

Ensemble Learning

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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.

Ensemble Methods

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

Based on [Ensemble methods in ML by Dietterich](#)

Three reasons why ensembles make sense:

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Three reasons why ensembles make sense:

1) Statistical: Sometimes if **data is less, many competing hypothesis can be learnt** all giving same accuracy on training data.

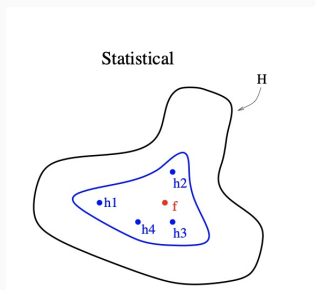
Intuition

Based on [Ensemble methods in ML by Dietterich](#)

Three reasons why ensembles make sense:

1) Statistical: Sometimes if **data is less, many competing hypothesis can be learnt** all giving same accuracy on training data.

Eg. We can learn many decision trees for the same data giving same accuracy.

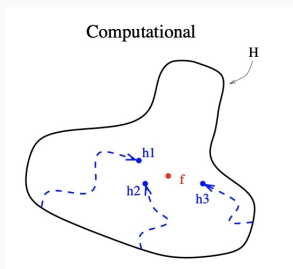


2) Computational: Even if data is enough, some **classifiers/regressors can get stuck in local optima/apply greedy strategies**. Computationally learning the “best” hypothesis can be non-trivial.

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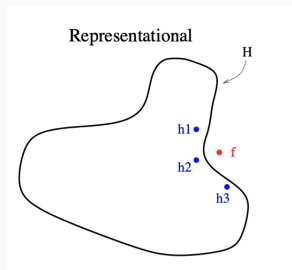
Eg. Decision Trees employ greedy criteria



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

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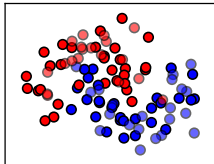
Eg. Decision Trees can only learn axis-parallel splits.



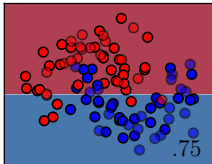
Representation of Limited Depth DTs vs RFs

Notebook: [ensemble-representation.html](#)

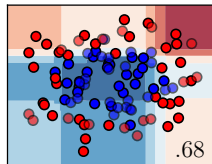
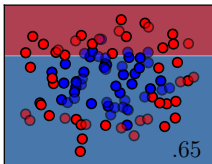
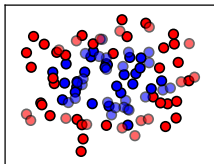
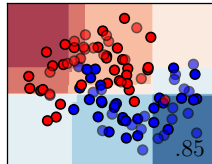
Input data



Decision Tree (Depth 1)



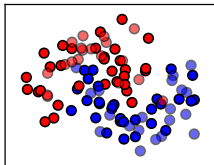
Random Forest



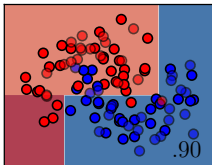
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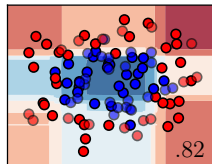
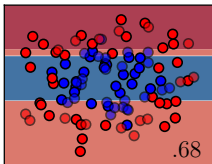
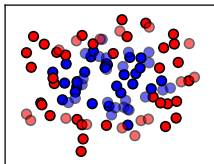
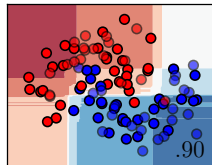
Input data



Decision Tree (Depth 2)



Random Forest



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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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

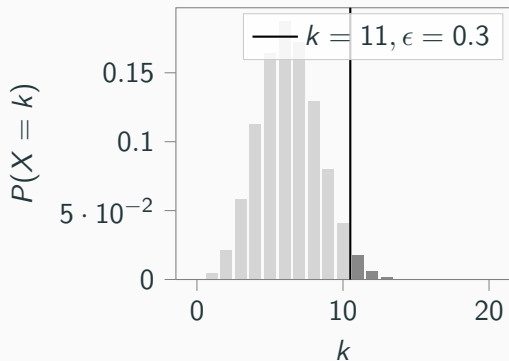
Intuition for Ensemble Methods from Quantitative Perspective

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

$$\begin{aligned}Pr(\text{ensemble being wrong}) &= {}^3C_2(\varepsilon^2)(1-\varepsilon)^{3-2} + {}^3C_3(\varepsilon^3)(1-\varepsilon)^{3-3} \\ &= 0.19 \leq 0.3\end{aligned}$$

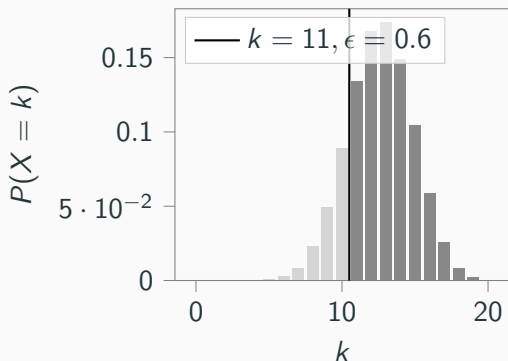
Some calculations

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



Where does ensemble learning not work well?

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

Also known as *Bootstrap Aggregation*.

Bagging

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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, $D_1, D_2, D_3, \dots, D_n$.

For each model in the ensemble, we create a new dataset of size n by sampling uniformly with replacement.

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Round 1 : $D_1, D_3, D_6, D_1, \dots, D_n$

Round 2 : $D_2, D_4, D_1, D_{80}, \dots, D_3$

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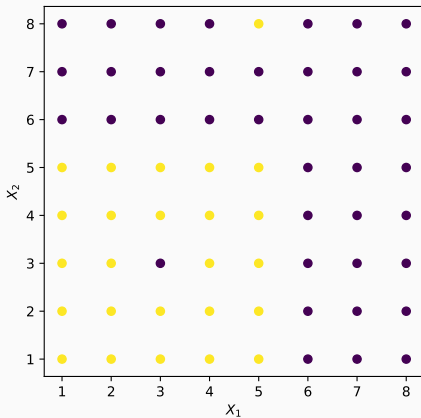
⋮

Repetition of samples is possible.

We can train the same classifier/models on each of these different “Bagging Rounds”.

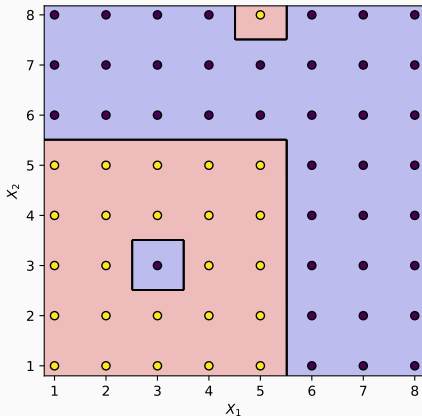
Bagging : Classification Example

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



Bagging : Classification Example

Decision Boundary for decision tree with depth 6.



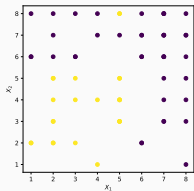
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Lets use bagging with ensemble of 5 trees.

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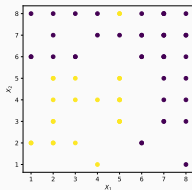
Round - 1



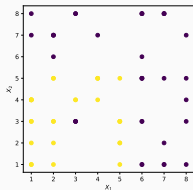
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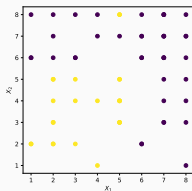
Round - 2



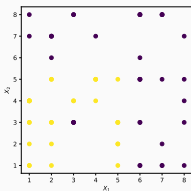
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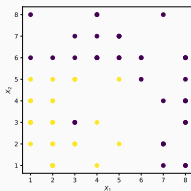
Round - 1



Round - 2



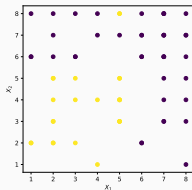
Round - 3



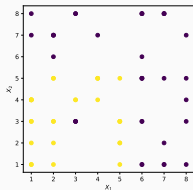
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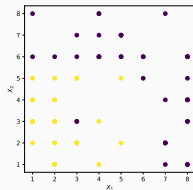
Round - 1



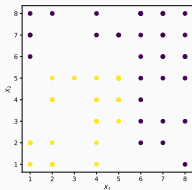
Round - 2



Round - 3



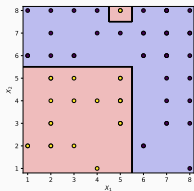
Round - 4



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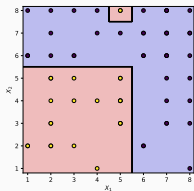
Round - 1



Tree Depth = 4

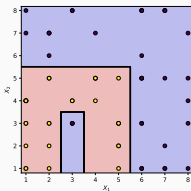
Bagging : Classification Example

Round - 1



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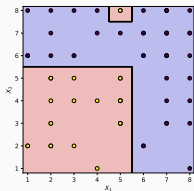
Round - 2



Tree Depth = 5

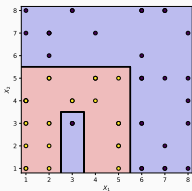
Bagging : Classification Example

Round - 1



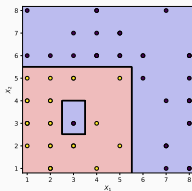
Tree Depth = 4

Round - 2



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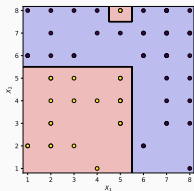
Round - 3



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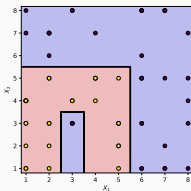
Bagging : Classification Example

Round - 1



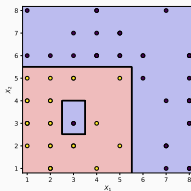
Tree Depth = 4

Round - 2



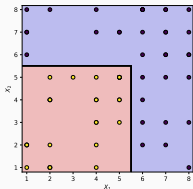
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Round - 3



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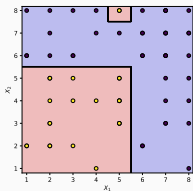
Round - 4



Tree Depth = 2

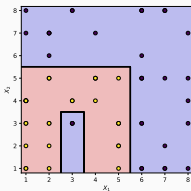
Bagging : Classification Example

Round - 1



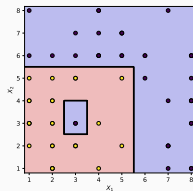
Tree Depth = 4

Round - 2



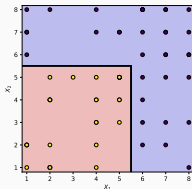
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Round - 3



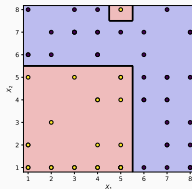
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Round - 4



Tree Depth = 2

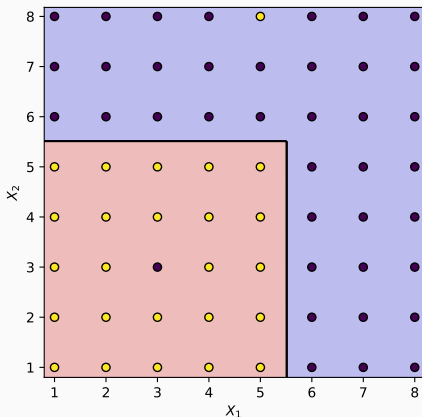
Round - 5



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Bagging : Classification Example

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



Summary

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

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

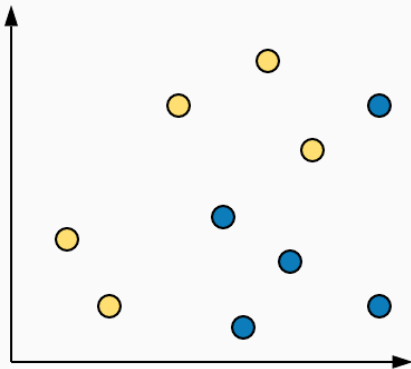
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- All learners are incrementally built.
- Incremental building: Incrementally try to classify “harder” samples correctly.

Boosting : AdaBoost

Consider we have a dataset of N samples.

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

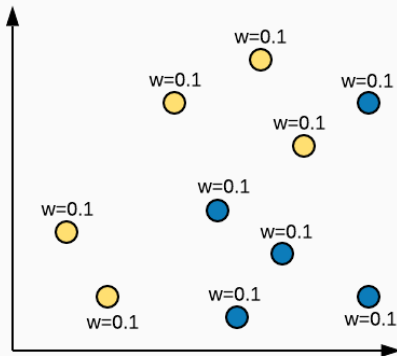


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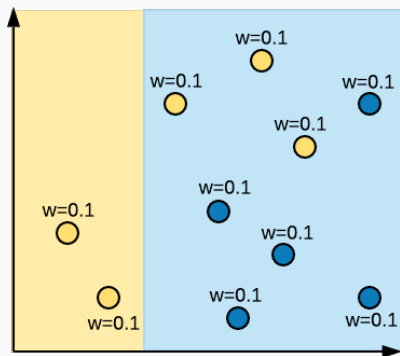


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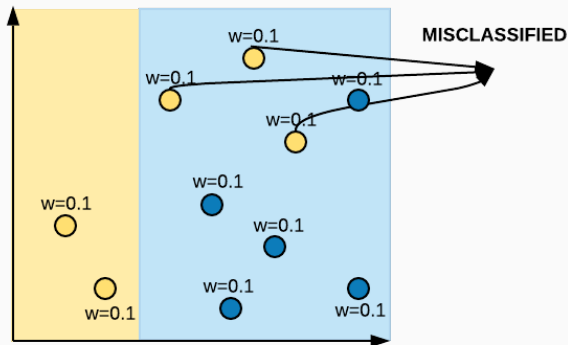


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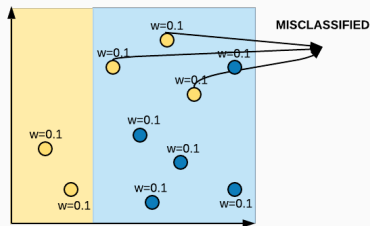
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2.2 Compute the weighted error, $err_m = \frac{\sum_i w_i(\text{incorrect})}{\sum_i w_i}$



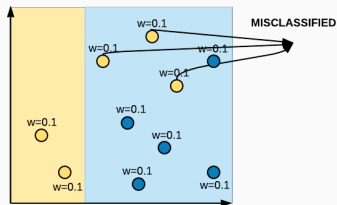
$$err_1 = \frac{0.3}{1}$$

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



$$err_1 = \frac{0.3}{1}$$
$$\alpha_1 = \frac{1}{2} \log \left(\frac{1 - 0.3}{0.3} \right) = 0.42$$

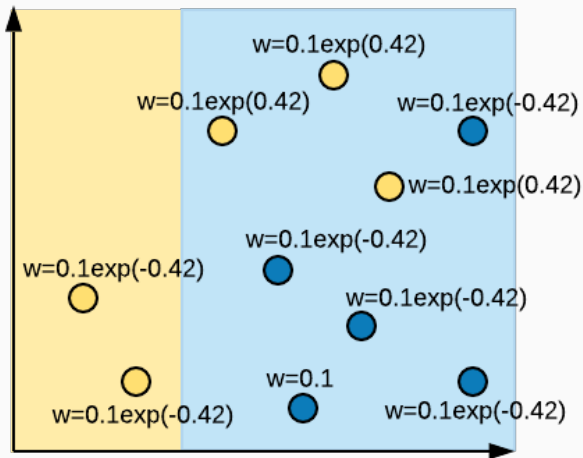
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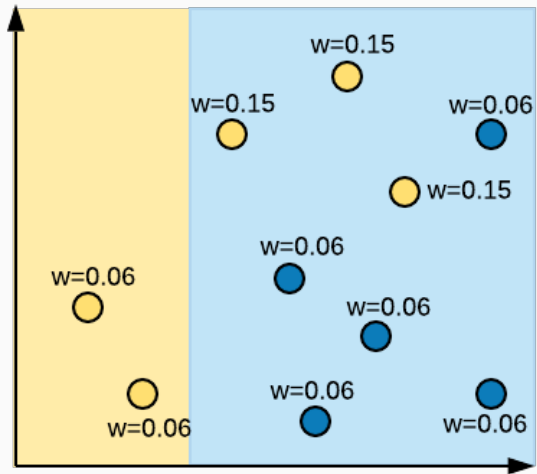
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Boosting : AdaBoost



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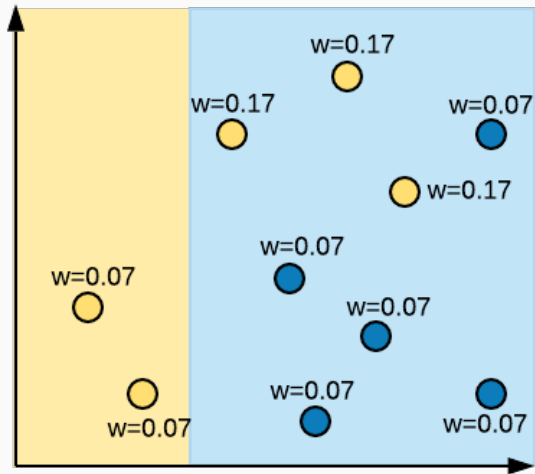
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 - 2.5 For samples which were predicted incorrectly, $w_i = w_i e^{\alpha_m}$
 - 2.6 Normalize w_i 's to sum up to 1.

Boosting : AdaBoost



Boosting : AdaBoost

Consider we have a dataset of N samples.

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

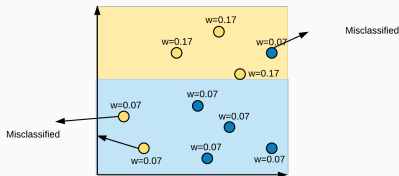
1. Initialize weights of data samples, $w_i = \frac{1}{N}$

2. For $m = 1 \dots M$

2.1 Learn classifier using current weights w_i 's

2.2 Compute the weighted error, $err_m = \frac{\sum_i w_i(\text{incorrect})}{\sum_i w_i}$

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



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

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

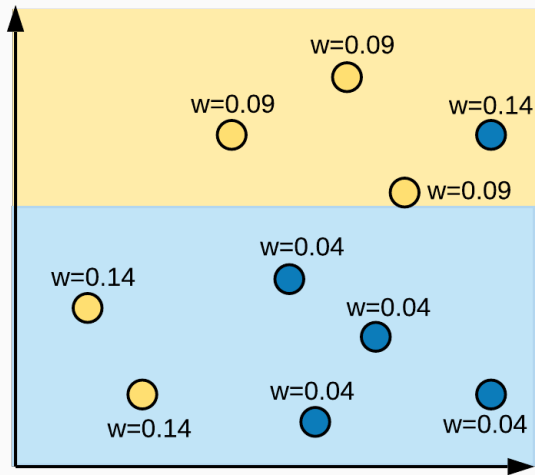
Boosting : AdaBoost

Consider we have a dataset of N samples.

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1. Initialize weights of data samples, $w_i = \frac{1}{N}$
2. For $m = 1 \dots M$
 - 2.1 Learn classifier using current weights w_i 's
 - 2.2 Compute the weighted error, $err_m = \frac{\sum_i w_i(\text{incorrect})}{\sum_i w_i}$
 - 2.3 Compute $\alpha_m = \frac{1}{2} \log_e \left(\frac{1 - err_m}{err_m} \right)$
 - 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



Boosting : AdaBoost

Consider we have a dataset of N samples.

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

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

2. For $m = 1 \dots M$

2.1 Learn classifier using current weights w_i 's

2.2 Compute the weighted error, $err_m = \frac{\sum_i w_i(\text{incorrect})}{\sum_i w_i}$

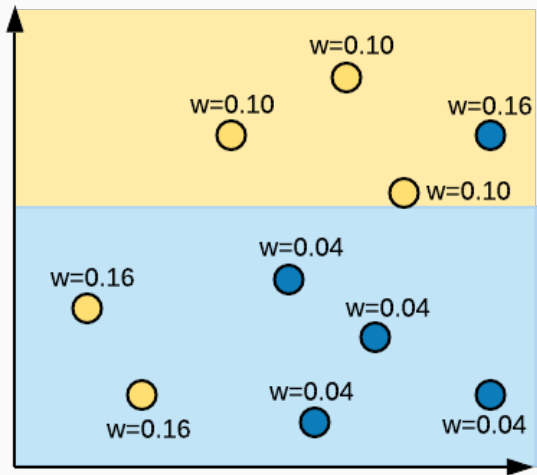
2.3 Compute $\alpha_m = \frac{1}{2} \log_e \left(\frac{1 - err_m}{err_m} \right)$

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



Boosting : AdaBoost

Consider we have a dataset of N samples.

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

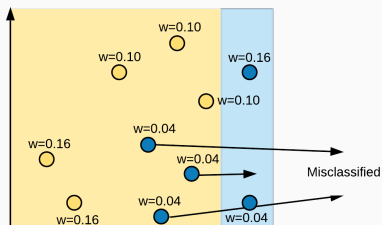
1. Initialize weights of data samples, $w_i = \frac{1}{N}$

2. For $m = 1 \dots M$

2.1 Learn classifier using current weights w_i 's

2.2 Compute the weighted error, $err_m = \frac{\sum_i w_i(\text{incorrect})}{\sum_i w_i}$

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



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

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

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.

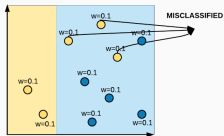
Testing

- 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:
- $\text{SIGN}(\alpha_1 h_1(x) + \alpha_2 h_2(x) + \dots + \alpha_M h_M(x))$

Example

Boosting: Adaboost

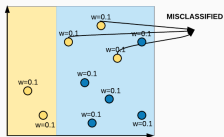
Example



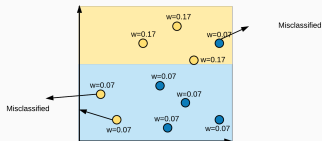
$$\alpha_1 = 0.42$$

Boosting: Adaboost

Example



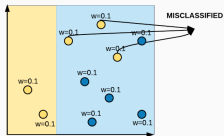
$$\alpha_1 = 0.42$$



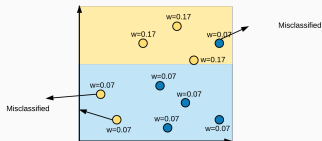
$$\alpha_2 = 0.66$$

Boosting: Adaboost

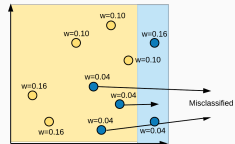
Example



$$\alpha_1 = 0.42$$



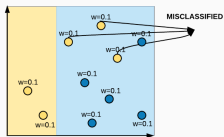
$$\alpha_2 = 0.66$$



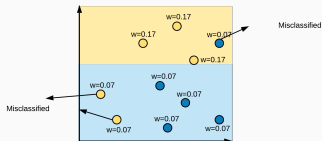
$$\alpha_3 = 0.99$$

Boosting: Adaboost

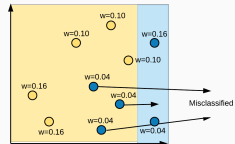
Example



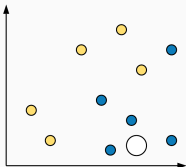
$$\alpha_1 = 0.42$$



$$\alpha_2 = 0.66$$

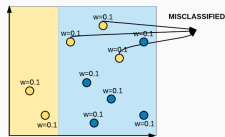


$$\alpha_3 = 0.99$$

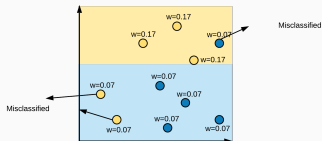


Boosting: Adaboost

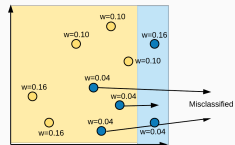
Example



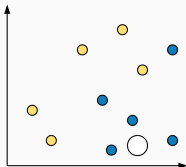
$$\alpha_1 = 0.42$$



$$\alpha_2 = 0.66$$



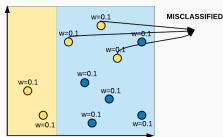
$$\alpha_3 = 0.99$$



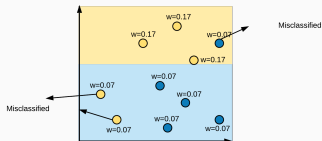
Let us say, yellow class is +1 and blue class is -1

Boosting: Adaboost

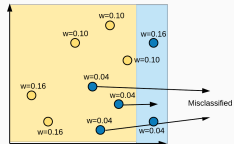
Example



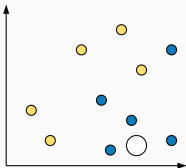
$$\alpha_1 = 0.42$$



$$\alpha_2 = 0.66$$



$$\alpha_3 = 0.99$$



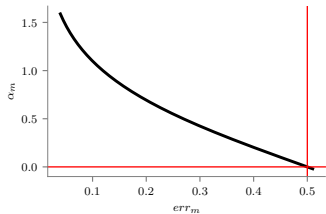
Let us say, yellow class is +1 and blue class is -1

$$\text{Prediction} = \text{SIGN}(0.42 * -1 + 0.66 * -1 + 0.99 * +1) = \text{Negative} = \text{blue}$$

Intuition behind weight update formula

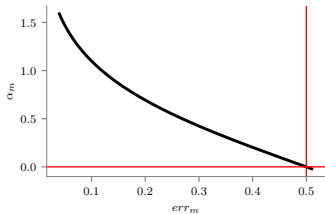
Intuition behind weight update formula

Notebook: [boosting-explanation.ipynb](#)

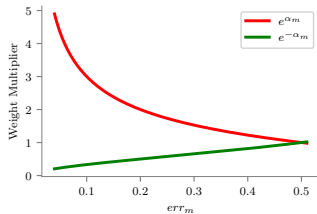


Intuition behind weight update formula

Notebook: [boosting-explanation.ipynb](#)



Notebook: [boosting-explanation.ipynb](#)



From Paper: Improving Regressors using Boosting Techniques

Our problem will be that the modeling error is also nonzero because we have to determine the model in the presence of noise. Since we don't know the probability distributions, we approximate the expectation of the ME and PE using the sample ME (if the truth is known) and sample PE and then average over multiple experiments.

In the following discussion, we detail both bagging and boosting. We then discuss how to build trees which are the basic building blocks of our regression machines and use these ensembles on some standard test functions.

2. BAGGING

The following is a paraphrase of Breiman (1996b) with some difference in notation. Suppose we pick with replacement N_1 examples from the training set of size N_1 and call the k 'th set of observations O_k . Based on these observations, we form a predictor $y^{(k)}(\mathbf{x}, O_k)$. Because we are sampling with replacement, we may have multiple observations or no observations of a particular training example. Sampling with replacement is sometimes termed bootstrap sampling [Efron and Tibshirani (1993)] and therefore this method is called bootstrap aggregating or bagging for short. The ensemble predictor is formed from the approximation to the expectation over all the observation sets, i.e. $E_{O_k}[y^{(k)}(\mathbf{x}, O_k)]$ by using the average of the outputs of all the predictors. Breiman discusses which algorithms are good candidates for predictors and concludes that the best predictors are unstable, i.e., a small change in the training set O_k causes a large change in the predictor $y^{(k)}(\mathbf{x}, O_k)$. Good candidates are regression trees and neural nets.

3. BOOSTING

In bagging, each training example is equally likely to be picked. In boosting, the probability of a particular example being in the training set of a particular machine depends on the performance of the prior machines on that example. The following is a modification of *Adaboost.R* [Freund and Schapire (1996a)].

Initially, for each training pattern we assign a weight $w_i=1$ $i=1, \dots, N_1$

Repeat the following while the average loss \bar{L} defined

set. Each machine makes a hypothesis: $h_i: \mathbf{x} \rightarrow y$

3. Pass *every* member of the training set through this machine to obtain a prediction $y^{(i)}(\mathbf{x}_i)$ $i=1, \dots, N_1$.

4. Calculate a loss for each training sample $L_i = L \left[\left| y^{(i)}(\mathbf{x}_i) - y_i \right| \right]$. The loss L may be of any functional form as long as $L \in [0, 1]$. If we let

$$D = \sup \left| y^{(i)}(\mathbf{x}_i) - y_i \right| \quad i=1, \dots, N_1$$

then we have three candidate loss functions:

$$L_1 = \frac{\left| y^{(i)}(\mathbf{x}_i) - y_i \right|}{D} \quad (\text{linear})$$

$$L_2 = \frac{\left| y^{(i)}(\mathbf{x}_i) - y_i \right|^2}{D^2} \quad (\text{square law})$$

$$L_3 = 1 - \exp \left[\frac{- \left| y^{(i)}(\mathbf{x}_i) - y_i \right|}{D} \right] \quad (\text{exponential})$$

5. Calculate an average loss: $\bar{L} = \sum_{i=1}^{N_1} L_i \beta_i$

6. Form $\beta = \frac{\bar{L}}{1 - \bar{L}}$. β is a measure of confidence in the predictor. Low β means high confidence in the prediction.

7. Update the weights: $w_i \rightarrow w_i \beta^{**} [1 - L_i]$, where $**$ indicates exponentiation. The smaller the loss, the more the weight is reduced making the probability smaller that this pattern will be picked as a member of the training set for the next machine in the ensemble.

8. For a particular input \mathbf{x}_i , each of the T machines makes a prediction h_i , $i=1, \dots, T$. Obtain the cumulative prediction h_T using the T predictors:

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 ($i \in \{1 \dots N\}$), 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

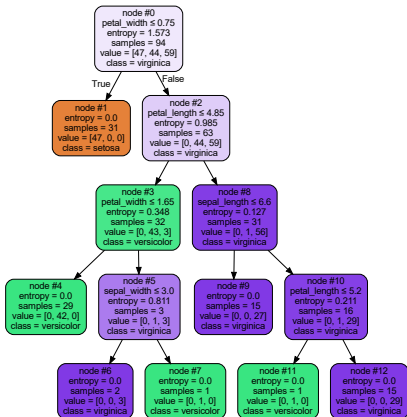
Dataset

	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

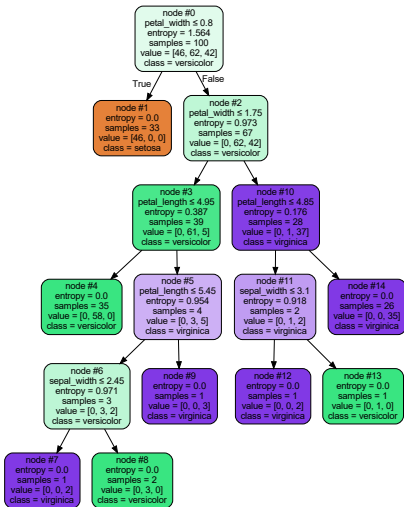
Decision Tree # 0

Notebook: ensemble-feature-importance.ipynb



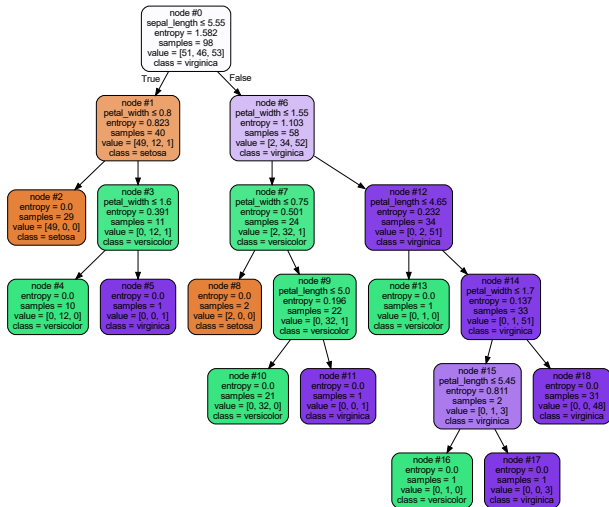
Decision Tree # 1

Notebook: ensemble-feature-importance.ipynb



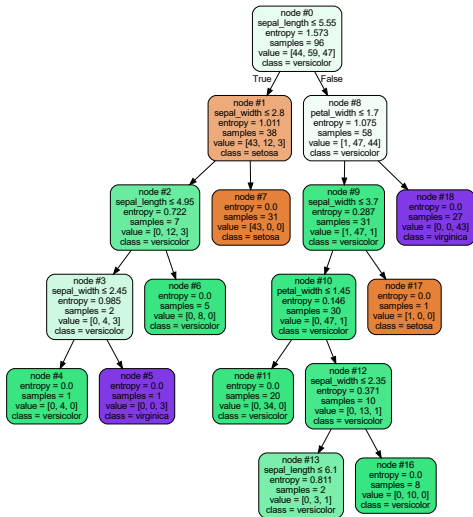
Decision Tree # 2

Notebook: ensemble-feature-importance.ipynb



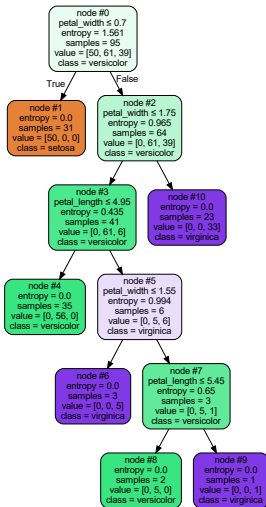
Decision Tree # 3

Notebook: ensemble-feature-importance.ipynb



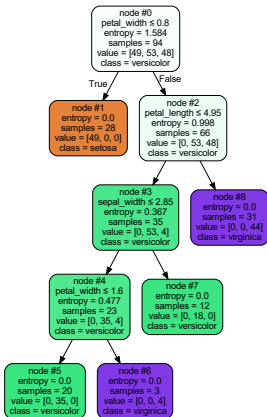
Decision Tree # 4

Notebook: ensemble-feature-importance.ipynb



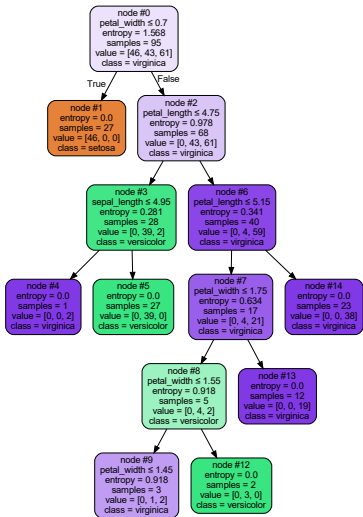
Decision Tree # 5

Notebook: ensemble-feature-importance.ipynb



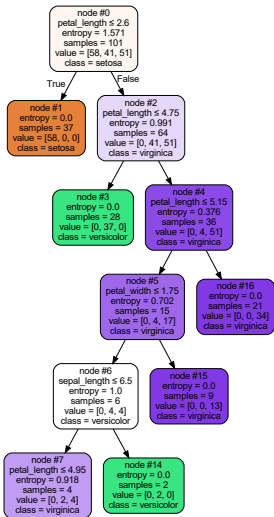
Decision Tree # 6

Notebook: ensemble-feature-importance.ipynb



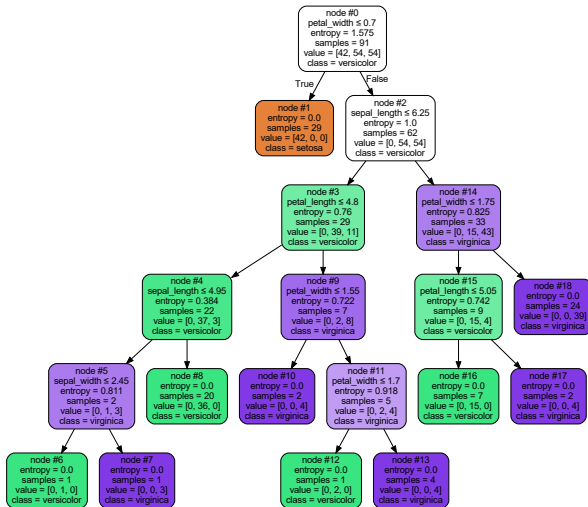
Decision Tree # 7

Notebook: ensemble-feature-importance.ipynb



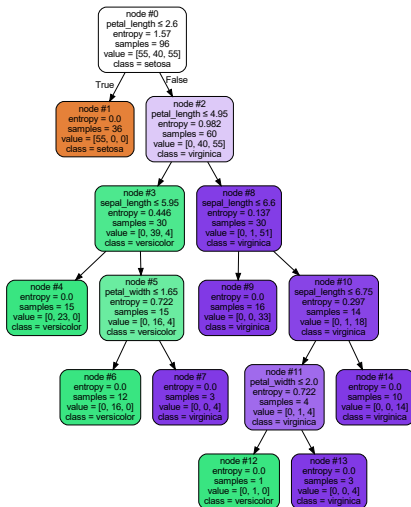
Decision Tree # 8

Notebook: ensemble-feature-importance.ipynb

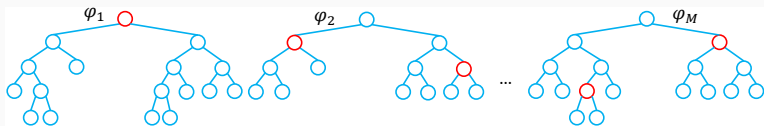


Decision Tree # 9

Notebook: ensemble-feature-importance.ipynb



Feature Importance¹



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

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

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 :

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

¹Slide Courtesy Gilles Louppe

Computed Feature Importance

Notebook: ensemble-feature-importance.ipynb

