Ensemble Model

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Contents

Notation

symbol	meaning
$a, b, c, N \ldots$	scalar number
$\boldsymbol{w}, \boldsymbol{v}, \boldsymbol{x}, \boldsymbol{y} \ldots$	column vector
$\boldsymbol{X}, \boldsymbol{Y} \ldots$	matrix
$\mathbb{R}$	set of real numbers
$\mathbb{Z}$	set of integer numbers
$\mathbb{N}$	set of natural numbers
$\mathbb{R}^D$	set of vectors
$\mathcal{X}, \mathcal{Y}, \ldots$	set
$\mathcal{A}$	algorithm

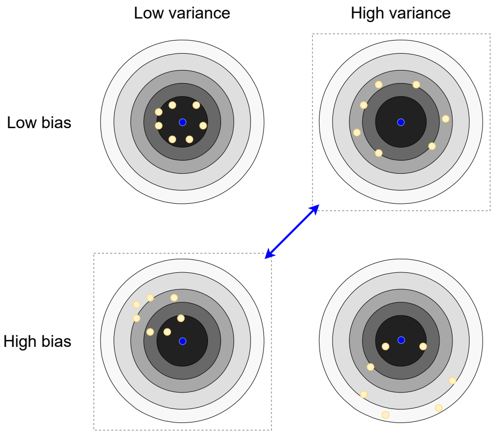
operator	meaning
$\boldsymbol{w}^\mathsf{T}$	transpose
$\boldsymbol{X}\boldsymbol{Y}$	matrix multiplication
$\boldsymbol{X}^{-1}$	inverse

Big Picture

Ensemble Model

Bias vs. Variance

- Low-bias models tend to have high variance, and vice versa.



Basics of Ensembles

Concept 1

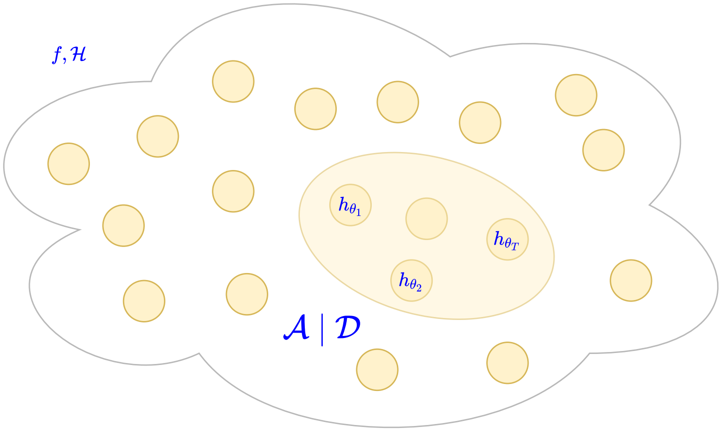
Instead of providing **one model,** an **ensemble** approach proposes **many models** to the same problem, and **combine** them

- The simplest ensemble H over models $\{h_i \in \mathcal{H}, i = 1 \ldots T\}$

$$H(\boldsymbol{x}) = \sum_{i=1}^{T} \alpha_i h_i(\boldsymbol{x}) \text{ with } \sum_{i=1}^{T} \alpha_i = 1 \quad (1)$$

- Why should this be a good idea?
  - combine models $\rightarrow$ reduce the variance $\rightarrow$ enhance expected performance.
- However, increase the performance cost

Basics of Ensembles (cont.)



Why Does it Work?

It has been shown that the expected risk of the average of a set of models is better than the average of the expected risk of these models

- Let us consider the simplest ensemble H over models h_i

$$H(\boldsymbol{x}) = \sum_{i=1}^{T} \alpha_i h_i(\boldsymbol{x}) \text{ with } \sum_{i=1}^{T} \alpha_i = 1 \tag{2}$$

- The MSE risk of h_i at $\boldsymbol{x}$ is

$$e_i(\boldsymbol{x}) = \mathbb{E}_y[(y - h_i(\boldsymbol{x}))^2] \tag{3}$$

Why Does it Work? (cont.)

- The average risk $\bar{e}(\boldsymbol{x})$ of a model is

$$\bar{e}(\boldsymbol{x}) = \sum_i \alpha_i e_i(\boldsymbol{x}) \tag{4}$$

- The average risk $e(\boldsymbol{x})$ of the ensemble is

$$e(\boldsymbol{x}) = \mathbb{E}_y[(y - H(\boldsymbol{x}))^2] \tag{5}$$

- Let us define diversity

$$d_i(\boldsymbol{x}) = (h_i(\boldsymbol{x}) - H(\boldsymbol{x}))^2 \tag{6}$$

- The average diversity is

$$\bar{d}(\boldsymbol{x}) = \sum_i \alpha_i d_i(\boldsymbol{x}) \tag{7}$$

Why Does it Work? (cont.)

- It can then be shown that

$$e(\boldsymbol{x}) = \bar{e}(\boldsymbol{x}) - \bar{d}(\boldsymbol{x}) \quad (8)$$

$$e(\boldsymbol{x}) < \bar{e}(\boldsymbol{x}) \quad (9)$$

Bagging

- Bootstrap
- Algorithm
- Random Forests

Bagging

Underlying idea

A part of the **variance** is due to the specific choice of the training data set

- Let us create many **similar** training data sets,
- For each of them, let us train a new function f_i
- The final function will be the *average* of each function outputs.

- How similar? using **bootstrap aggregating**

Bootstrap

Concept 2

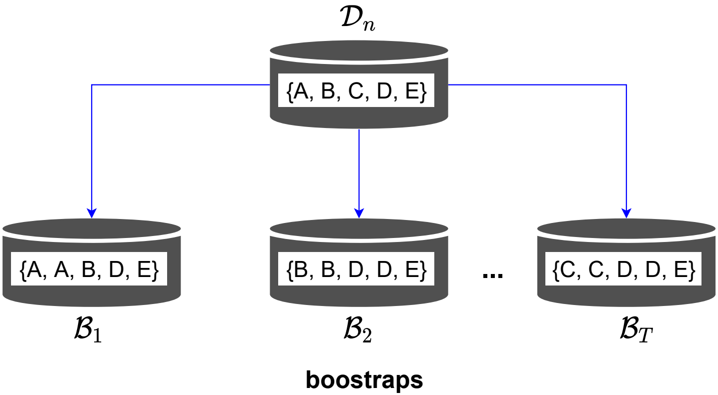
Given a data set $\mathcal{D}_n$ with n examples drawn from $p(\mathcal{Z}) = p(\mathcal{X}, \mathcal{Y})$, a bootstrap $\mathcal{B}_i, i = 1 \ldots T$ of $\mathcal{D}_n$ also contains n examples:

for $j = 1 \to n$

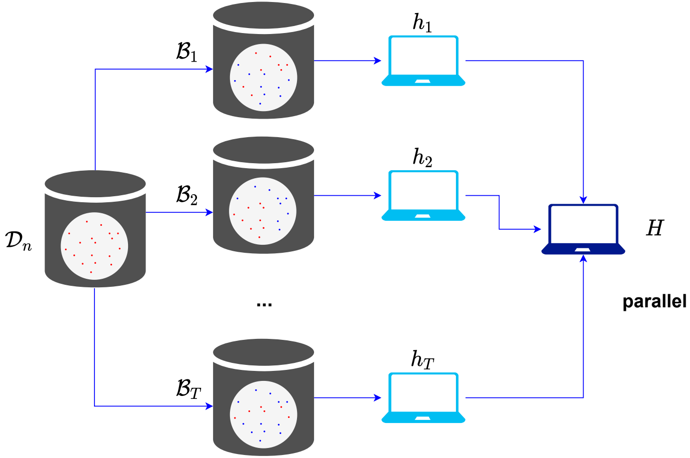
the j-th example of B_i is drawn independently with replacement from $\mathcal{D}_n$

- Some examples from $\mathcal{D}_n$ are in multiple copies in $\mathcal{B}_i$
- Some examples from $\mathcal{D}_n$ are not in $\mathcal{B}_i$
- The examples were i.i.d. drawn from $p(Z) \to$ the datasets $\mathcal{B}_i$ are as plausible as $\mathcal{D}_n$, but drawn from $\mathcal{D}_n$ instead of $p(Z)$.

Example


$\mathcal{D}_n$
{A, B, C, D, E}
{A, A, B, D, E}
{B, B, D, D, E}
...
{C, C, D, D, E}
$\mathcal{B}_1$
$\mathcal{B}_2$
$\mathcal{B}_T$
boostraps

Diagram


$\mathcal{D}_n$
$\mathcal{B}_1$
$\mathcal{B}_2$
...
$\mathcal{B}_T$
h_1
h_2
h_T
H
parallel

Algorithm

Training:

- Given a training set $\mathcal{D}_n$, create T bootstraps $\mathcal{B}_i$ of $\mathcal{D}_n$
- For each bootstrap $\mathcal{B}_i$, select

$$h_i = \arg\min_{h \in \mathcal{H}} E(h \mid \mathcal{B}_i) \tag{10}$$

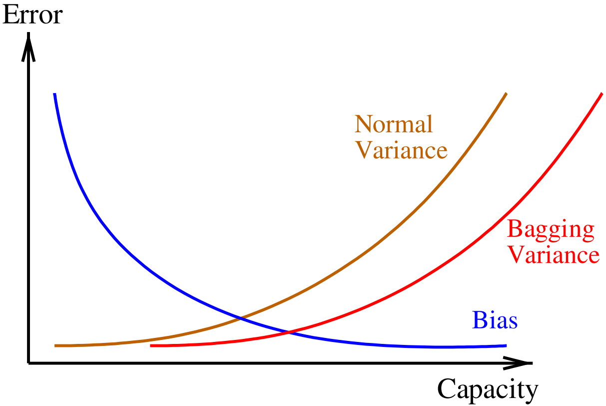
Running:

- Given an input $\boldsymbol{x}$, the corresponding output $\hat{y}$ is:

$$\hat{y} = H(\boldsymbol{x}) = \frac{1}{T} \sum_{i=1}^{T} h_i(\boldsymbol{x}) \tag{11}$$

Bias + Variance

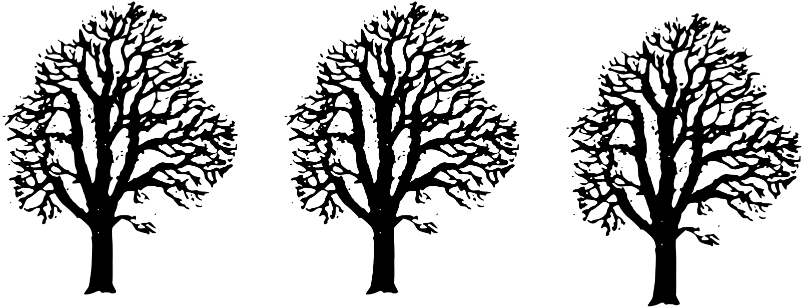
- **Analysis**: if generalization error is decomposed into **bias** and **variance** terms then **bagging reduces variance**.



Random Forests

Concept 3

A **random forest** is an ensemble of decision trees.



Random Forests (cont.)

Each decision tree h_i is trained as follows:

- Create a **bootstrap** of the training set
- Select a subset $m \ll d$ input variables as **potential** split nodes (m is constant over all trees)
- No pruning of the trees

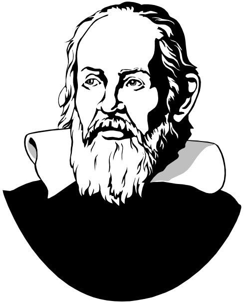
A decision is taken by **voting** amongst the trees

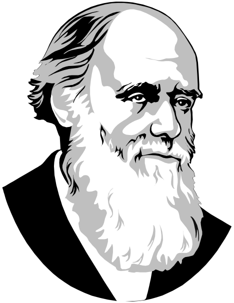
- Somehow, m controls the capacity.

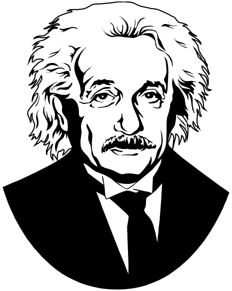
Boosting

- AdaBoost
- Face Detection

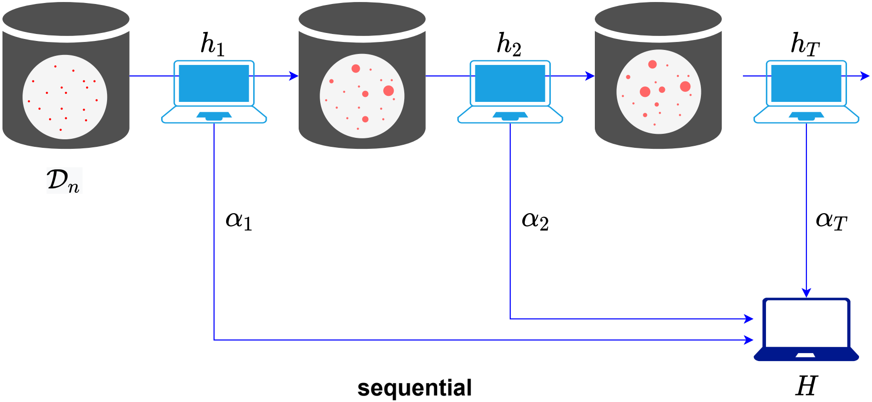
Big Picture







Diagram



Weak vs. Strong Learning Model

Concept 4

A learning model is **strong** iff every hypothesis h has low error

Concept 5

A learning model is **weak** iff every hypothesis h has high error

Examples of weak classifiers:

- Simple decision trees such as **stumps**
- Simple neural networks such as **perceptrons**
- Haar-like features

Boosting

Boosting involves three elements:

- A loss function to be optimized $\ell(.,.)$
- A set of weak learners $\{h_t(x)\}$
- An additive model $H(x)$ to add weak learners to minimize the loss function

$$H(x) = \sum_{t=1}^{T} \alpha_t h_t(x) \tag{12}$$

Loss function

- Square loss
$$\ell(\hat{y}, y) = (\hat{y} - y)^2 \tag{13}$$
- Absolute loss
$$\ell(\hat{y}, y) = |\hat{y} - y| \tag{14}$$
- Huber loss
$$\ell(\hat{y}, y) = \begin{cases} \frac{1}{2}(\hat{y} - y)^2 & (\hat{y} - y) \leq \delta \\ \delta(|\hat{y} - y| - \delta/2) & (\hat{y} - y) > \delta \end{cases} \tag{15}$$
- Exponential loss
$$\ell(\hat{y}, y) = e^{-\hat{y}\, y} \tag{16}$$

Algorithm

- **Initialize** $H_0 \leftarrow \emptyset$ or α_0
- At each time step t,
  - **Choose** h_t given the performance obtained by previous H_{t-1}.
  - **Train** a new weak classifier
  - **Find** the new weight α_t by minimizing the loss function

$$H_t \leftarrow H_{t-1} + \alpha_t h_t \tag{17}$$

AdaBoost

Concept 6

AdaBoost, short for Adaptive Boosting, is the most popular algorithm in the family of **boosting** algorithms

- **Simplest framework**: binary classification $H(x)$
- **Simplest requirement**: each weak classifier $y = h_t(x)$, $y \in \{-1, +1\}$ should perform better than chance
- **Loss function**:

$$\ell((H(x), y)) = e^{-yH(x)} \tag{18}$$

Algorithm

Inputs: training data $\mathcal{D} = \{(\boldsymbol{x}_1, y_1), \cdots, (\boldsymbol{x}_N, y_N)\}$ and a set of weak binary classifiers $\{h_i \in \mathcal{H}\}$

Initialize the weights' distribution of training data

$$(w_1^{(1)}, w_2^{(1)}, \cdots, w_N^{(1)}) = \left(\frac{1}{N}, \frac{1}{N}, \cdots, \frac{1}{N}\right) \tag{19}$$

Iterate over $t = 1, 2, \ldots, T$, use training data with current weights' distribution

1. **Find** a weak classifier $h_t(\boldsymbol{x})$ that that minimizes the error rate e_t of over the training data

$$e_t = P(h_t(\boldsymbol{x}_i) \neq y_i) = \sum_{i=1}^{N} w_i^{(t)} \mathbb{I}(h_t(\boldsymbol{x}_i) \neq y_i) \tag{20}$$

Algorithm (cont.)

2. **Compute** the weight of classifier $h_t(\boldsymbol{x})$

$$\alpha_t = \frac{1}{2}\log\frac{1-e_t}{e_t} \tag{21}$$

3. **Update** the weights' distribution of training data

$$w_i^{(t+1)} = w_i^{(t)}\exp(-\alpha_t y_i h_t(\boldsymbol{x}_i)) \tag{22}$$

4. **Normalize** the weights of data points

$$w_i = \frac{w_i}{\sum_i w_i} \tag{23}$$

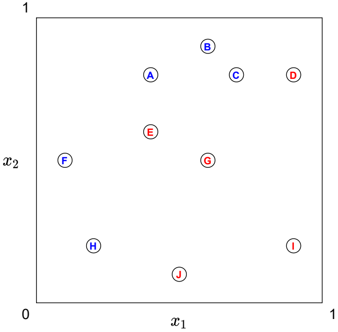
Ensemble T weak classifiers

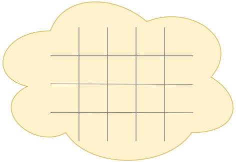
$$\text{sign}\left[H(\boldsymbol{x})\right] = \text{sign}\left[\sum_{t=1}^{T}\alpha_t h_t(\boldsymbol{x})\right] \tag{24}$$

Example

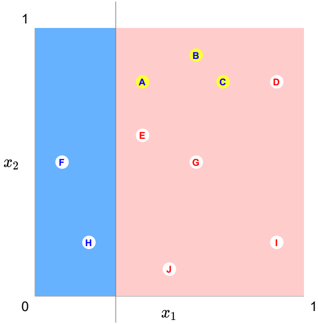
- Given a training data set $\mathcal{D} = \{$A, B, C, D, E, F, G, H, I, J$\}$, find a strong classifier from weak classifiers (vertical or horizontal lines)

#	x_1	x_2	label
A	0.4	0.8	1
B	0.6	0.9	1
C	0.7	0.8	1
D	0.9	0.8	-1
E	0.4	0.6	-1
F	0.1	0.5	1
G	0.6	0.5	-1
H	0.2	0.2	1
I	0.9	0.2	-1
J	0.5	0.1	-1



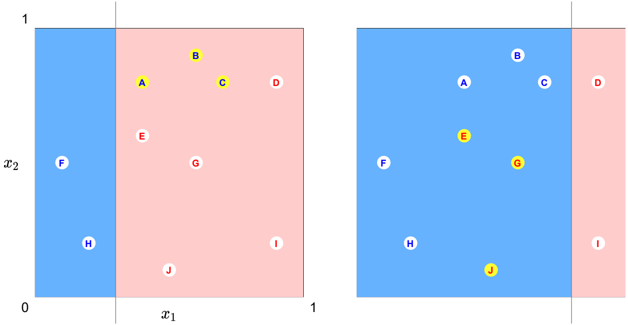


Round 1



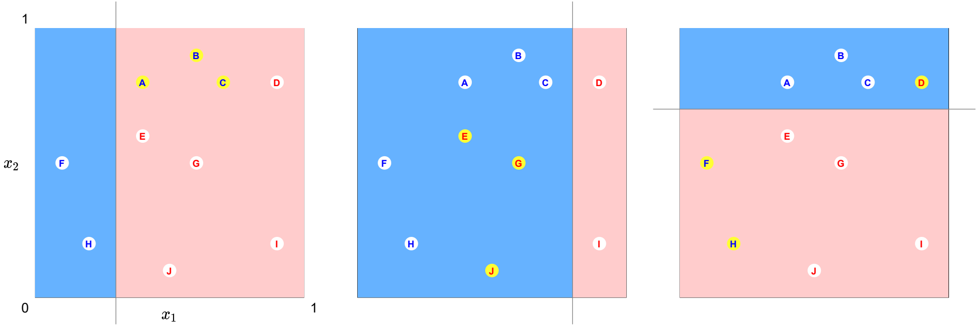
$\epsilon_1 = 0.30, \alpha_1 = 0.42$

Round 2



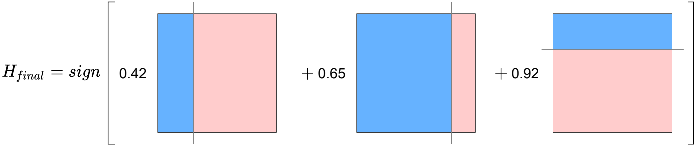
$\epsilon_2 = 0.21, \alpha_2 = 0.65$

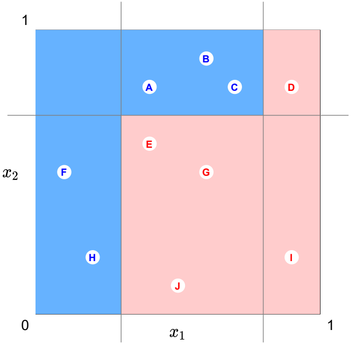
Round 3



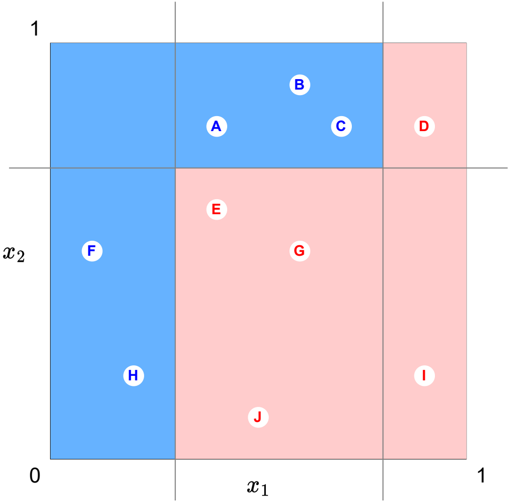
$\epsilon_3 = 0.14, \alpha_3 = 0.92$

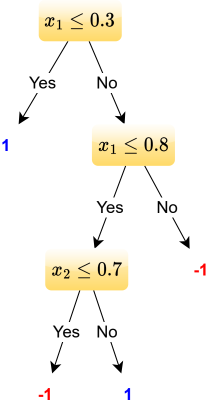
The combined classifier





Tree based classifier





Analysis

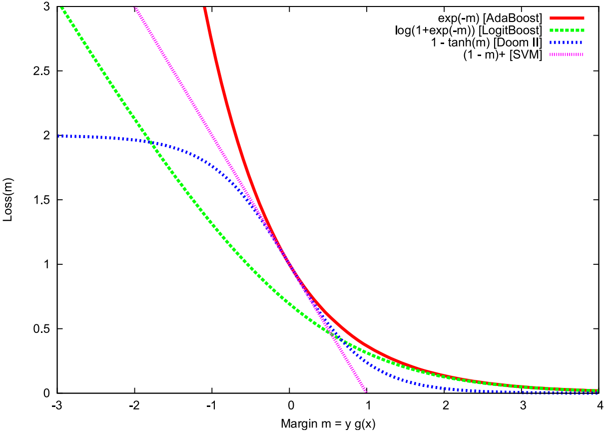
- Selection of α_t comes from minimizing

$$\arg\min_{\alpha_t} \sum_{i=1}^{N} \exp\left(-y_i \left[H_{t-1}(\boldsymbol{x}_i) + \alpha_t h_t(\boldsymbol{x}_i)\right]\right) \tag{25}$$

- If each weak classifier is always better than chance, then AdaBoost can be proven to **converge to 0 training error**
- Even after training error is 0, generalization error continues to improve: the **margin** continues to grow
- **Sampling** can often be replaced by **weighting**

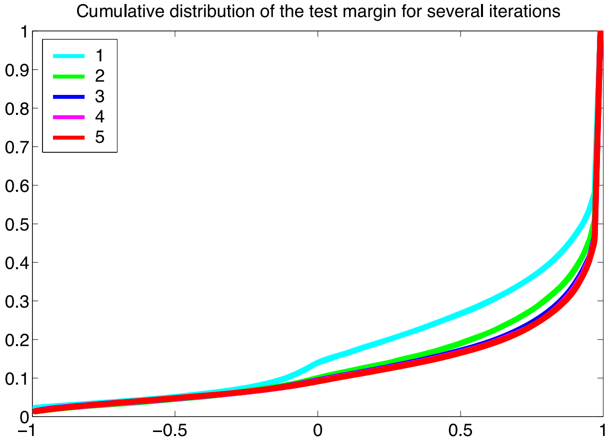
Cost Functions

- Comparison of various cost functions related to AdaBoost



Margin

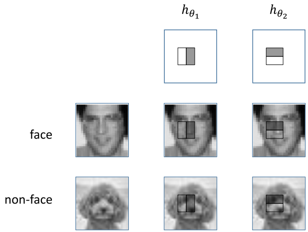
- The AdaBoost margin is defined as the distribution of $y \cdot h(x)$



Face Detection

Face detection framework was proposed in 2001 by Paul Viola and Michael Jones using AdaBoost

- Some hypotheses h_θ



- Haar-like features for each hypothesis

$$h_\theta = \sum_{(x,y)\in \text{dark area}} image(x, y) - \sum_{(x,y)\in \text{white area}} image(x, y) \tag{26}$$

Gradient Boosting

What is Gradient Boosting

$$\textit{\textbf{Gradient Boosting}} = \textit{\textbf{Gradient Descent}} + \textit{\textbf{Boosting}}$$

- In Adaboost, “losses” are identified by high-weight data points
- In Gradient Boosting, “losses” are identified by gradients
- Gradient Boosting can be applied for different problems

$$\text{Regression} \rightarrow \text{Classification} \rightarrow \text{Ranking}$$

Algorithm

Input: training set $\{(x_i, y_i)\}_{i=1}^{n}$ and a differentiable loss function $\ell(y, H(x))$, number of iterations M.

1. Initialize model with a constant value:

$$H_0(x) = \gamma_0 = \arg\min_{\gamma} \sum_{i=1}^{n} \ell(y_i, \gamma). \tag{27}$$

2. For $m = 1$ to M:

    2.1 Compute so-called pseudo-residuals:

$$r_{im} = -\left[\frac{\partial \ell(y_i, H(x_i))}{\partial H(x_i)}\right]_{H(x)=H_{m-1}(x)}, \quad \text{for } i = 1, \ldots, m \tag{28}$$

Algorithm (cont.)

2.2 Fit a base learner (or weak learner, e.g. tree) closed under scaling $h_m(x)$ to pseudo-residuals, i.e. train it using the training set $\{(x_i, r_{im})\}_{i=1}^n$.

2.3 Compute multiplier by solving the following one-dimensional optimization problem:

$$\gamma_m = \arg\min_{\gamma} \sum_{i=1}^{n} \ell\left(y_i, H_{m-1}(x_i) + \gamma h_m(x_i)\right). \tag{29}$$

2.4 Update the model:

$$H_m(x) = H_{m-1}(x) + \gamma_m h_m(x) \tag{30}$$

3. Output $H_M(x)$

Important points to remember

- Bagging is predominantly a variance-reduction technique, while boosting is primarily a bias-reduction technique.
- This explains why bagging is often used in combination with high-variance models such as tree models, whereas boosting is typically used with high-bias models such as linear classifiers.

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