Ensemble Model

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Contents

Notation

symbol	meaning
$a, b, c, N \dots$	scalar number
$\boldsymbol{w}, \boldsymbol{v}, \boldsymbol{x}, \boldsymbol{y} \dots$	column vector
$\boldsymbol{X}, \boldsymbol{Y} \dots$	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
$\mathcal{X}, \mathcal{Y}, \dots$	set
$\mathcal{A}$	algorithm

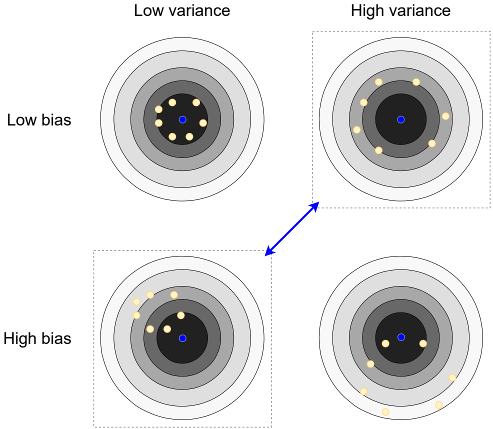
operator	meaning
$\boldsymbol{w}^\intercal$	transpose
$\boldsymbol{X}\boldsymbol{Y}$	matrix multiplication
$\boldsymbol{X}^{-1}$	inverse

Big Picture

Ensemble Model

Bias vs. Variance

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



Basics of Ensembles

Concept 1

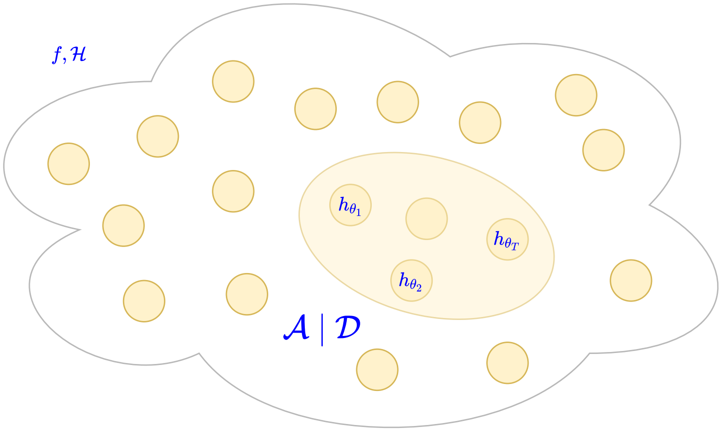
Instead of providing **one model,** an **ensemble** approach proposes **many models** to the same problem, and **combine** them

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

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

- 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

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

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

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

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

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

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

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**

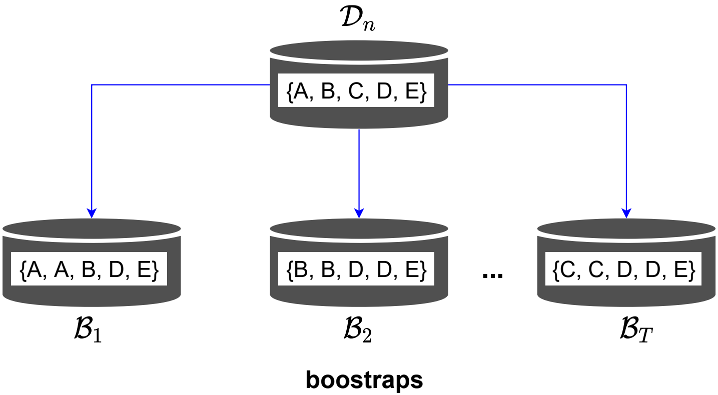
Bootstrap

Concept 2

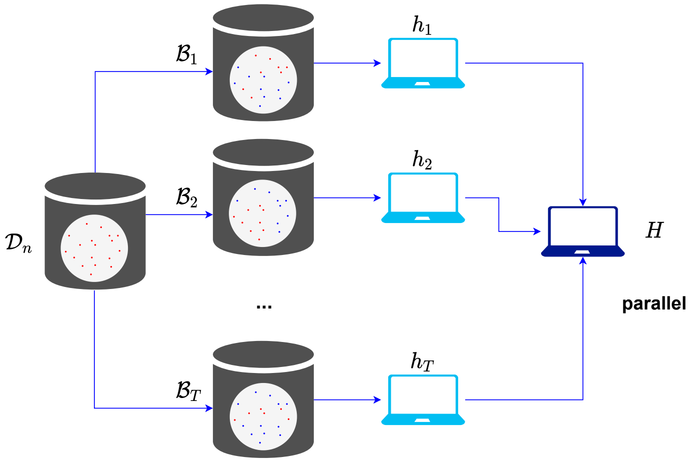
Given a data set $\mathcal{D}_n$ with n examples drawn from $p(\mathcal{Z}) = p(\mathcal{X}, \mathcal{Y})$, a bootstrap $\mathcal{B}_i, i = 1 \dots T$ of $\mathcal{D}_n$ also contains n examples:
for $j = 1 \to n$
the j-th example of B_i is drawn independently with replacement from $\mathcal{D}_n$

- 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

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

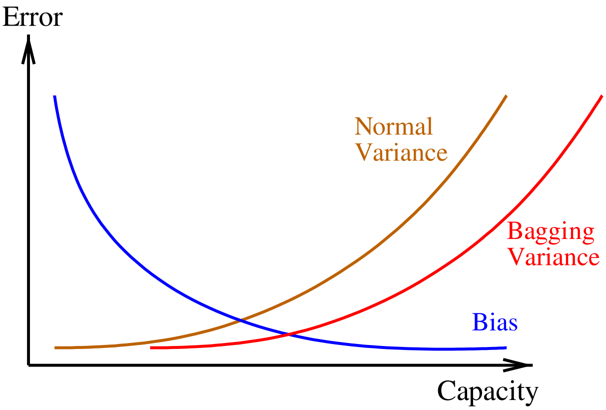
Running:

- 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

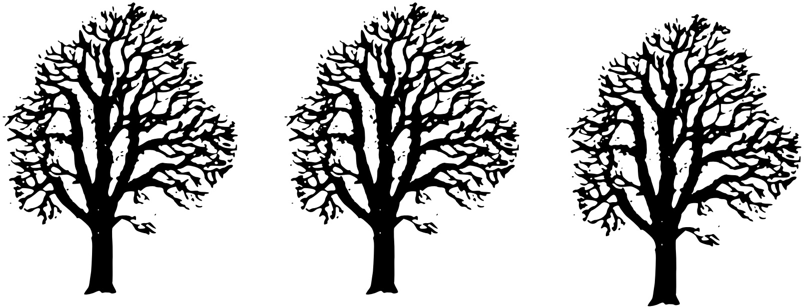
- **Analysis**: if generalization error is decomposed into **bias** and **variance** terms then **bagging reduces variance**.



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

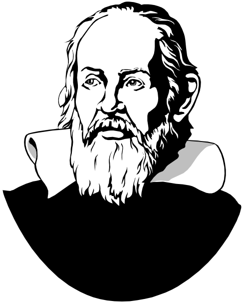
A decision is taken by **voting** amongst the trees

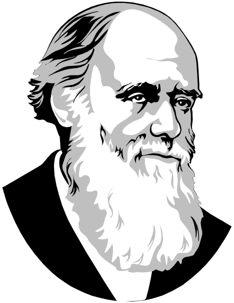
- Somehow, m controls the capacity.

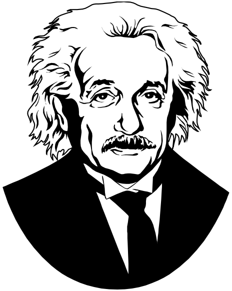
Boosting

- AdaBoost
- Face Detection

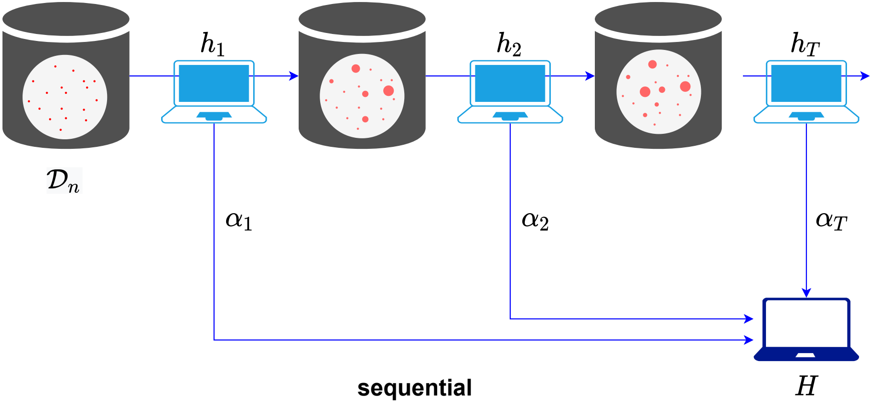
Big Picture







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

- Is there a **boosting** algorithm that turns a weak learner into a strong learner?

Robert Schapire

Yoav Fruend

- Yes! There is boosting algorithm that uses simple (**weak**) classifiers h_t and combine them **iteratively** to a strong classifier.
- General combination classifier

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

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
- **Error function**:

$$\ell((H(x), y)) = e^{-yH(x)} \tag{13}$$

Concepts

- **Initialize** $H_0 \leftarrow \emptyset$
- At each time step t,
  - **Select** h_t given the performance obtained by previous H_{t-1}.
  - **Modify** training sample distribution in order to favor difficult **examples**.
  - **Train** a new weak classifier
  - **Select** the new weight α_t by optimizing a global criterion

$$H_t \leftarrow H_{t-1} + \alpha_t h_t \tag{14}$$

- **Stop** when impossible to find a weak classifier satisfying the simplest condition (being better than chance)

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

$$(w_1^{(1)}, w_2^{(1)}, \cdots, w_N^{(1)}) = \left(\frac{1}{N}, \frac{1}{N}, \cdots, \frac{1}{N}\right) \tag{15}$$

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

$$e_t = P(h_t(\boldsymbol{x}_i) \neq y_i) = \sum_{i=1}^{N} w_i^{(t)} \mathbb{I}(h_t(\boldsymbol{x}_i) \neq y_i) \tag{16}$$

Algorithm (cont.)

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

$$\alpha_t = \frac{1}{2} \log \frac{1 - e_t}{e_t} \tag{17}$$

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

$$w_i^{(t+1)} = w_i^{(t)} \exp(-\alpha_t y_i h_t(\boldsymbol{x}_i)) \tag{18}$$

4. **Normalize** the weights

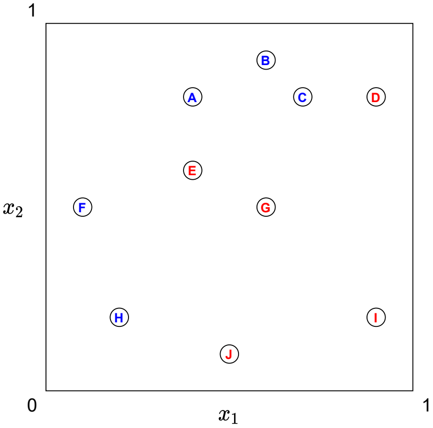
$$w_i = \frac{w_i}{\sum_i w_i} \tag{19}$$

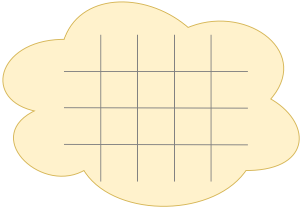
Ensemble T weak classifiers

$$\text{sign}\left[H(\boldsymbol{x})\right] = \text{sign}\left[\sum_{t=1}^{T} \alpha_t h_t(\boldsymbol{x})\right] \tag{20}$$

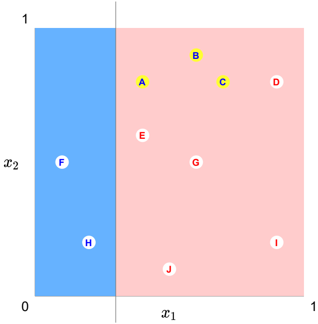
Example

- 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)



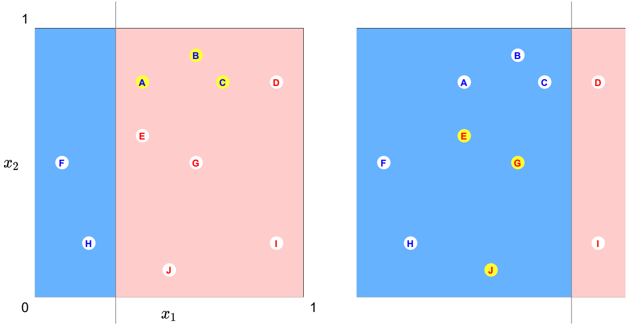


Round 1



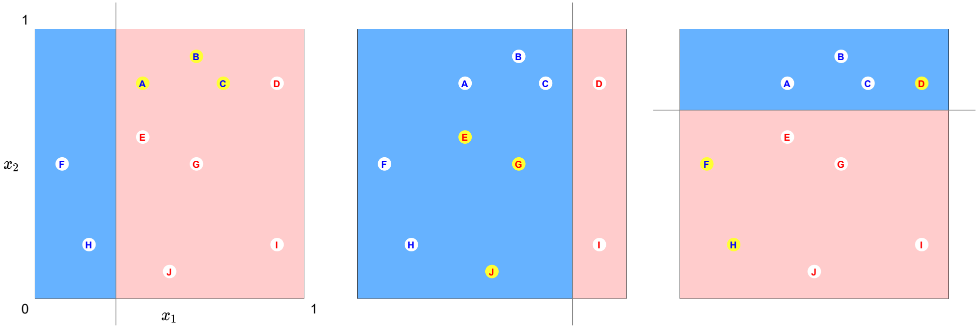
$\epsilon_1 = 0.30, \alpha_1 = 0.42$

Round 2



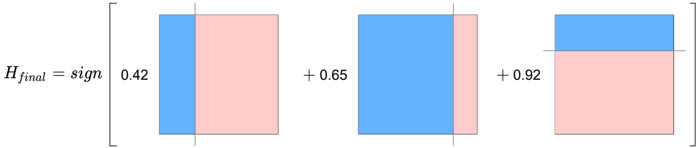
$\epsilon_2 = 0.21, \alpha_2 = 0.65$

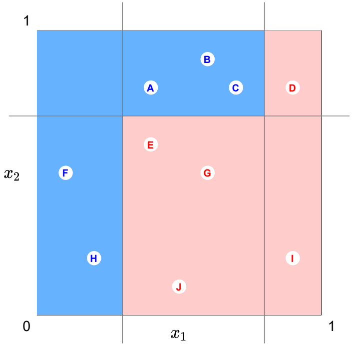
Round 3



$\epsilon_3 = 0.14, \alpha_3 = 0.92$

The combined classifier





Analysis

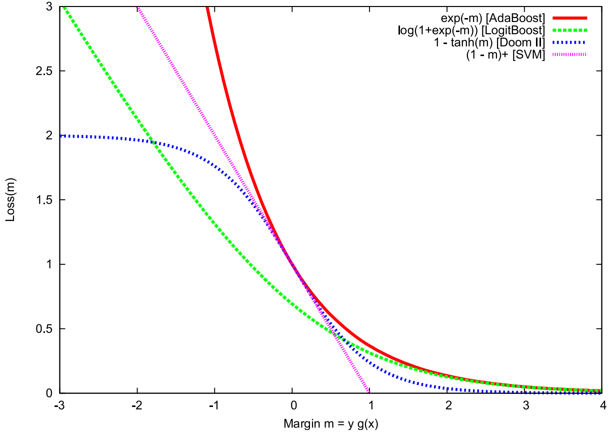
- Selection of α_t comes from minimizing

$$\arg\min_{\alpha_t} \sum_{i=1}^{N} \exp\left(-y_i \left[H_{t-1}(\boldsymbol{x}_i) + \alpha_t h_t(\boldsymbol{x}_i)\right]\right) \tag{21}$$

- 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**

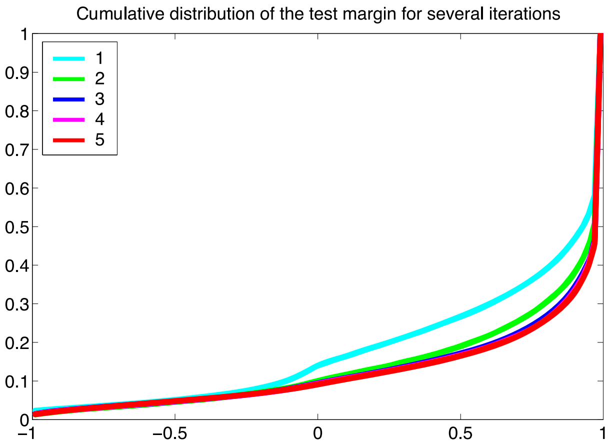
Cost Functions

- Comparison of various cost functions related to AdaBoost



Margin

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



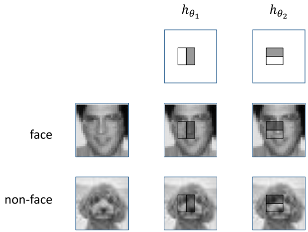
Extensions

- **Multi-class** classification
- **Single-class classification**: estimating quantiles
- **Regression**: transform the problem into a binary classification task
- **Localized Boosting**: similar to **mixtures of experts**

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

$$h_\theta = \sum_{(x,y)\in \text{dark area}} image(x, y) - \sum_{(x,y)\in \text{white area}} image(x, y) \tag{22}$$

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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