Ensemble Learning

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IIT Gandhinagar

Ensemble Methods

Use multiple models for prediction.
Most winning entries of Kaggle competition using ensemble learning.

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Example:
Classifier 1 - Good
Classifier 2 - Good
Classifier 3 - Bad

Using Majority Voting, we predict Good.

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Use multiple models for prediction.
Most winning entries of Kaggle competition using ensemble learning.

Example:

Regressor 1 - 20
Regressor 2 - 30
Regressor 3 - 30

Using Average, we predict $\frac{80}{3}$

Intuition

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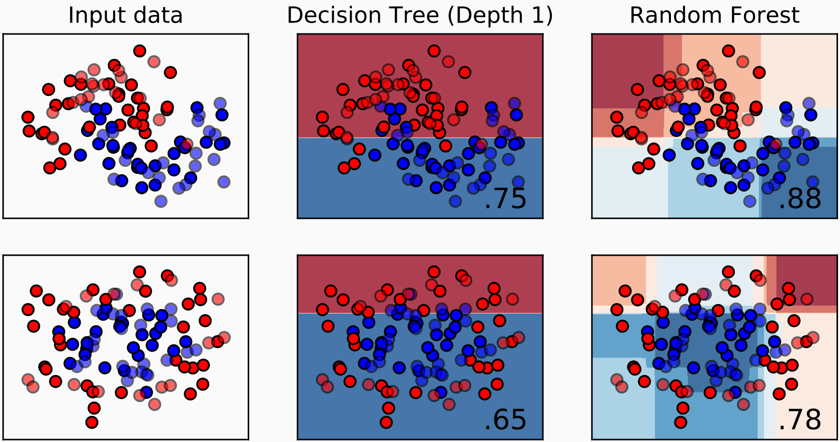
3) Representational: Some classifiers/regressors can not learn the true form/representation.

Representation of Limited Depth DTs vs RFs



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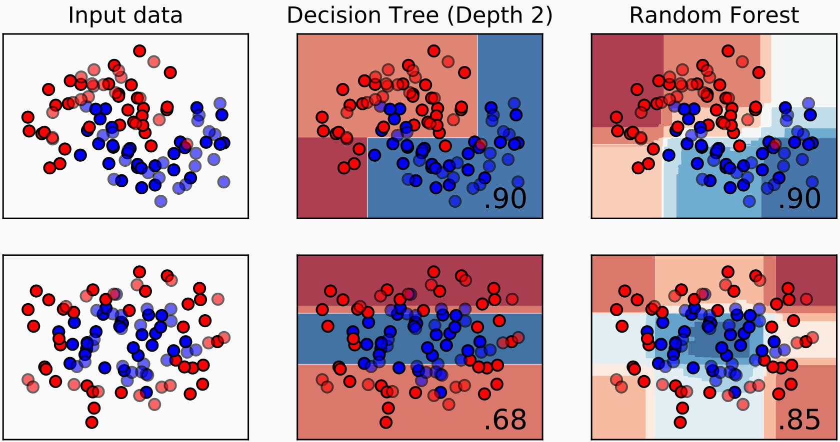

Necessary and Sufficient Conditions

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3) Two classifiers are diverse: if they make different errors on new data points

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If the three classifiers are identical, i.e. not diverse, then when $h_1(x)$ is wrong $h_2(x)$ and $h_3(x)$ will also be wrong.

Necessary and Sufficient Conditions

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If the three classifiers are identical, i.e. not diverse, then when $h_1(x)$ is wrong $h_2(x)$ and $h_3(x)$ will also be wrong.

However, if the errors made by the classifiers are uncorrelated, then when $h_1(x)$ is wrong, $h_2(x)$ and $h_3(x)$ may be correct, so that a majority vote will correctly class.

Intuition for Ensemble Methods from Quantitative Perspective

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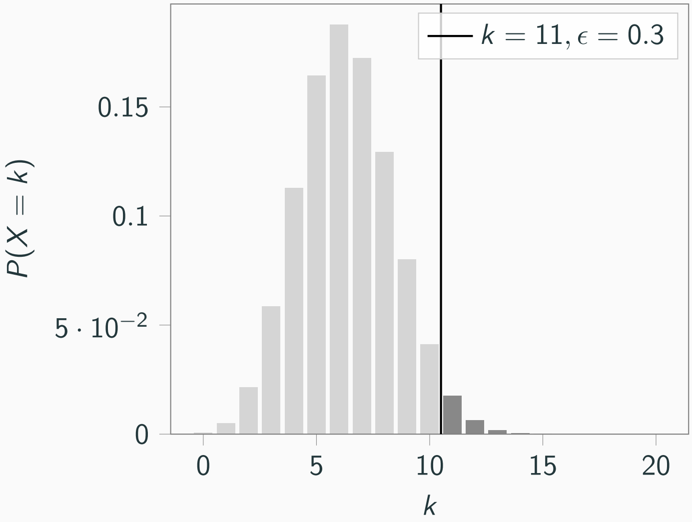
Error Probability of each model $= \varepsilon = 0.3$

$$Pr(\text{ensemble being wrong}) = {}^3C_2(\varepsilon^2)(1-\varepsilon)^{3-2} + {}^3C_3(\varepsilon^3)(1-\varepsilon)^{3-3}$$

$$= 0.19 \leq 0.3$$

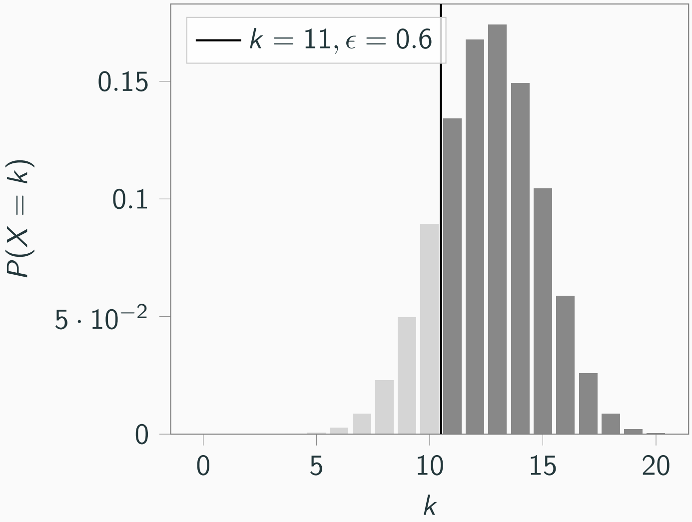
Some calculations

Probability that majority vote (11 out of 21) is wrong $= 0.026$



Some calculations

Probability that majority vote (11 out of 21) is wrong $= 0.826$



Ensemble Methods

Where does ensemble learning not work well?

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Where does ensemble learning not work well?

- The base model is bad.
- All models give similar prediction or the models are highly correlated.

Bagging

Also known as *Bootstrap Aggregation*.

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Key idea : Reduce Variance

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Think about cross-validation!

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How to learn different classifiers while feeding in the same data?

Think about cross-validation!

We will create multiple datasets from our single dataset using "*sampling with replacement*".

Bagging

Consider our dataset has n samples, $D_1, D_2, D_3, \ldots, D_n$.
For each model in the ensemble, we create a new dataset of size n by sampling uniformly with replacement.

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$$\begin{aligned}
&\text{Round 1}: D_1, D_3, D_6, D_1, \ldots, D_n \\
&\text{Round 2}: D_2, D_4, D_1, D_{80}, \ldots, D_3 \\
&\vdots
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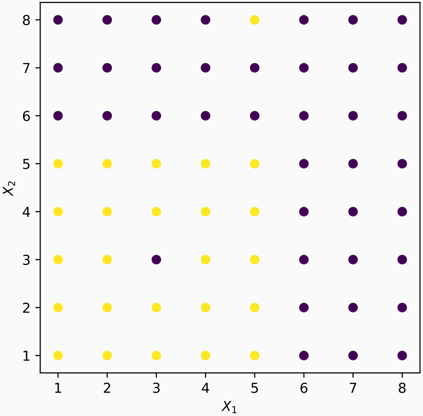
$\vdots$

Repetition of samples is possible.
We can train the same classifier/models on each of these different "Bagging Rounds".

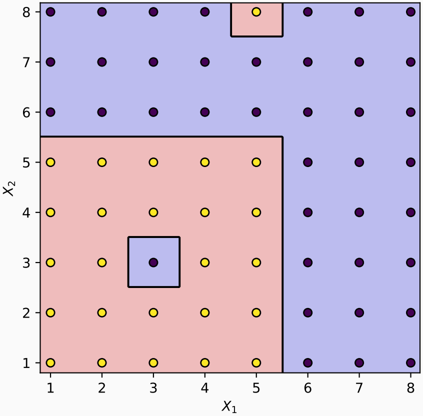
Bagging : Classification Example

Consider the dataset below. Points (3,3) and (5,8) are anomalies.



Bagging : Classification Example

Decision Boundary for decision tree with depth 6.



Bagging : Classification Example

Lets use bagging with ensemble of 5 trees.

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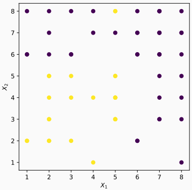

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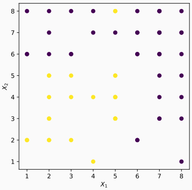
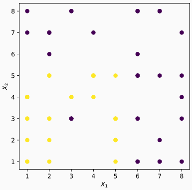


Round - 2



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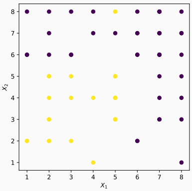

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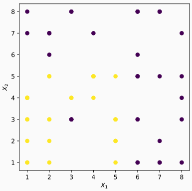
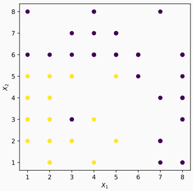


Round - 3



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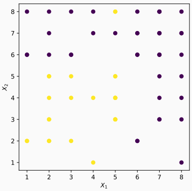

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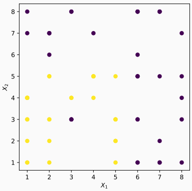

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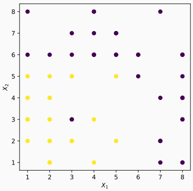
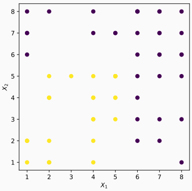


Round - 4



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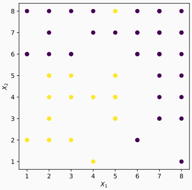

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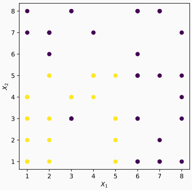

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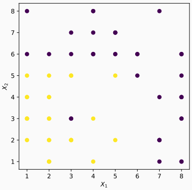

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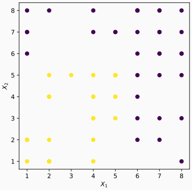
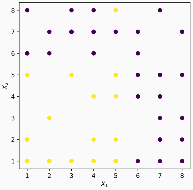


Round - 5



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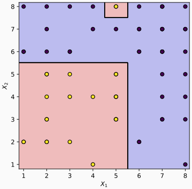

Tree Depth $= 4$

Bagging : Classification Example

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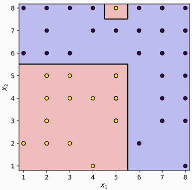
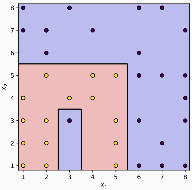


Tree Depth = 4

Round - 2



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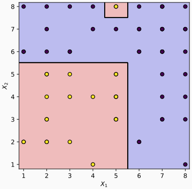
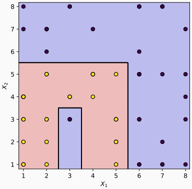


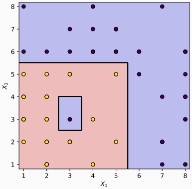
Tree Depth = 4

Round - 2



Tree Depth = 5

Round - 3



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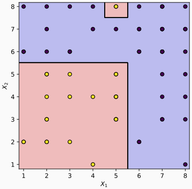

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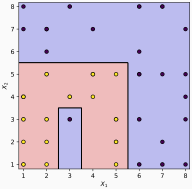

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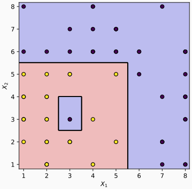
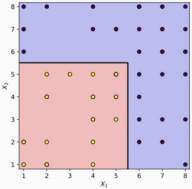


Tree Depth = 5

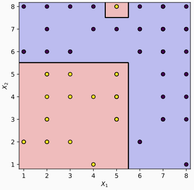
Round - 4



Tree Depth = 2

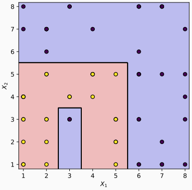
Bagging : Classification Example

Round - 1



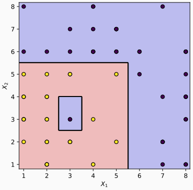
Tree Depth = 4

Round - 2



Tree Depth = 5

Round - 3



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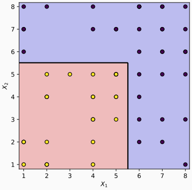
Round - 4



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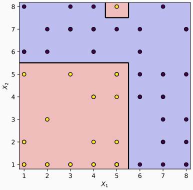
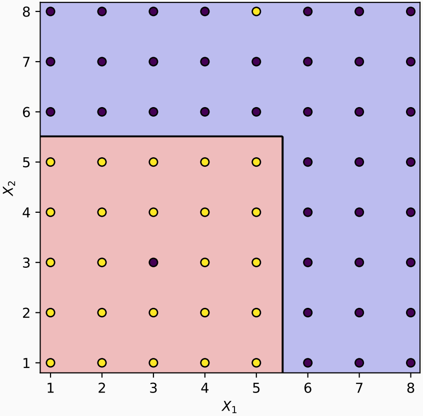
Round - 5



Tree Depth = 4

Bagging : Classification Example

Using majority voting to combine all predictions, we get the decision boundary below.



Bagging

Summary

- We take “strong” learners and combine them to reduce variance.
- All learners are independent of each other.

Boosting

- We take “weak” learners and combine them to reduce bias.

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- All learners are incrementally built.

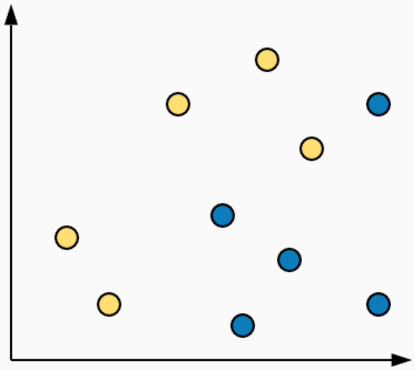
Boosting

- We take "weak" learners and combine them to reduce bias.
- All learners are incrementally built.
- Incremental building: Incrementally try to classify "harder" samples correctly.

Boosting : AdaBoost

Consider we have a dataset of N samples.

Sample i has weight w_i. There are M classifers in ensemble.



Boosting : AdaBoost

Consider we have a dataset of N samples.

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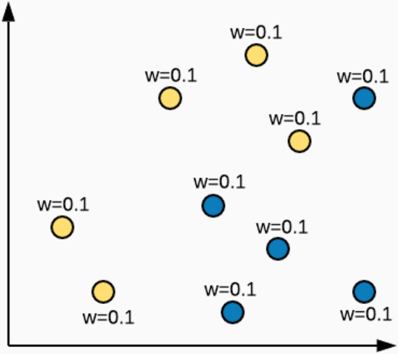
1. Initialize weights of data samples, $w_i = \dfrac{1}{N}$



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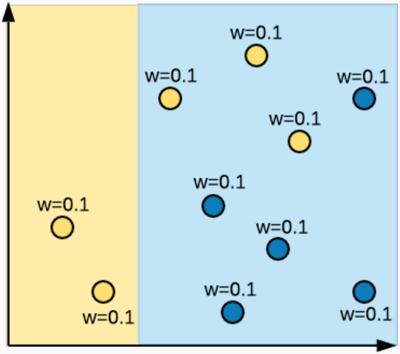
   2.1 Learn classifier using current weights $w_i^{\prime} s$



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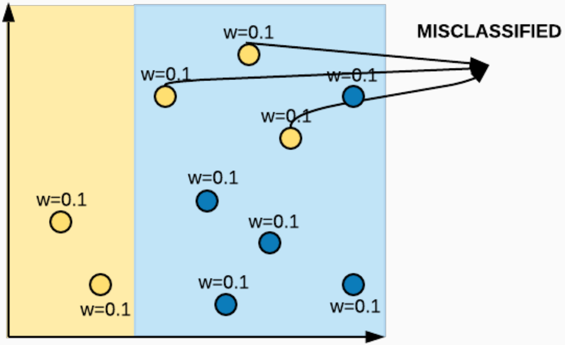

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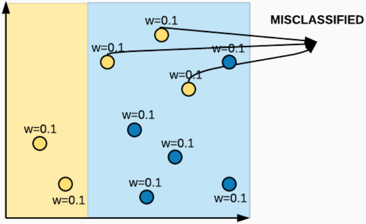
2. For $m = 1 \dots M$
    2.1 Learn classifier using current weights $w_i's$
    2.2 Compute the weighted error, $err_m = \dfrac{\sum_i w_i(incorrect)}{\sum_i w_i}$



$$err_1 = \frac{0.3}{1}$$

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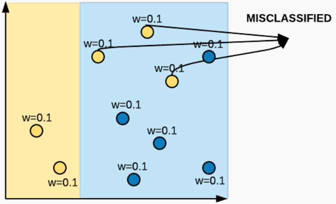
    - 2.3 Compute $\alpha_m = \dfrac{1}{2} log_e \left(\dfrac{1 - err_m}{err_m} \right)$



$$err_1 = \frac{0.3}{1}$$

$$\alpha_1 = \frac{1}{2} log \left(\frac{1 - 0.3}{0.3} \right) = 0.42$$

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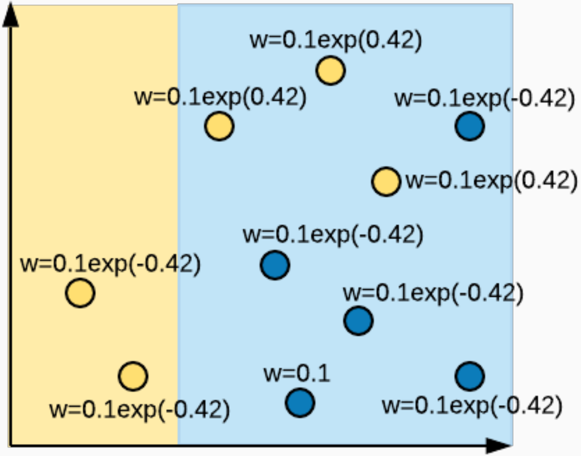
   2.2 Compute the weighted error, $err_m = \dfrac{\sum_i w_i(incorrect)}{\sum_i w_i}$
   2.3 Compute $\alpha_m = \dfrac{1}{2} log_e \left(\dfrac{1 - err_m}{err_m} \right)$
   2.4 For samples which were predicted correctly, $w_i = w_i e^{-\alpha_m}$
   2.5 For samples which were predicted incorrectly, $w_i = w_i e^{\alpha_m}$

Boosting : AdaBoost



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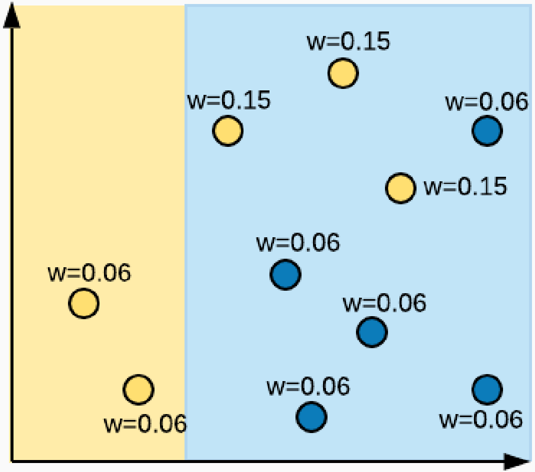

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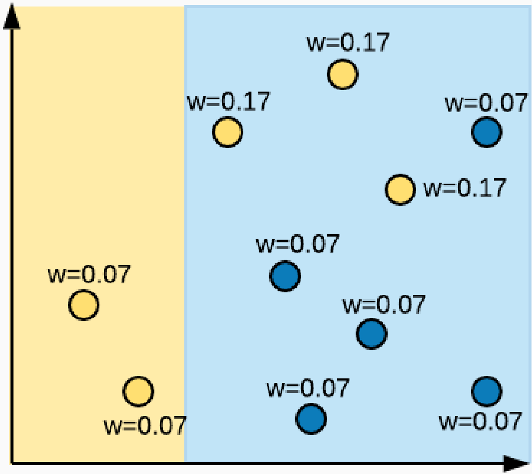
Sample i has weight w_i. There are M classifers in ensemble.

1. Initialize weights of data samples, $w_i = \dfrac{1}{N}$
2. For $m = 1 \dots M$
   2.1 Learn classifier using current weights $w_i's$
   2.2 Compute the weighted error, $err_m = \dfrac{\sum_i w_i(incorrect)}{\sum_i w_i}$
   2.3 Compute $\alpha_m = \dfrac{1}{2} log_e \left(\dfrac{1 - err_m}{err_m} \right)$
   2.4 For samples which were predicted correctly, $w_i = w_i e^{-\alpha_m}$
   2.5 For samples which were predicted incorrectly, $w_i = w_i e^{\alpha_m}$
   2.6 Normalize $w_i's$ to sum up to 1.

Boosting : AdaBoost



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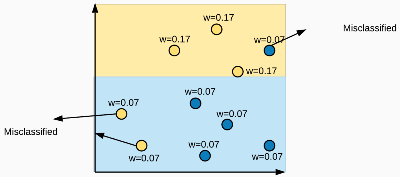

$$err_2 = \frac{0.21}{1}$$

$$\alpha_2 = \frac{1}{2} log \left(\frac{1 - 0.21}{0.21} \right) = 0.66$$

Boosting : AdaBoost

Consider we have a dataset of N samples.

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1. Initialize weights of data samples, $w_i = \dfrac{1}{N}$
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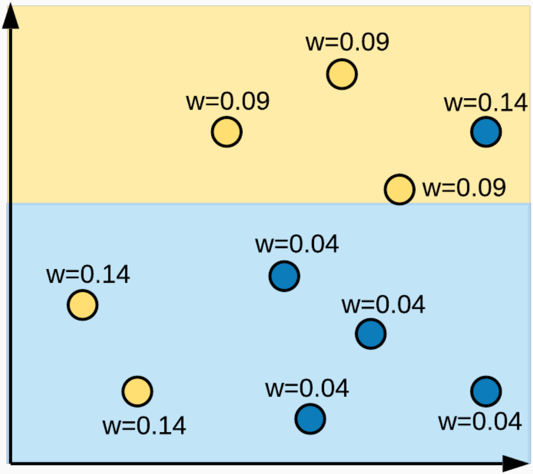

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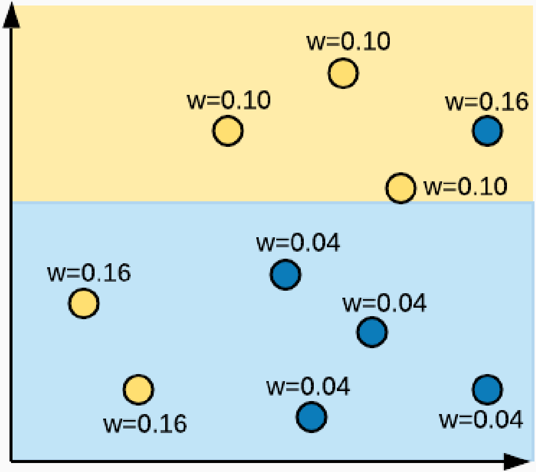

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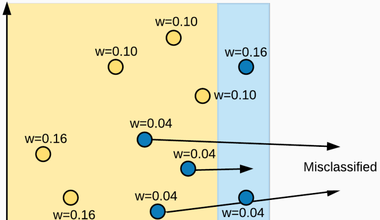


$$err_3 = \frac{0.12}{1}$$

$$\alpha_3 = \frac{1}{2} log \left(\frac{1 - 0.12}{0.12} \right) = 0.99$$

Boosting: Adaboost

Intuitively, after each iteration, importance of wrongly classified samples is increased by increasing their weights and importance of correctly classified samples is decreased by decreasing their weights.

Boosting: Adaboost

Testing

- For each sample x, compute the prediction of each classifier $h_m(x)$.
- Final prediction is the sign of the sum of weighted predictions, given as:
- $\text{SIGN}(\alpha_1 h_1(x) + \alpha_2 h_2(x) + \ldots + \alpha_M h_M(x))$

Boosting: Adaboost

Example

Example

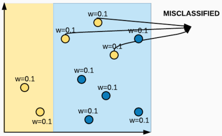
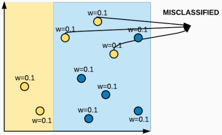


Figure 1: $\alpha_1 = 0.42$

Example



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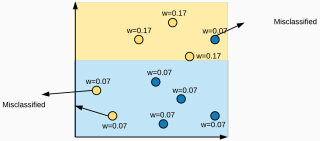
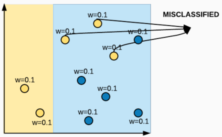


Figure 2: $\alpha_2 = 0.66$

Boosting: Adaboost

Example



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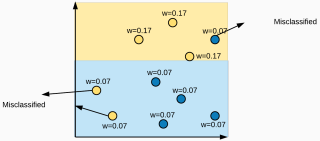

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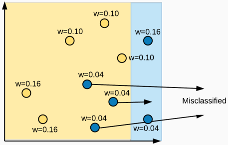
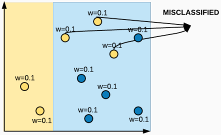


Figure 3: $\alpha_3 = 0.99$

Example



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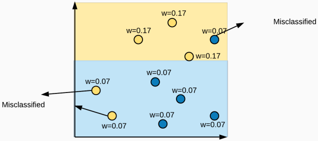
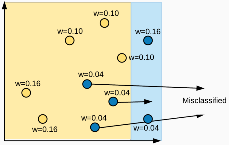


Figure 2: $\alpha_2 = 0.66$



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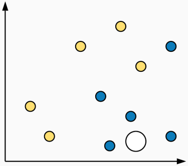
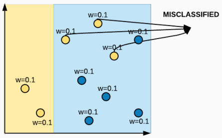


Boosting: Adaboost

Example



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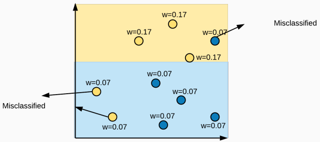

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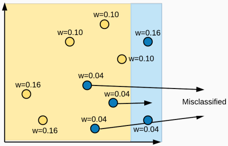

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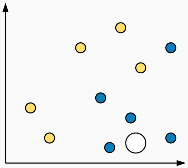
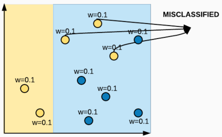


Let us say, yellow class is $+1$ and blue class is -1

Boosting: Adaboost

Example



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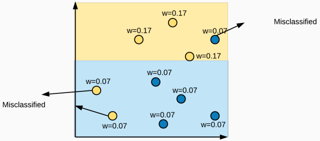

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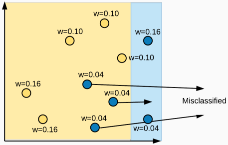

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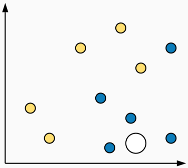

Let us say, yellow class is $+1$ and blue class is -1

Prediction $=$ SIGN(0.42*-1 $+$ 0.66*-1 $+$ 0.99*+1) $=$ Negative $=$ blue

Intuition behind weight update formula

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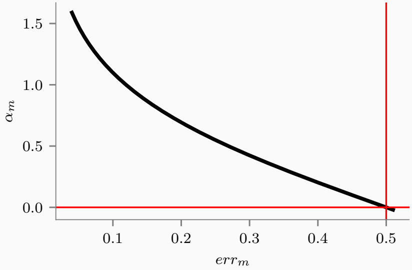
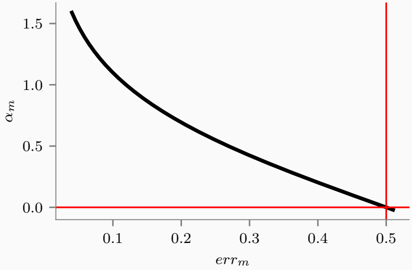
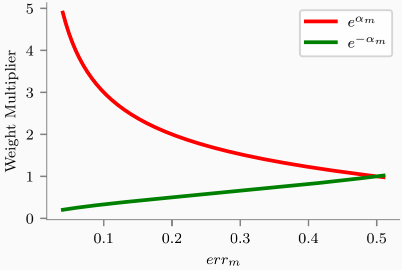


Intuition behind weight update formula





Random Forest

- Random Forest is an ensemble of decision trees.
- We have two types of bagging: bootstrap (on data) and random subspace (of features).
- As features are randomly selected, we learn decorrelated trees and helps in reducing variance.

Random Forest

There are 3 parameters while training a random forest number of trees, number of features (m), maximum depth.

Training Algorithm

- For i^{th} tree ($i \in \{1 \cdots N\}$), select n samples from total N samples with replacement.
- Learn Decision Tree on selected samples for i^{th} round.

Learning Decision Tree (for RF)

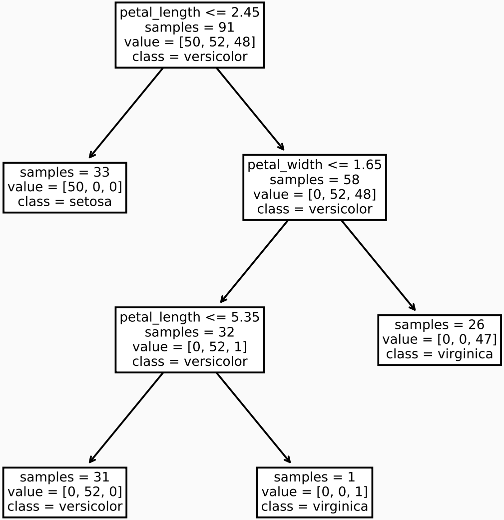
- For each split, select m features from total available M features and train a decision tree on selected features

Dataset

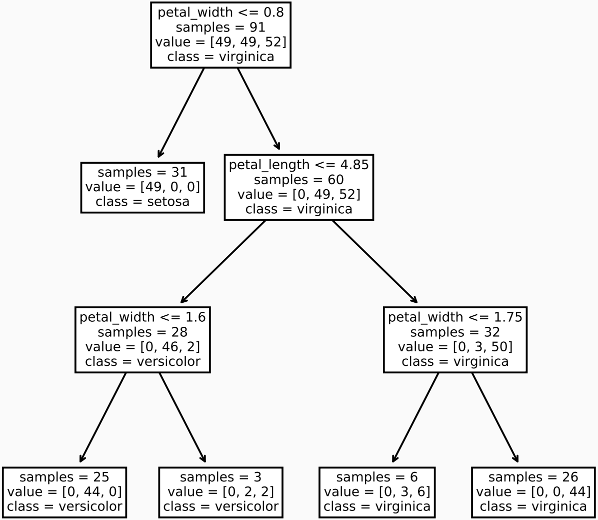
	sepal_length	sepal_width	petal_length	petal_width	species
0	5.1	3.5	1.4	0.2	setosa
1	4.9	3.0	1.4	0.2	setosa
2	4.7	3.2	1.3	0.2	setosa
3	4.6	3.1	1.5	0.2	setosa
4	5.0	3.6	1.4	0.2	setosa
...	...	...	...	...	...
145	6.7	3.0	5.2	2.3	virginica
146	6.3	2.5	5.0	1.9	virginica
147	6.5	3.0	5.2	2.0	virginica
148	6.2	3.4	5.4	2.3	virginica
149	5.9	3.0	5.1	1.8	virginica

150 rows × 5 columns

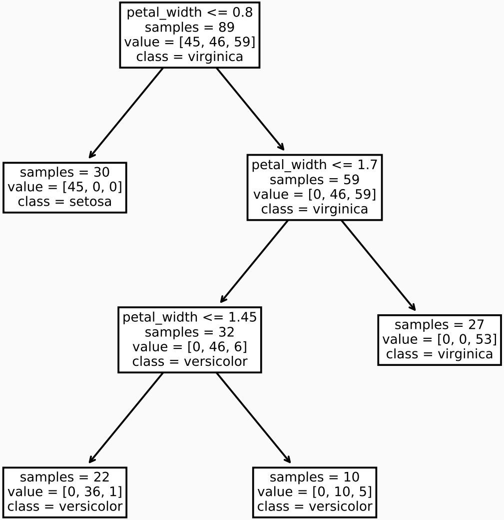
Decision Tree # 0



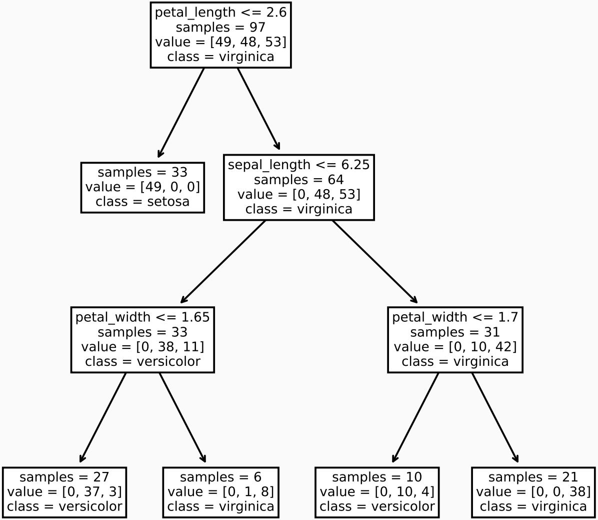
Decision Tree # 1



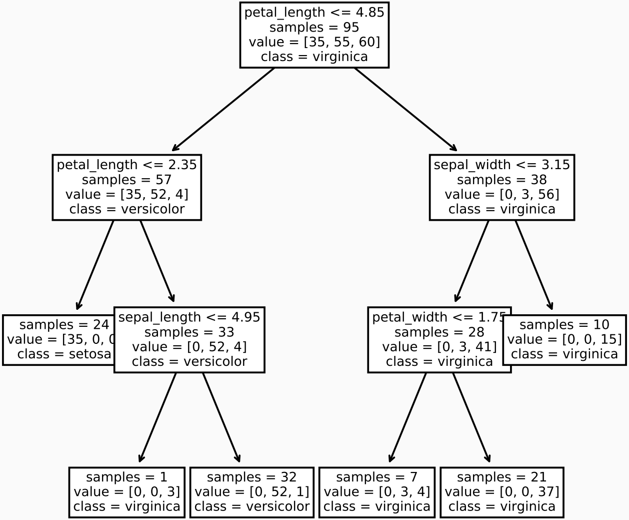
Decision Tree # 2



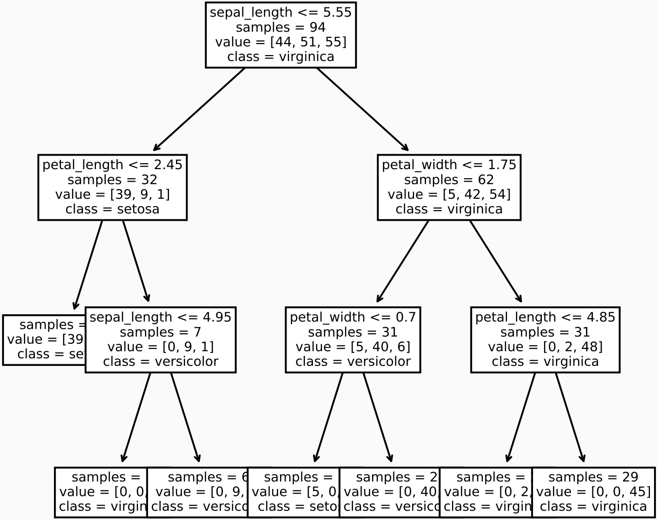
Decision Tree # 3



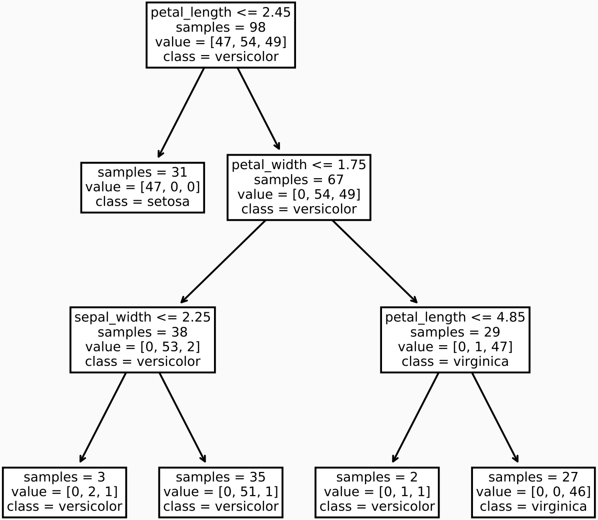
Decision Tree # 4



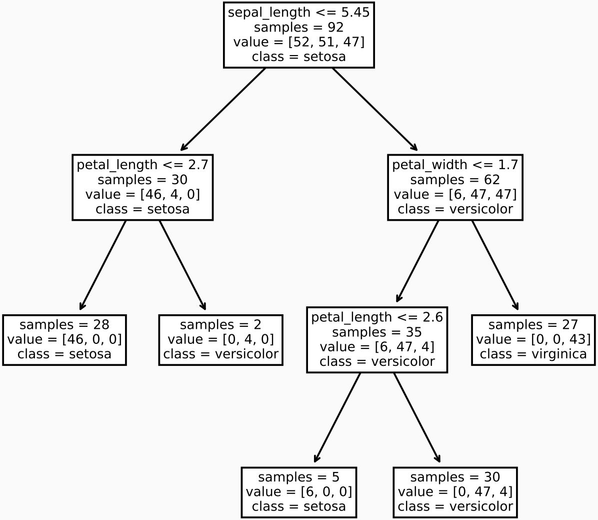
Decision Tree # 5



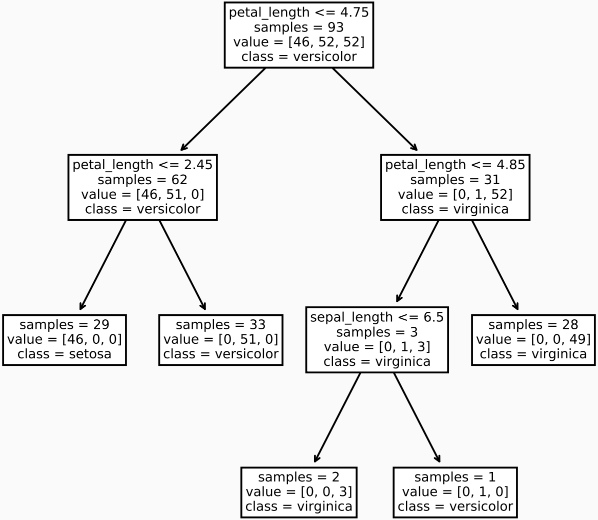
Decision Tree # 6



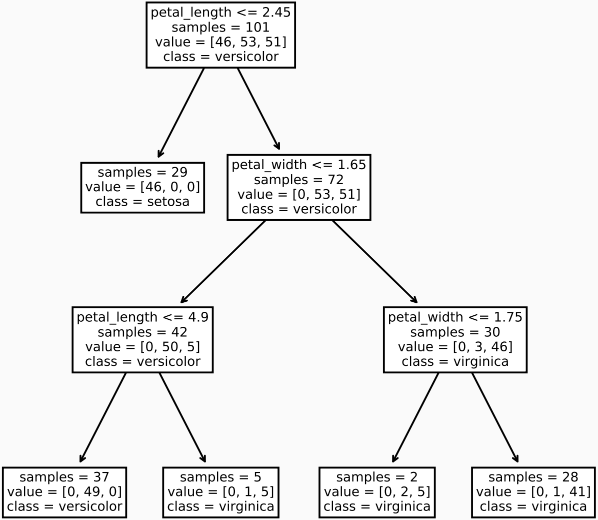
Decision Tree # 7



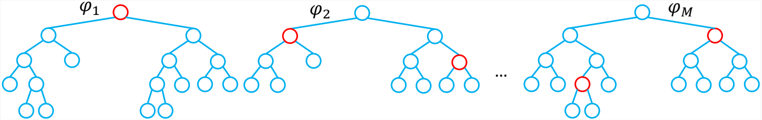
Decision Tree # 8



Decision Tree # 9



Feature Importance[1]



Importance of variable X_j for an ensemble of M trees φ_m is:

$$\text{Imp}(X_j) = \frac{1}{M} \sum_{m=1}^{M} \sum_{t \in \varphi_m} 1(j_t = j) \Big[p(t) \Delta i(t) \Big],$$

where j_t denotes the variable used at node t, $p(t) = N_t / N$ and $\Delta i(t)$ is the impurity reduction at node t:

$$\Delta i(t) = i(t) - \frac{N_{t_L}}{N_t} i(t_L) - \frac{N_{t_r}}{N_t} i(t_R)$$

[1] Slide Courtesy Gilles Louppe

Computed Feature Importance