

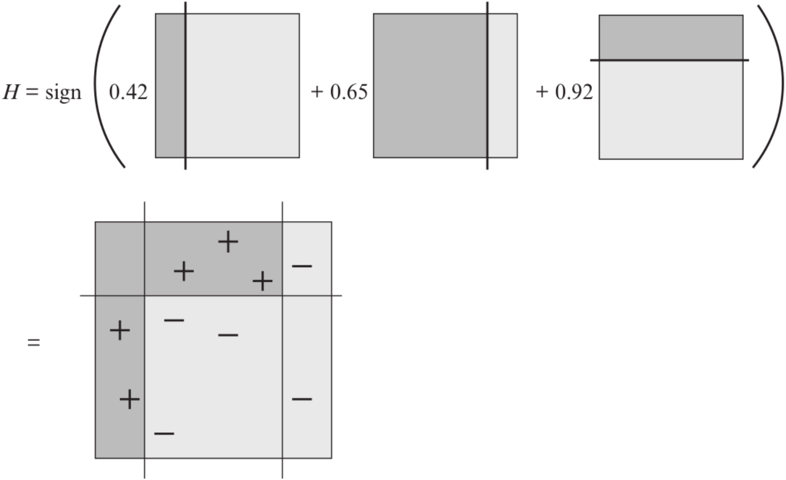
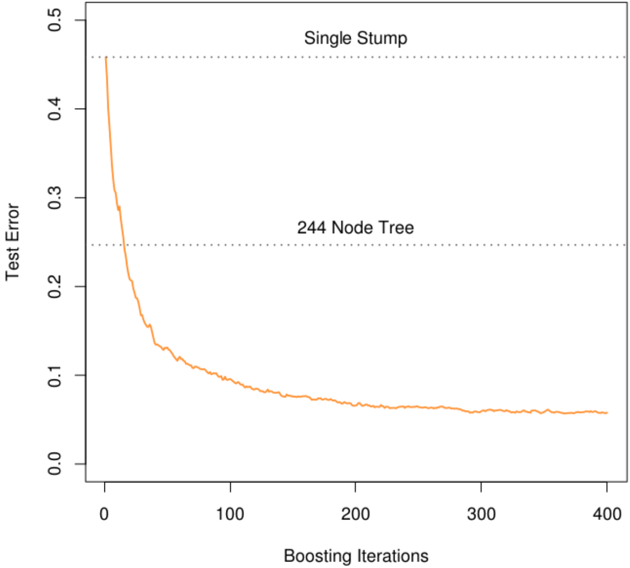


figure from Schapire & Freund (2014)

AdaBoost: example



Statistical Boosting: Boosting as a forward stagewise additive modelling

The statistical view of boosting is based on the concept of **forward stagewise additive modelling**:

- minimizes a loss function $L(y_i, f(x_i))$;
- using an additive model,
$$f(x) = \sum_{m=1}^{M} \beta_m b(x; \gamma_m);$$
  - $b(x; \gamma_m)$ is the basis, or weak learner;
- at each step,
$$(\beta_m, \gamma_m) = \text{argmin}_{\beta,\gamma} \sum_{i=1}^{N} L(y_i, f_{m-1}(x_i) + \beta b(x_i; \gamma));$$
- the estimate is updated as $f_m(x) = f_{m-1}(x) + \beta_m b(x; \gamma_m)$
- e.g., in AdaBoost, $\beta_m = \alpha_m/2$, $b(x; \gamma_m) = G(x)$;

Statistical Boosting: Boosting as a forward stagewise additive modelling

(see notes)

Statistical Boosting: Why exponential loss?

The statistical view of boosting:

- allows to interpret the results;
- by studying the properties of the exponential loss;

It is easy to show that

$$f^*(x) = \text{argmin}_{f(x)} E_{Y|X=x}[e^{-Yf(x)}] = \frac{1}{2}\log\frac{Pr(Y=1|x)}{Pr(Y=-1|x)},$$

i.e.

$$Pr(Y=1|x) = \frac{1}{1+e^{-2f^*(x)}};$$

therefore AdaBoost estimates 1/2 the log-odds of $Pr(Y=1|x)$.

Statistical Boosting: Why exponential loss?

Note:

- the exponential loss is not the only possible loss-function;
- deviance (cross/entropy): binomial negative log-likelihood,

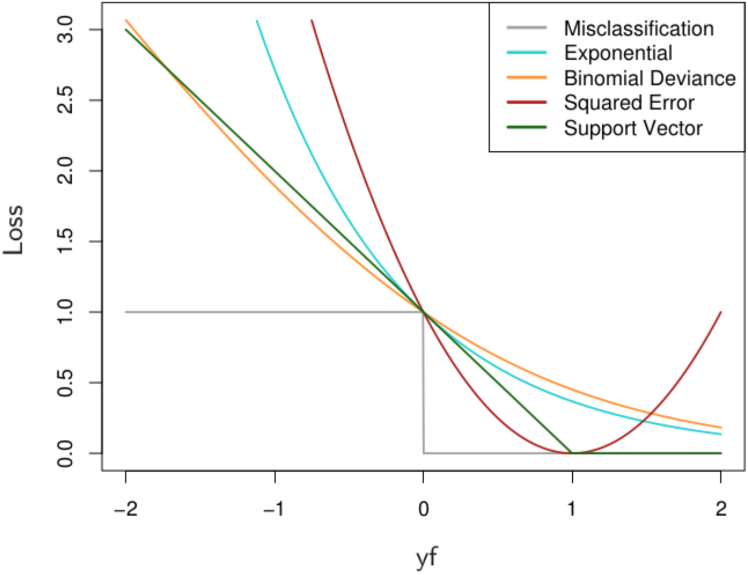
$$-\ell(\pi_x) = -y' \log(\pi_x) - (1 - y') \log(1 - \pi_x),$$

  where:
  - $y' = (y + 1)/2$, i.e., $y' \in \{0, 1\}$;
  - $\pi_x = \Pr(Y = 1|X = x) = \frac{e^{f(x)}}{e^{-f(x)}+e^{f(x)}} = \frac{1}{1+e^{-2f(x)}}$;
- equivalently,

$$-\ell(\pi_x) = \log(1 + e^{-2yf(x)}).$$

- same population minimizers for $E[-\ell(\pi_x)]$ and $E[e^{-Yf(x)}]$.

Statistical Boosting: Why exponential loss?



Statistical Boosting: Gradient boosting

We saw that AdaBoost iteratively minimizes a loss function.

In general, consider

- $L(f) = \sum_{i=1}^{N} L(y_i, f(x_i))$;
- $\hat{f} = \text{argmin}_f L(f)$;
- the minimization problem can be solved by considering

$$f_{m_{\text{stop}}} = \sum_{m=0}^{m_{\text{stop}}} h_m$$

where:

  - $f_0 = h_0$ is the initial guess;
  - each f_m improves the previous f_{m-1} though h_m;
  - h_m is called "step".

Statistical Boosting: steepest descent

The steepest descent chooses

$$h_m = -\rho_m g_m$$

where

- $g_m \in \mathbb{R}^N$ is the gradient descent of $L(f)$ evaluated at $f = f_{m-1}$ and represents the direction for the minimization,

$$g_{im} = \left. \frac{\partial L(y_i, f(x_i))}{\partial f(x_i)} \right|_{f(x_i) = f_{m-1}(x_i)}$$

- ρ_m is a scalar and tells "how much" to minimize

$$\rho_m = \text{argmin}_\rho L(f_{m-1} - \rho g_m).$$

Statistical Boosting: example

Consider the linear Gaussian regression case:

- $L(y, f(x)) = \frac{1}{2}\sum_{i=1}^{N}(y_i - f(x_i))^2$;
- $f(x) = X^T\beta$;
- initial guess: $\beta \equiv 0$.

Therefore:

- $g = \frac{\partial \frac{1}{2}\sum_{i=1}^{N}(y_i - f(x_i))^2}{\partial f(x_i)} = -(y - X^T\beta)$;
- $g_m = -\left.(y - X^T\beta)\right|_{\beta=0} = -y$;
- $\rho_m = \text{argmin}_\rho \frac{1}{2}(y - \rho y)^2 \rightarrow \rho_m = X(X^TX)^{-1}X^T$.

Note:

- overfitting!

Statistical Boosting: shrinkage

To regularize the procedure, a shrinkage factor is introduced,

$$f_m(x) = f_{m-1}(x) + \nu h_m$$

where $0 < \nu < 1$.

Moreover, h_m can be a general weak learner (base learner):

- stump;
- spline;
- ...
- the idea is to fit the base learner to the gradient descent to iteratively minimize the loss function.

Statistical Boosting: Gradient boosting

Gradient boosting algorithm:

1. initialize the estimate, e.g., $f_0(x) = 0$;
2. for $m = 1, \dots, m_{\text{stop}}$,
   - 2.1 compute the negative gradient vector,
     $u_m = - \frac{\partial L(y, f(x))}{\partial f(x)}\Big|_{f(x) = \hat{f}_{m-1}(x)}$;
   - 2.2 fit the base learner to the negative gradient vector, $h_m(u_m, x)$;
   - 2.3 update the estimate, $f_m(x) = f_{m-1}(x) + \nu h_m(u_m, x)$.
3. final estimate, $\hat{f}_{m_{\text{stop}}}(x) = \sum_{m=1}^{m_{\text{stop}}} \nu h_m(u_m, x)$

Note:

- $u_m = -g_m$
- $\hat{f}_{m_{\text{stop}}}(x)$ is a GAM.

Statistical Boosting: example

Consider again the linear Gaussian regression case:

- $L(y, f(X)) = \frac{1}{2}\sum_{i=1}^{N}(y_i - f(x_i, \beta))^2$, $f(x_i, \beta) = x_i\beta$;
- $h(y, X) = X(X^TX)^{-1}X^Ty$.

Therefore:

- initialize the estimate, e.g., $\hat{f}_0(X, \beta) = 0$;
- $m = 1$,
  - $u_1 = -\left.\frac{\partial L(y, f(X,\beta))}{\partial f(X,\beta)}\right|_{f(X,\beta)=\hat{f}_0(X,\beta)} = (y - 0) = y$;
  - $h_1(u_1, X) = X(X^TX)^{-1}X^Ty$;
  - $\hat{f}_1(x) = 0 + \nu X(X^TX)^{-1}X^Ty$.
- $m = 2$,
  - $u_2 = -\left.\frac{\partial L(y, f(X,\beta))}{\partial f(X,\beta)}\right|_{f(X,\beta)=\hat{f}_1(X,\beta)} = (y - X^T(\nu\hat{\beta}))$;
  - $h_2(u_2, X) = X(X^TX)^{-1}X^T(y - X^T(\nu\hat{\beta}))$;
  - update the estimate, $\hat{f}_2(X, \beta) =$ $\nu X(X^TX)^{-1}X^Ty + \nu X(X^TX)^{-1}X^T(y - X^T(\nu\hat{\beta}))$.

Statistical Boosting: remarks

Note that:

- we do not need to have a linear effects,
  - $h(y, X)$ can be, e.g., a spline;
- using $f(X, \beta) = X^T\beta$, it makes more sense to work with β:
  1. initialize the estimate, e.g., $\hat{\beta}_0 = 0$;
  2. for $m = 1, \dots, m_{\text{stop}}$,
     - 2.1 compute the negative gradient vector, $u_m = -\left.\frac{\partial L(y, f(X,\beta))}{\partial f(X,\beta)}\right|_{\beta=\hat{\beta}_{m-1}}$;
     - 2.2 fit the base learner to the negative gradient vector, $b_m(u_m, X) = (X^T X)^{-1} X^T u_m$;
     - 2.3 update the estimate, $\hat{\beta}_m = \hat{\beta}_{m-1} + \nu b_m(u_m, x)$.
  3. final estimate, $\hat{f}_{m_{\text{stop}}}(x) = X^T\hat{\beta}_m$.

Statistical Boosting: remarks

Further remarks:

- for $m_{\text{stop}} \to \infty$, $\hat{\beta}_{m_{\text{stop}}} \to \hat{\beta}_{OLS}$;
- the shrinkage is controlled by both m_{stop} and ν;
- usually ν is fixed, $\nu = 0.1$
- m_{stop} is computed by cross-validation:
  - it controls the model complexity;
  - we need an early stop to avoid overfitting;
  - if it is too small $\to$ too much bias;
  - if it is too large $\to$ too much variance;

- the predictors must be centred, $E[X_j] = 0$.

References I

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