11.10.2024

Statistical Methods in AI (CS7.403)

Lecture-19: Ensemble Methods (Bagging, Boosting, Stacking)

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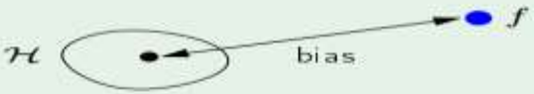
$$\mathbb{E}_{\mathcal{D}}\left[\left(g^{(\mathcal{D})}(\mathbf{x}) - f(\mathbf{x})\right)^2\right] = \underbrace{\mathbb{E}_{\mathcal{D}}\left[\left(g^{(\mathcal{D})}(\mathbf{x}) - \bar{g}(\mathbf{x})\right)^2\right]}_{\text{var}(\mathbf{x})} + \underbrace{\left(\bar{g}(\mathbf{x}) - f(\mathbf{x})\right)^2}_{\text{bias}(\mathbf{x})}$$

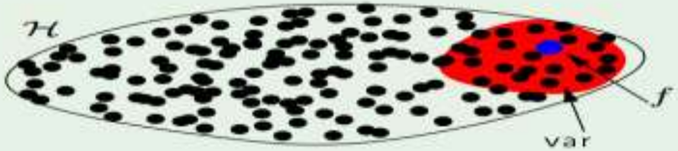
$$\mathbb{E}_{\mathbf{x}}[\text{bias}(\mathbf{x}) + \text{var}(\mathbf{x})]$$

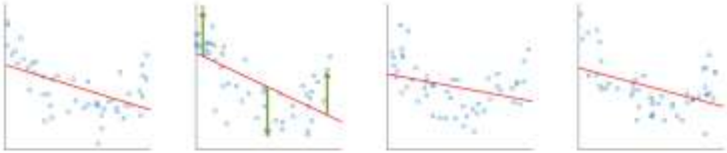
The tradeoff

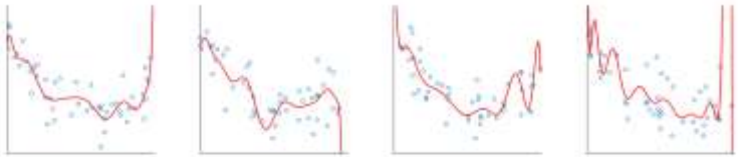
$$\text{bias} = \mathbb{E}_{\mathbf{x}}\left[\left(\bar{g}(\mathbf{x}) - f(\mathbf{x})\right)^2\right]$$

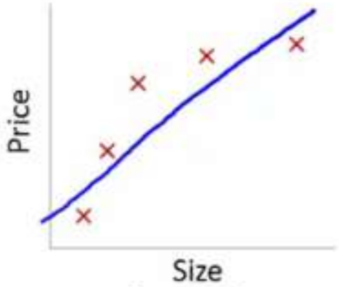
$$\text{var} = \mathbb{E}_{\mathbf{x}}\left[\mathbb{E}_{\mathcal{D}}\left[\left(g^{(\mathcal{D})}(\mathbf{x}) - \bar{g}(\mathbf{x})\right)^2\right]\right]$$





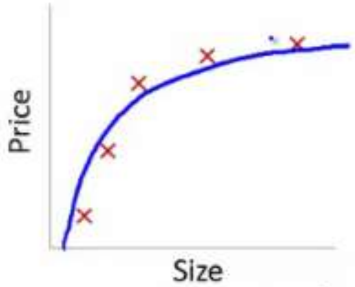






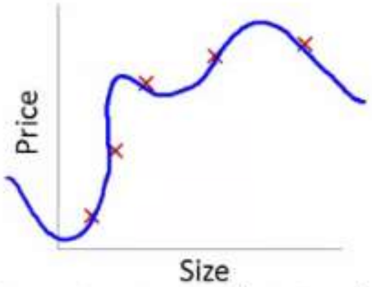
$\theta_0 + \theta_1 x$

High bias
(underfit)



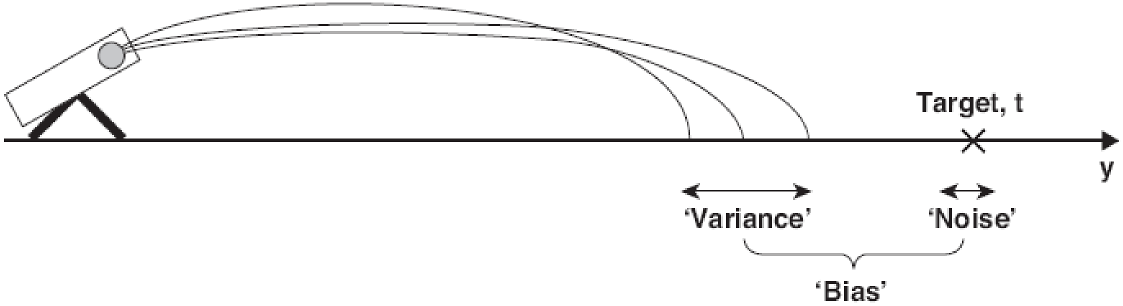
$\theta_0 + \theta_1 x + \theta_2 x^2$

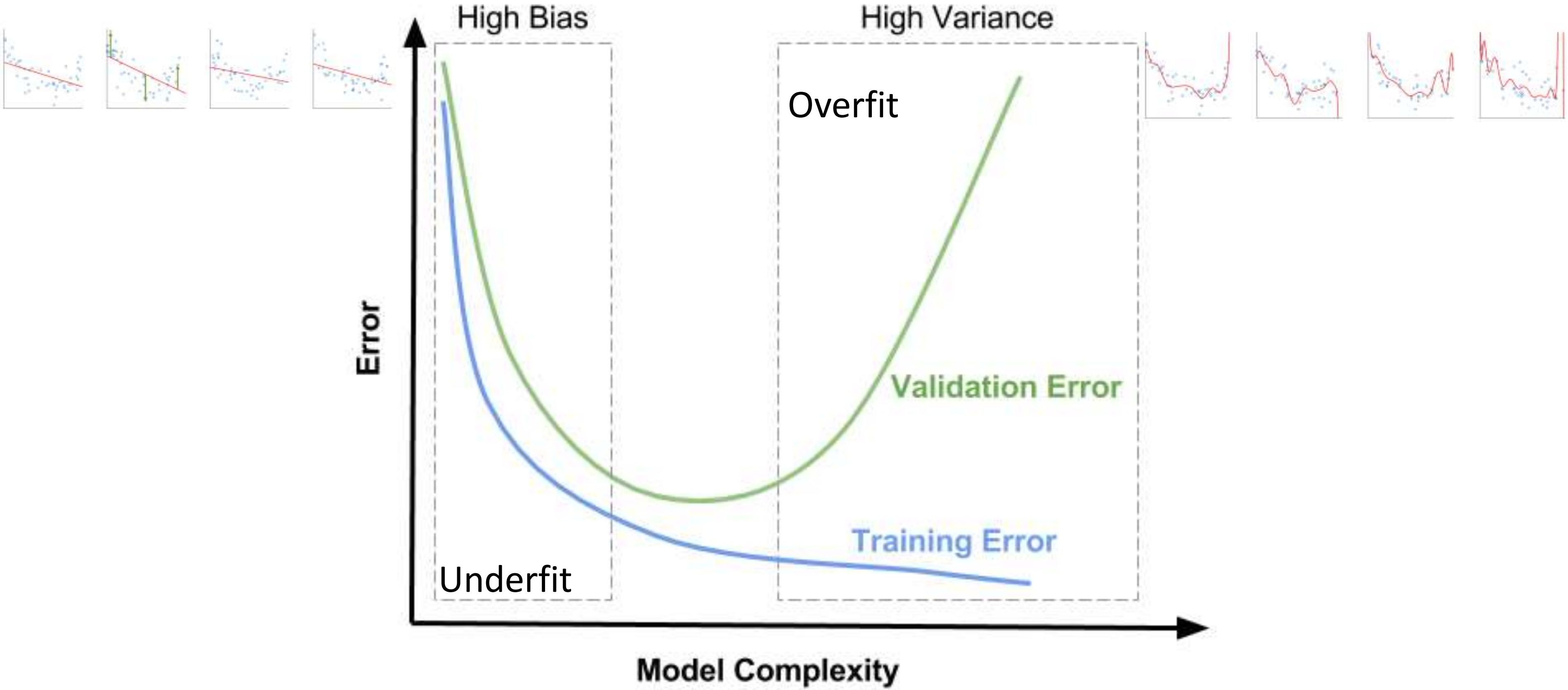
“Just right”



$\theta_0 + \theta_1 x + \theta_2 x^2 + \theta_3 x^3 + \theta_4 x^4$

High variance
(overfit)

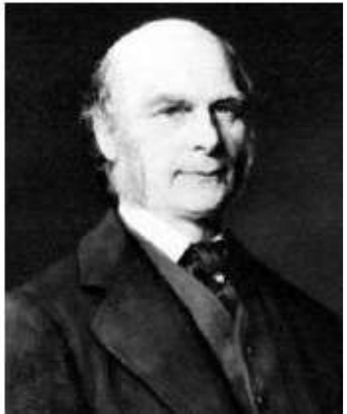




High Bias
High Variance
Overfit
Validation Error
Training Error
Underfit
Error
Model Complexity

Francis Galton

- Galton promoted statistics and invented the concept of correlation.
- In 1906 Galton visited a livestock fair and stumbled upon an intriguing contest.
- An ox was on display, and the villagers were invited to guess the animal's weight.
- Nearly 800 gave it a go and, not surprisingly, not one hit the exact mark: 1,198 pounds.



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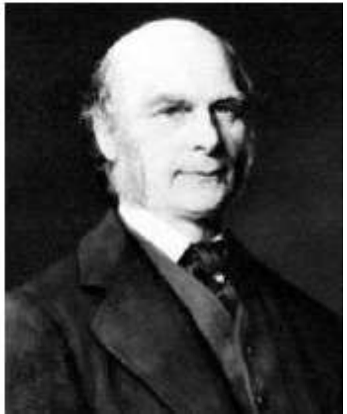
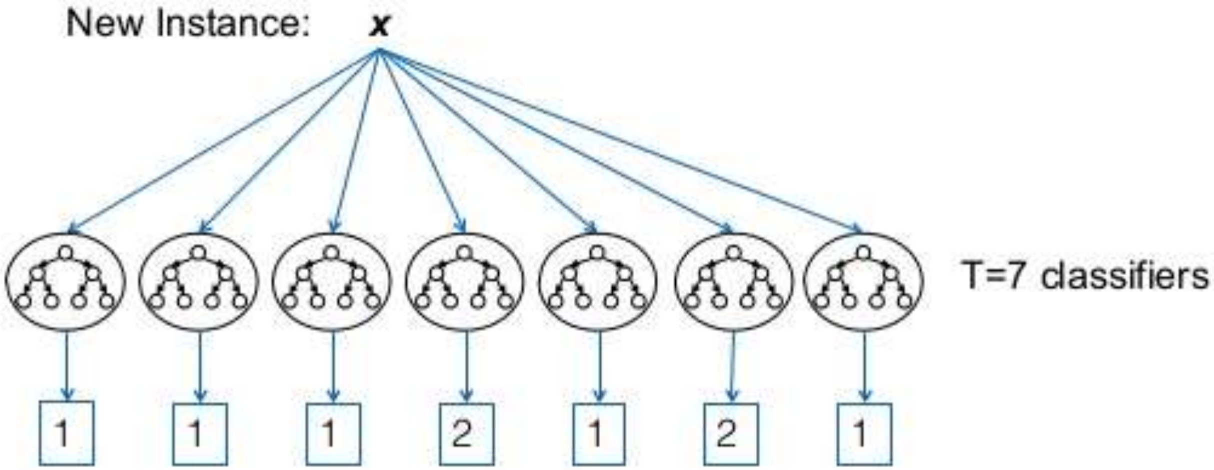
- An ox was on display, and the villagers were invited to guess the animal's weight.
- Nearly 800 gave it a go and, not surprisingly, not one hit the exact mark: 1,198 pounds.
- Astonishingly, however, the average of those 800 guesses came close - very close indeed. It was 1,197 pounds.



Ensemble Learning

- An ensemble is a combination of classifiers that output a final classification.



General idea

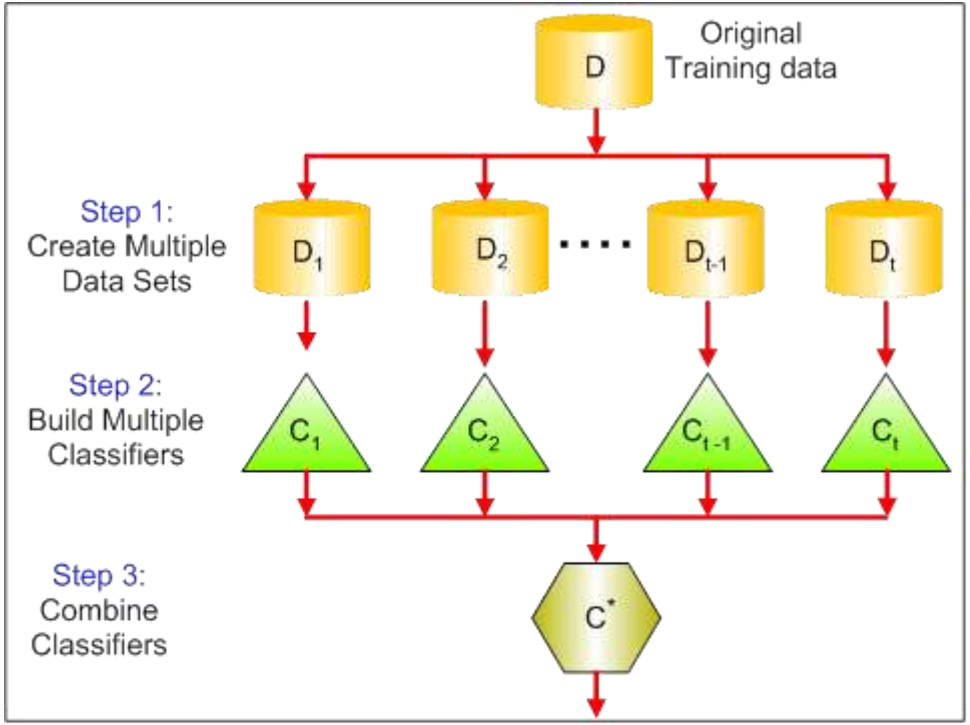
- Generate many classifiers and combine them to get a final classification
- They perform very good. In general better than any of the single learners they are composed of
- The classifiers should be different from one another
- It is important to generate diverse classifiers from the available data

How to build them?

- There are several techniques to build diverse base learners in an ensemble:
  - Use modified versions of the training set to train the base learners

- Modifications of the training set can be generated by
    - Resampling the dataset. By bootstrap sampling (e.g. bagging), weighted sampling (e.g. boosting).

Bootstrap Aggregating (Bagging)



"Bagging Predictors" [Leo Breiman, 1994]
http://statistics.berkeley.edu/sites/default/files/tech-reports/421.pdf

Why does it work?

- Suppose there are 25 base classifiers
  - Each classifier has error rate, $\varepsilon = 0.35$
  - Assume classifiers are independent
  - Probability that the ensemble classifier makes a wrong prediction:

Why does it work?

- Suppose there are 25 base classifiers
  - Each classifier has error rate, ε = 0.35
  - Assume classifiers are independent
  - Probability that the ensemble classifier makes a wrong prediction: $\sum_{i=13}^{25} \binom{25}{i} \varepsilon^i (1-\varepsilon)^{25-i} = 0.06$

```
Input:
  Dataset L
  Ensemble size T

for t=1 to T:
    sample = BootstrapSample(L)
    h_t = TrainClassifier(sample)
```

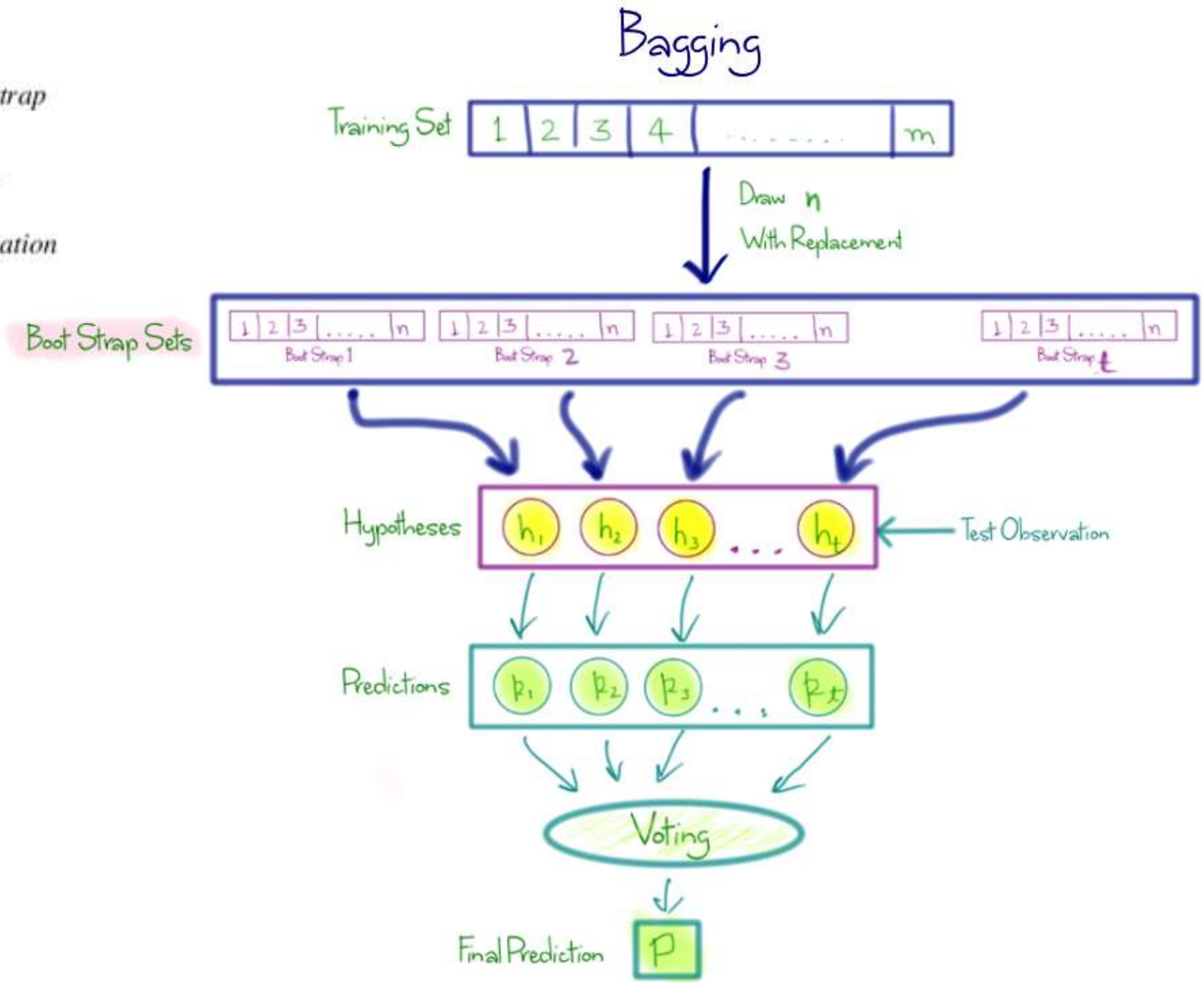
Bootstrap

+

Output:

$$H(\mathbf{x}) = \underset{j}{\operatorname{argmax}}\left(\sum_{t=1}^{T} I(h_t(\mathbf{x}) = j)\right)$$

Aggregation



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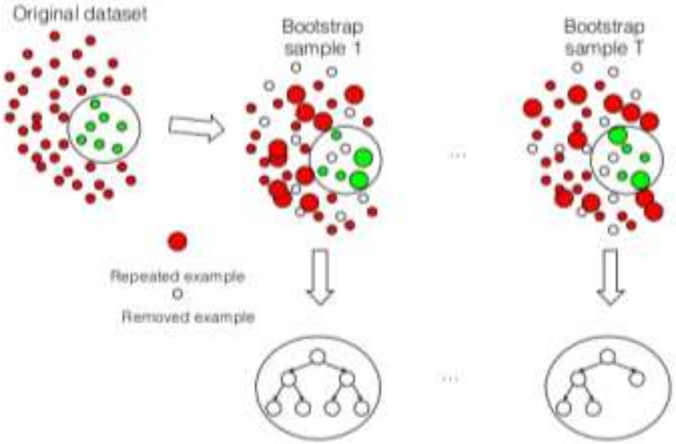
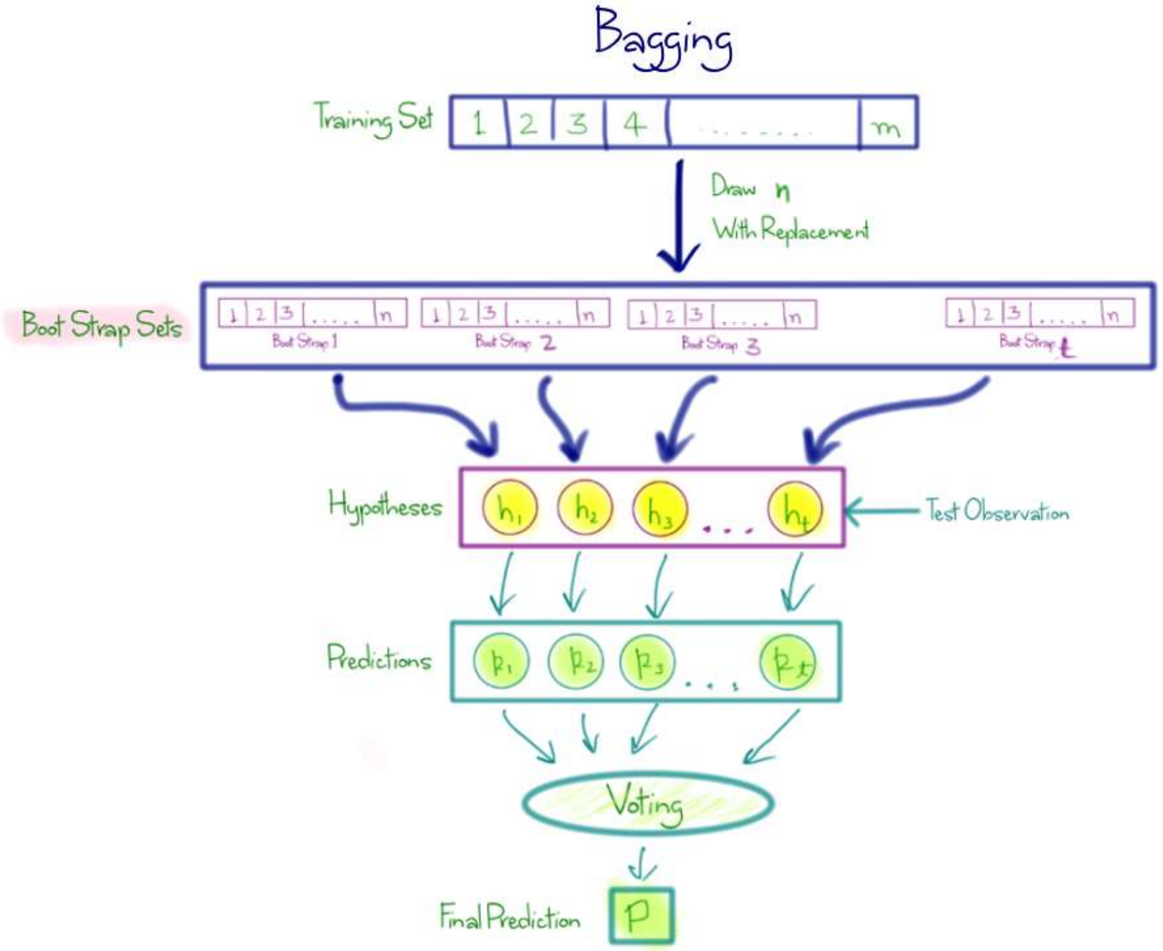
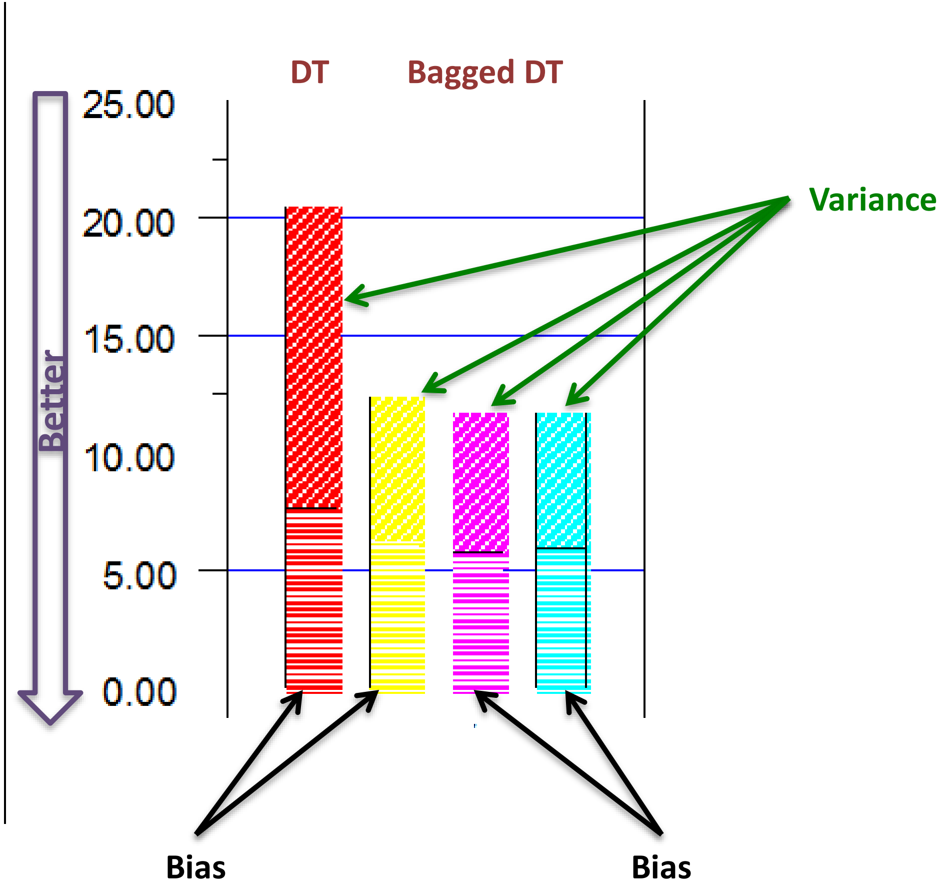
Aggregation



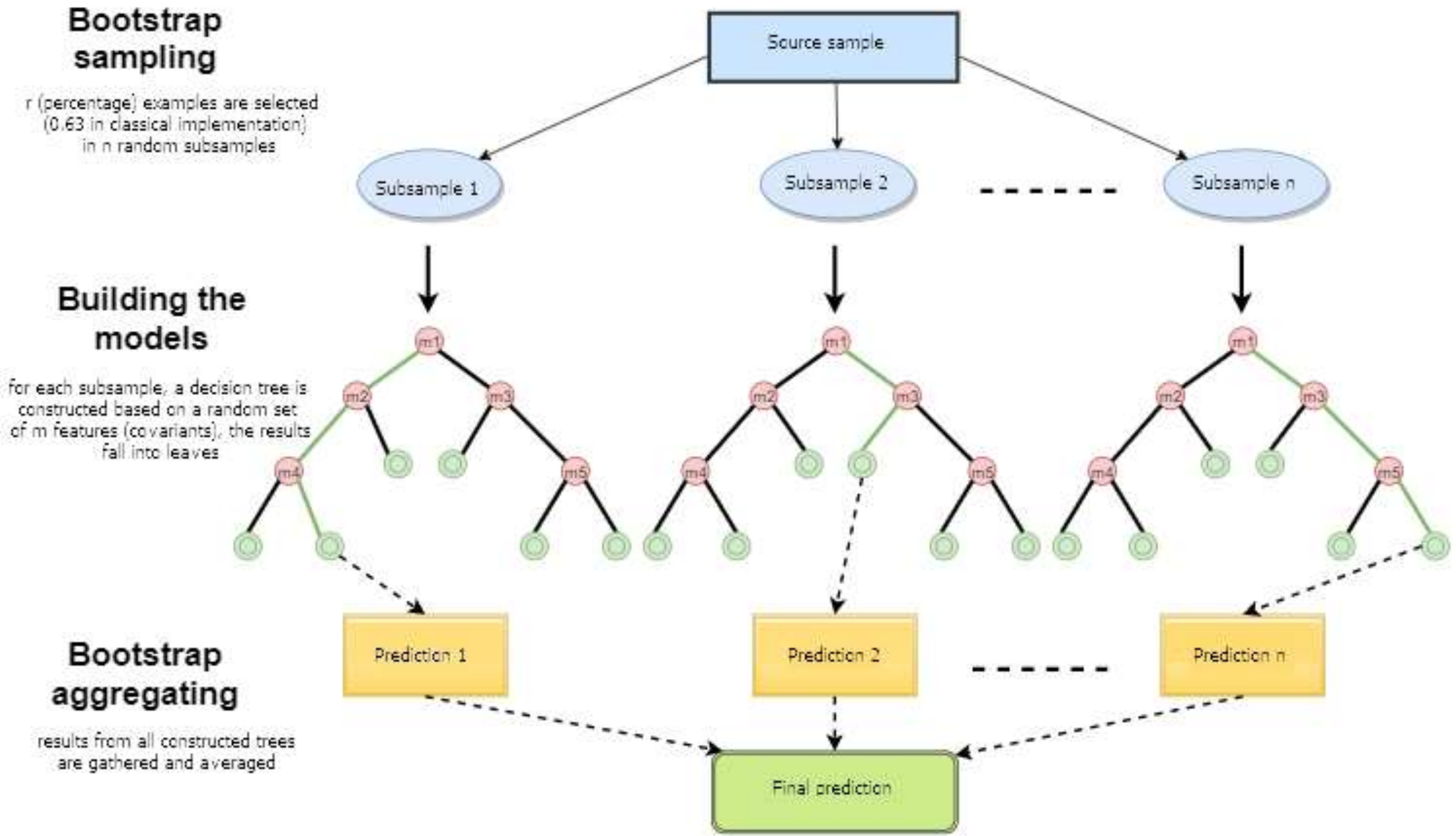




“An Empirical Comparison of Voting Classification Algorithms: Bagging, Boosting, and Variants”
Eric Bauer & Ron Kohavi, Machine Learning 36, 105–139 (1999)

- Modifications of the training set can be generated by
  - Resampling the dataset. By bootstrap sampling (e.g. bagging), weighted sampling (e.g. boosting).
  - Altering the attributes: The base learners are trained using different feature subsets (e.g Random subspaces)

Random Forests



Ensemble Learning

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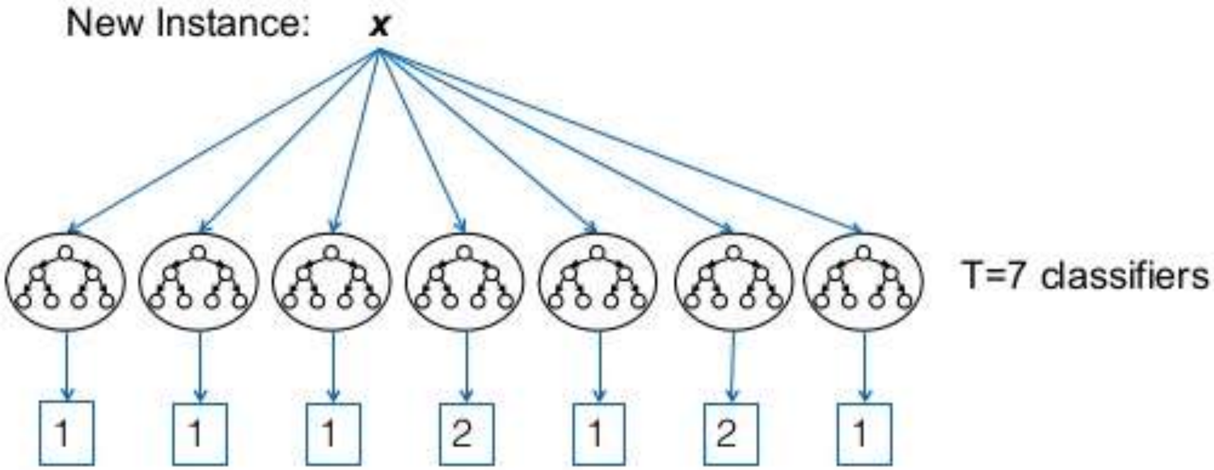
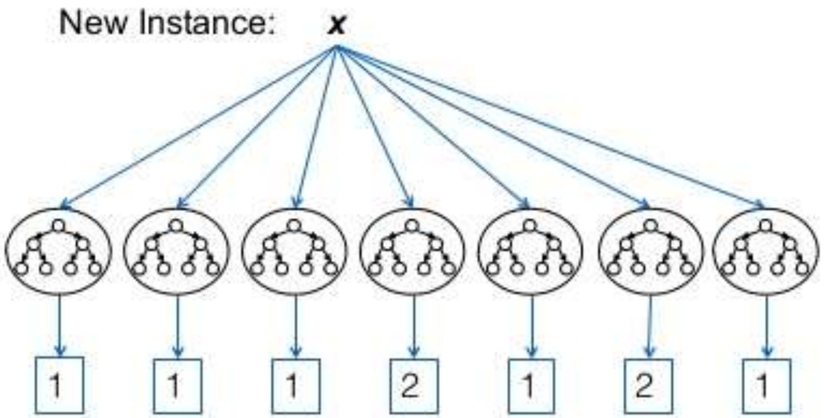
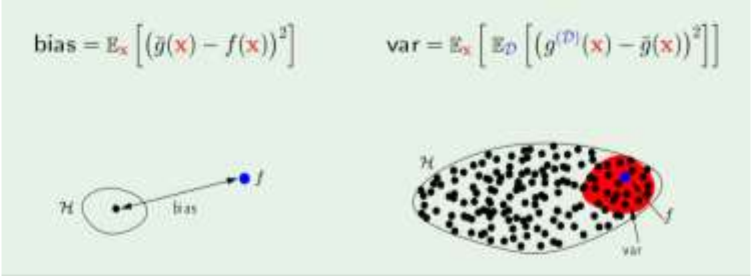
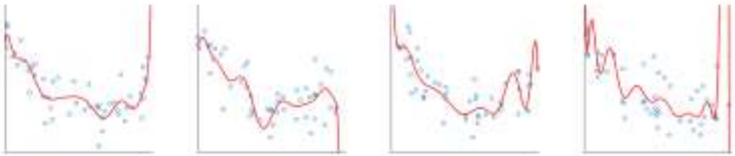


- **Ensemble methods that minimize variance**
  - Classifier Bagging
  - Classifier + Feature Bagging (e.g. Random Forests)

$$\mathbb{E}_{\mathcal{D}}\left[\left(g^{(\mathcal{D})}(\mathbf{x}) - f(\mathbf{x})\right)^2\right] = \underbrace{\mathbb{E}_{\mathcal{D}}\left[\left(g^{(\mathcal{D})}(\mathbf{x}) - \bar{g}(\mathbf{x})\right)^2\right]}_{\text{var}(\mathbf{x})} + \underbrace{\left(\bar{g}(\mathbf{x}) - f(\mathbf{x})\right)^2}_{\text{bias}(\mathbf{x})}$$



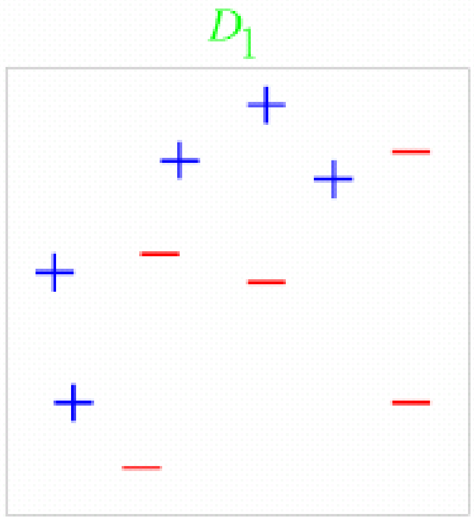




How to build them?

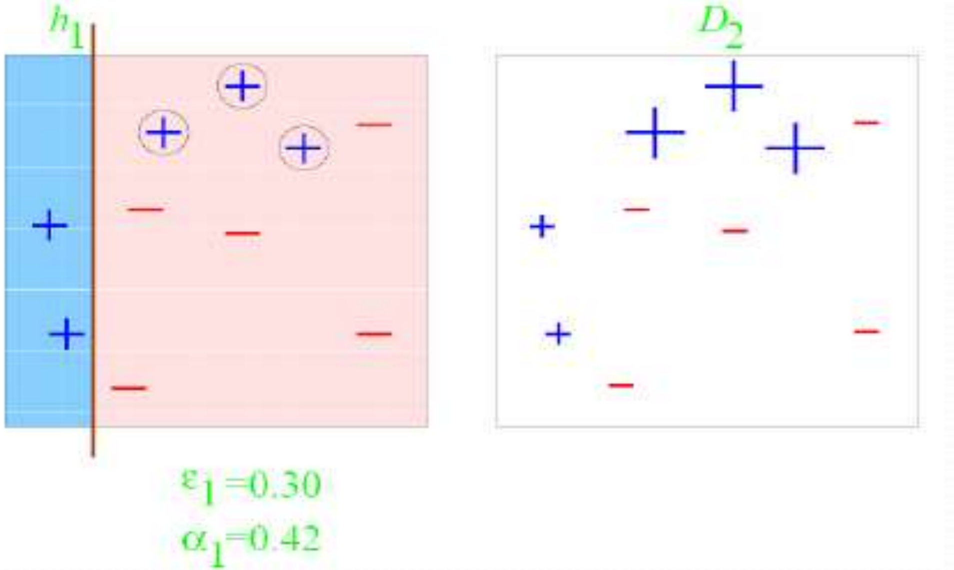
- There are several techniques to build diverse base learners in an ensemble:
  - Use modified versions of the training set to train the base learners
  - Introduce changes in the learning algorithms

A toy example[2]



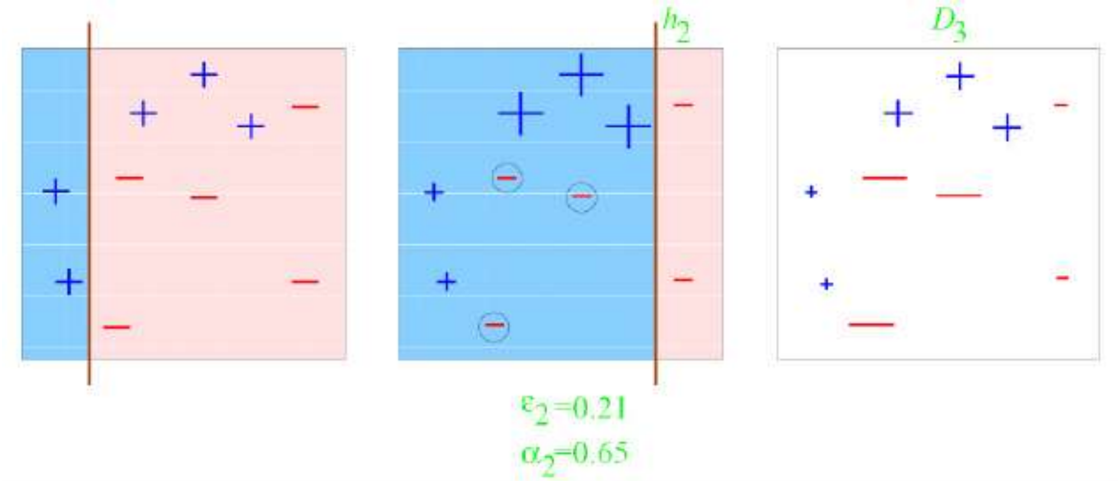
Training set: 10 points
(represented by plus or minus)
Original Status: Equal Weights
for all training samples

A toy example(cont'd)



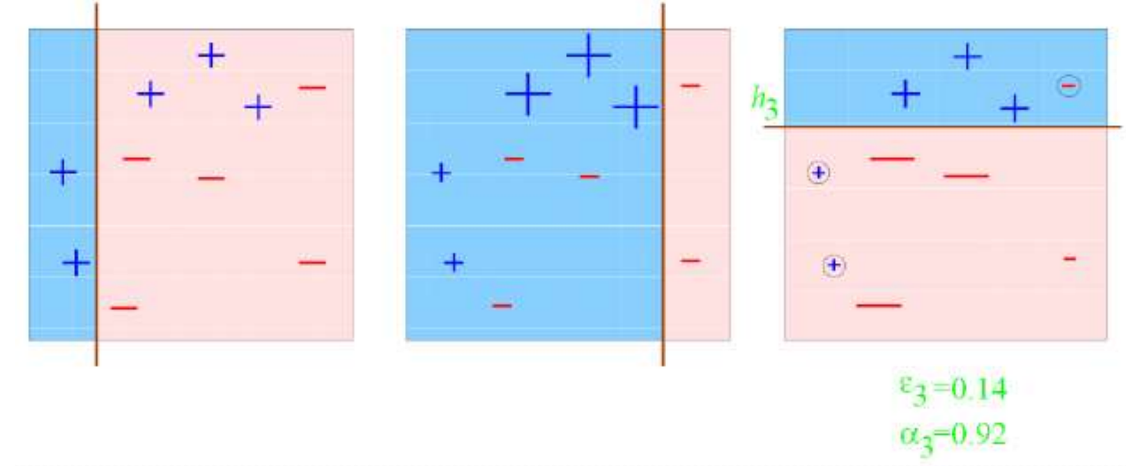
Round 1: Three "plus" points are not correctly classified;
They are given higher weights.

A toy example(cont'd)



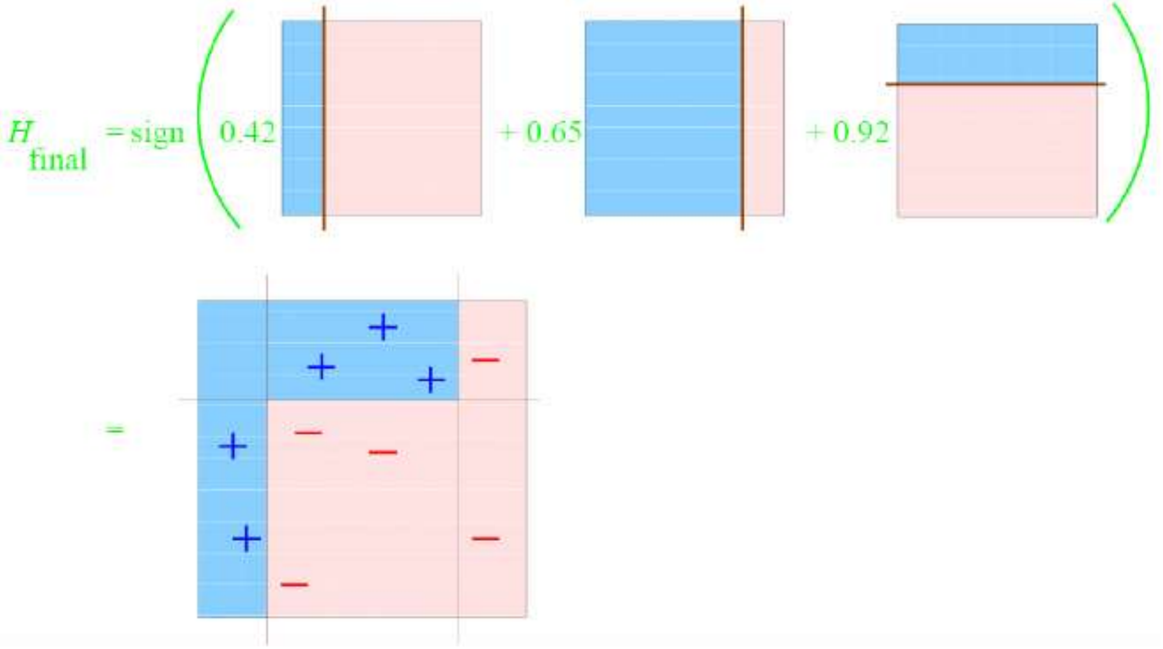
Round 2: Three "minus" points are not correctly classified;
They are given higher weights.

A toy example(cont'd)



Round 3: One "minus" and two "plus" points are not correctly classified;
They are given higher weights.

A toy example(cont'd)



Final Classifier: integrate the three "weak" classifiers and obtain a final strong classifier.

Given: $(x_1, y_1), \ldots, (x_m, y_m)$ where $x_i \in \mathscr{X}$, $y_i \in \{-1, +1\}$.
Initialize $\boxed{D_1(i) = 1/m \text{ for } i = 1, \ldots, m.}$ Initial Distribution of Data
For $t = 1, \ldots, T$:

- Train weak learner using distribution D_t.
- Get weak hypothesis $h_t : \mathscr{X} \to \{-1, +1\}$.

Train model

- Aim: select h_t with low weighted error:

$$\boxed{\varepsilon_t = \Pr_{i \sim D_t}[h_t(x_i) \neq y_i].}$$

Error of model

- Choose $\boxed{\alpha_t = \frac{1}{2} \ln\left(\frac{1 - \varepsilon_t}{\varepsilon_t}\right)}$.

Coefficient of model

- Update, for $i = 1, \ldots, m$:

$$\boxed{D_{t+1}(i) = \frac{D_t(i) \exp(-\alpha_t y_i h_t(x_i))}{Z_t}}$$

Update Distribution

where Z_t is a normalization factor (chosen so that D_{t+1} will be a distribution).

Output the final hypothesis:

$$\boxed{H(x) = \operatorname{sign}\left(\sum_{t=1}^{T} \alpha_t h_t(x)\right).}$$

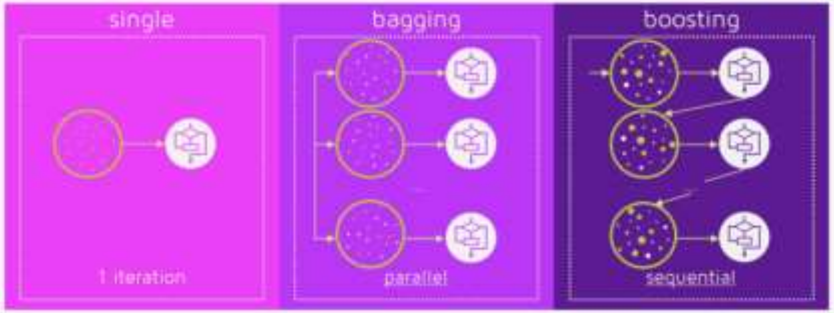
Final average

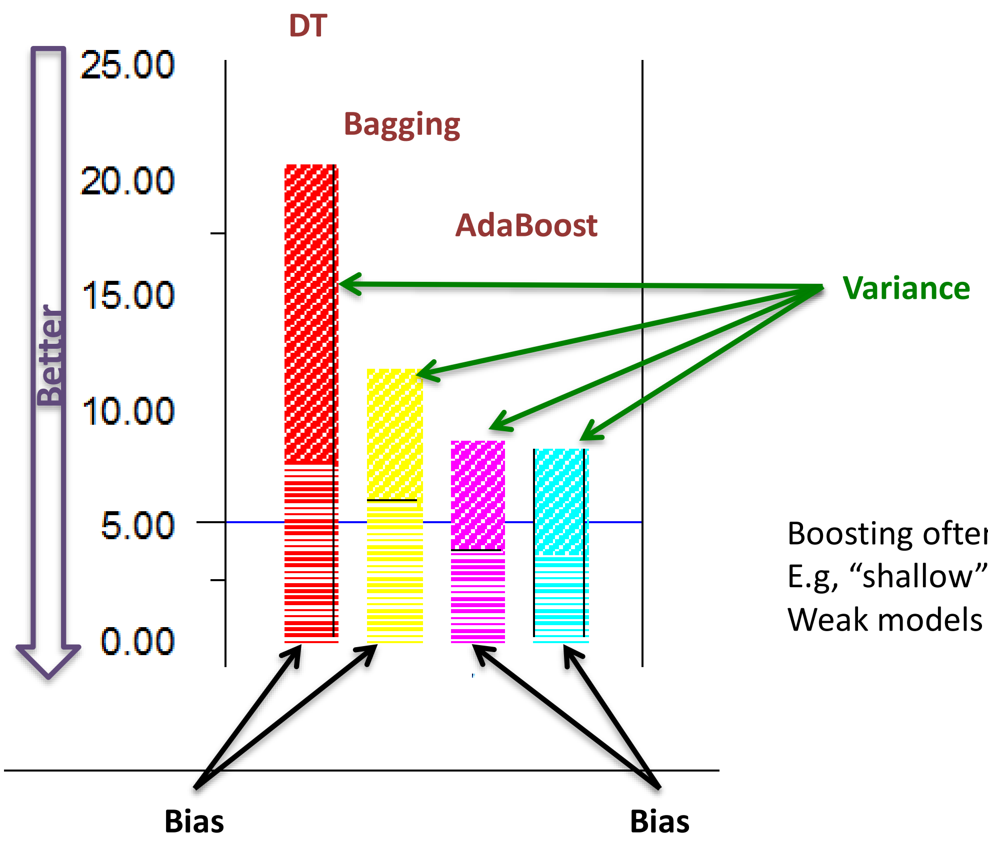
Theorem: training error drops exponentially fast

https://www.cs.princeton.edu/~schapire/papers/explaining-adaboost.pdf

Bagging *vs* Boosting

- Bagging
  - Construction of <u>complementary</u> base-learners is left to chance
  - .. and to the unstability of the learning methods.
- Boosting
  - Actively seek to generate complementary base-learner
  - Training the next base-learner based on the mistakes of the previous learners.





Boosting often uses weak models
E.g, “shallow” decision trees
Weak models have lower variance

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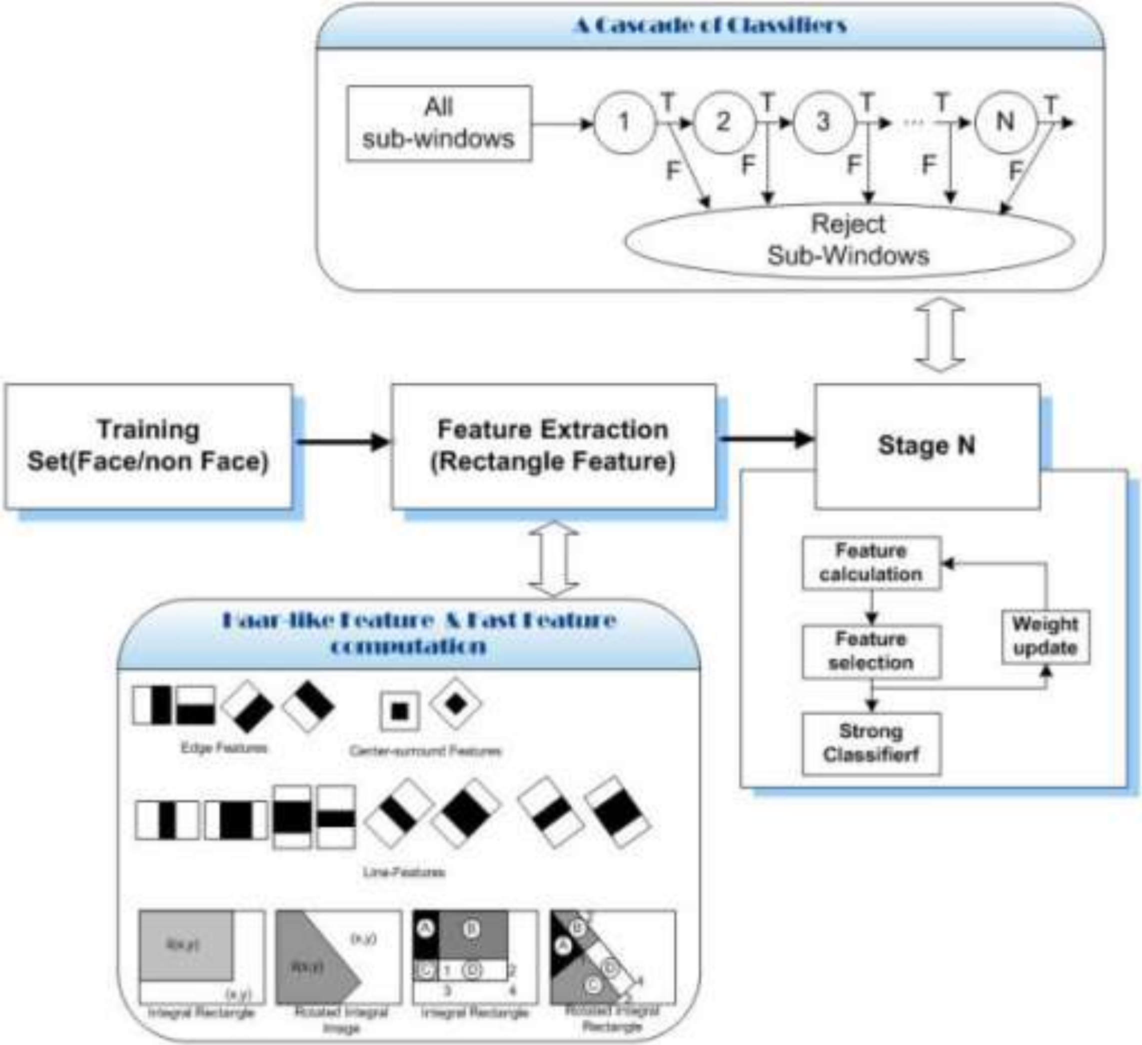
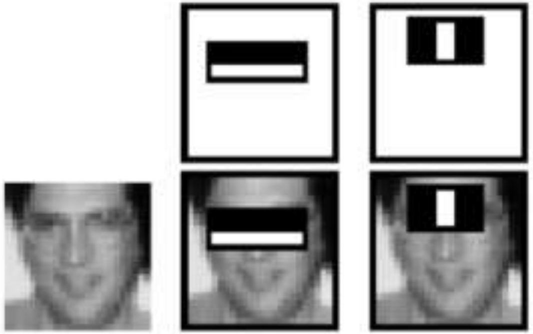
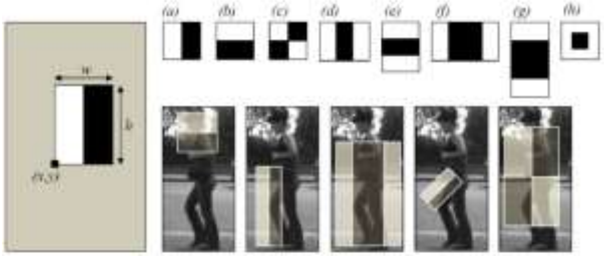
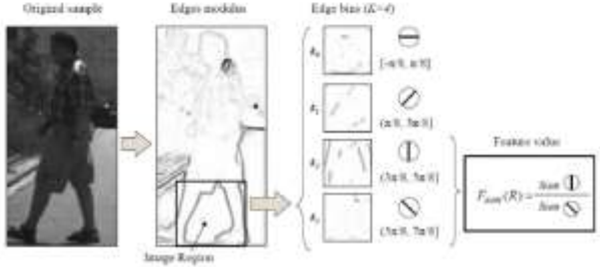

A Cascade of Classifiers
All sub-windows
1
2
3
N
T
F
Reject Sub-Windows
Training Set(Face/non Face)
Feature Extraction (Rectangle Feature)
Stage N
Feature calculation
Feature selection
Weight update
Strong Classifierf
Haar-like Feature & Fast Feature computation
Edge Features
Center-surround Features
Line Features
Integral Rectangle
Rotated Integral Image
Integral Rectangle
Rotated Integral Rectangle




(a)
(b)
(c)
(d)
(e)
(f)
(g)
(h)


Original sample
Edges modulus
Feature value
Image Region

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Error of model

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Output the final hypothesis:

$$\boxed{H(x) = \operatorname{sign}\left(\sum_{t=1}^{T} \alpha_t h_t(x) \right).}$$

Final average

Adaboost: Additive model with exponential loss function

$$\min_{\alpha_{n=1:N}, \beta_{n=1:N}} L\left(y, \sum_{n=1}^{N} \alpha_n f(x, \beta_n)\right)$$