

Ensemble Methods, Random Forests and Boosting

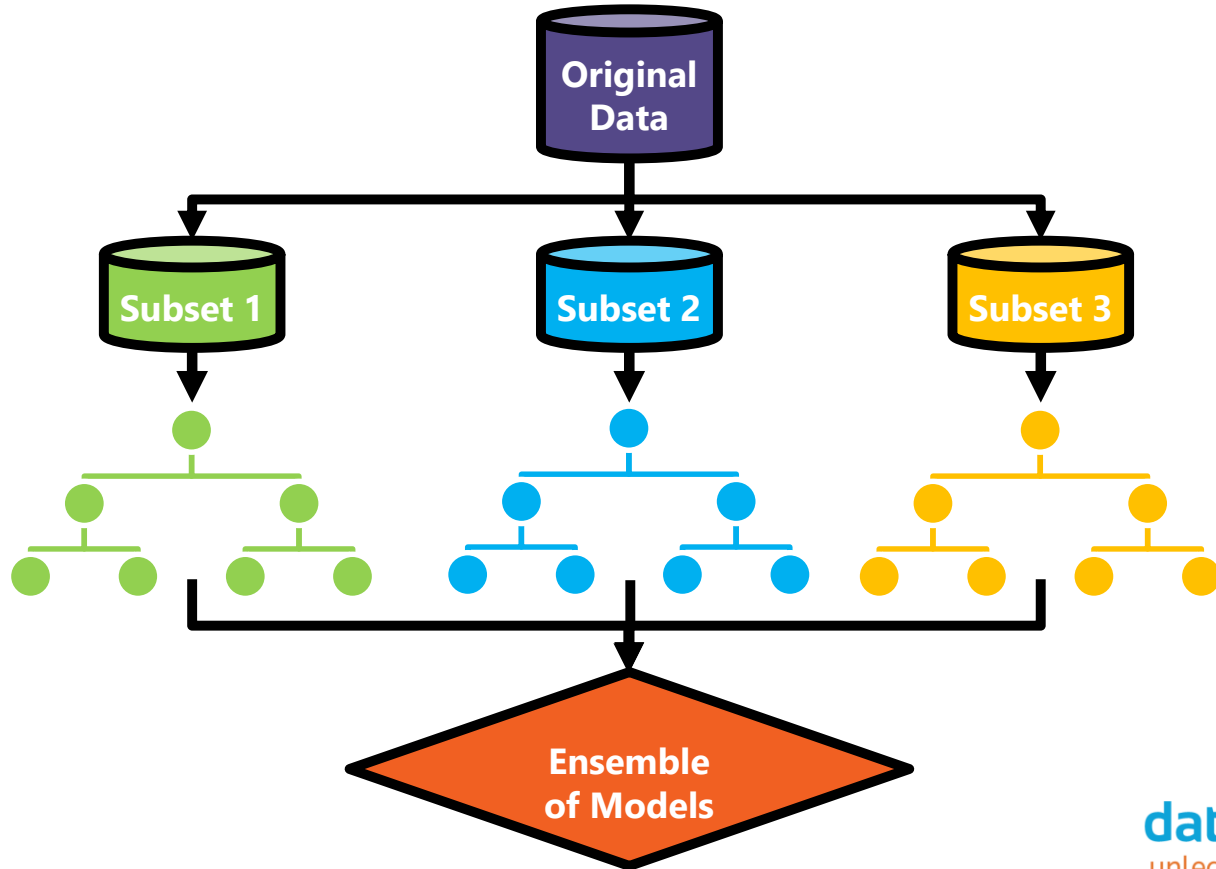
Ensemble Methods

- Overview and rationale
- Why ensemble?
 - Binomial Distribution
- Ensemble models
 - Bagging
 - Random Forests
 - Boosting

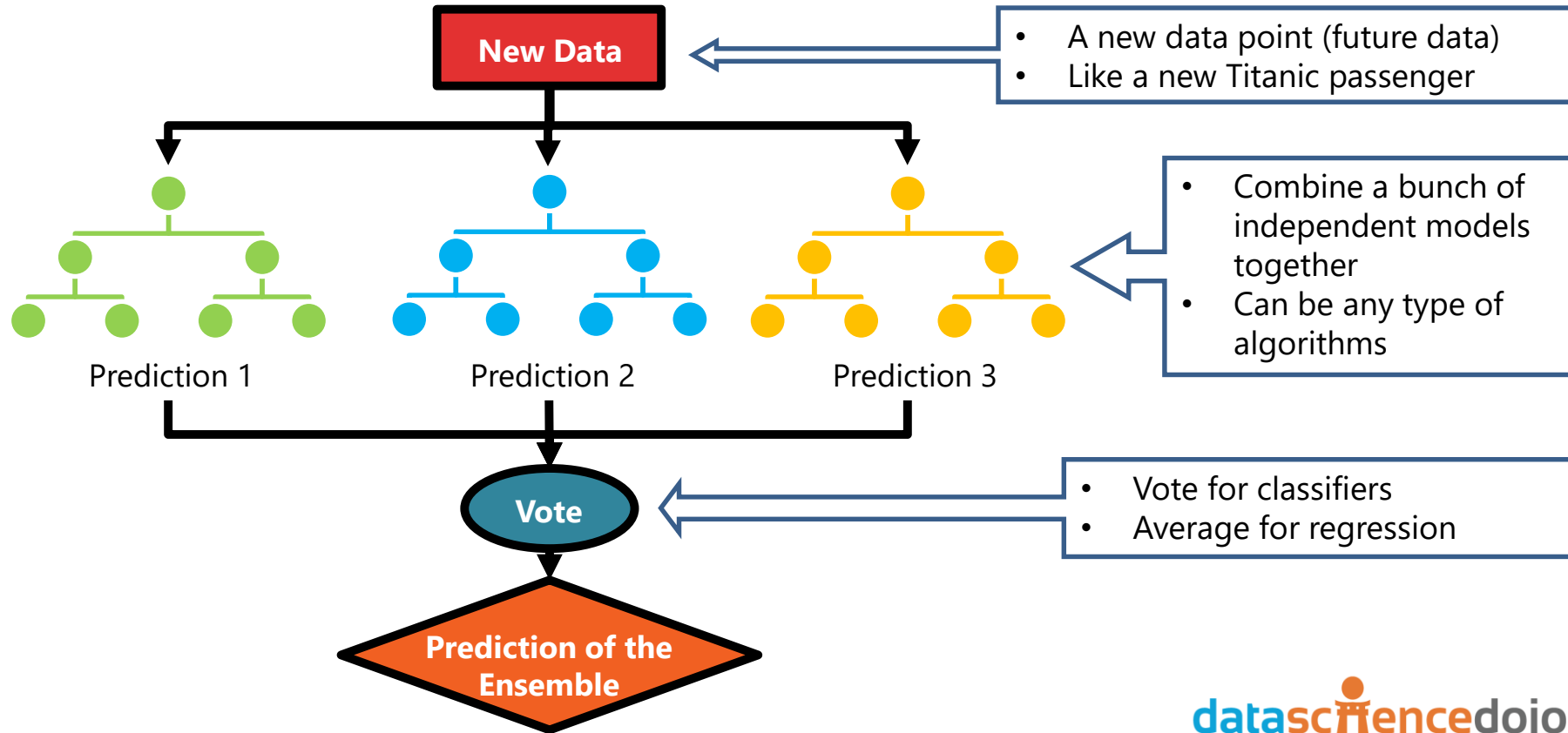
Ensemble Methods

- Improve model performance by combining multiple models
- Can be used for both **classification** and **regression**

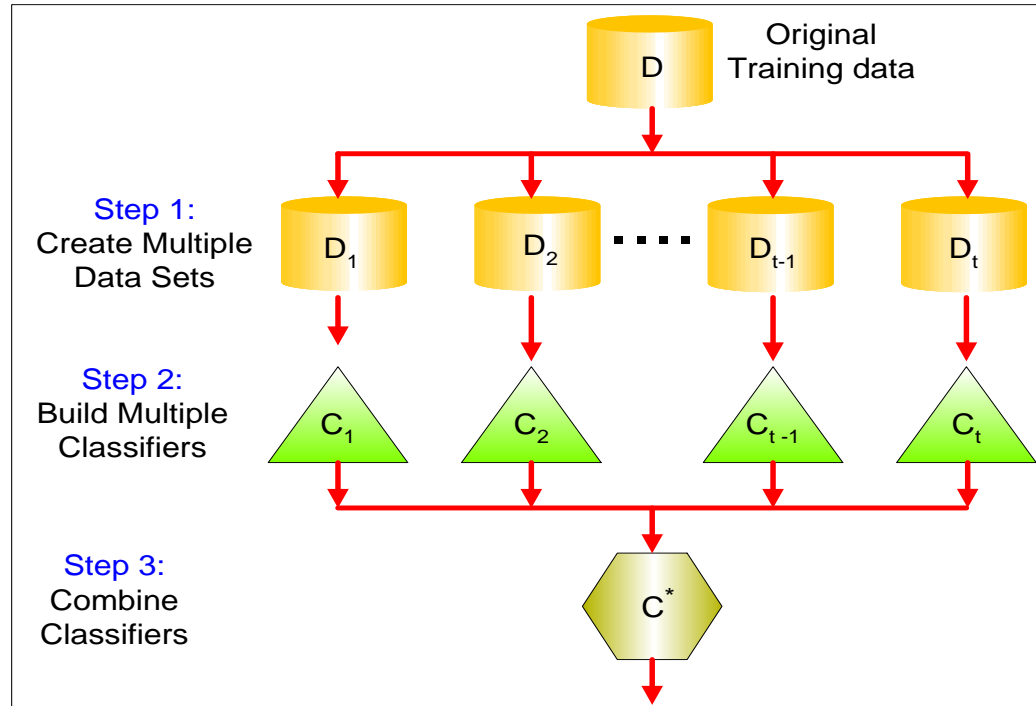
Ensemble of Decision Tree Models



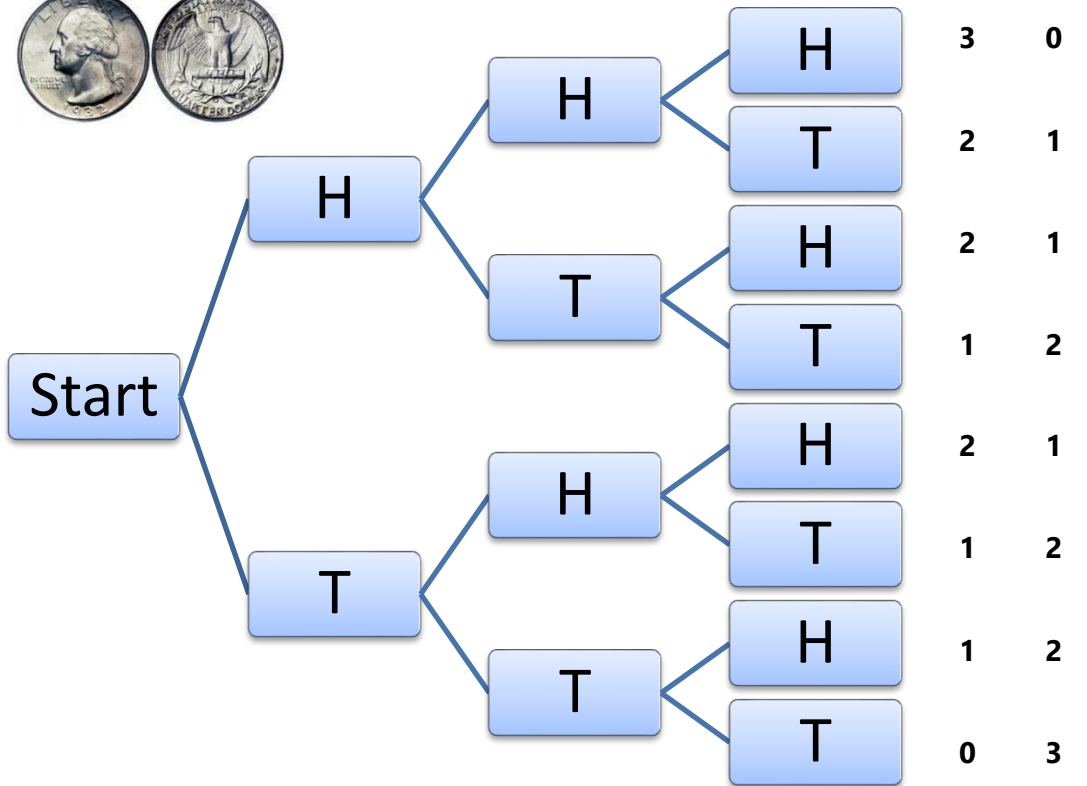
Ensemble of Decision Tree Models



General Idea of Ensemble Methods



Binomial Distribution



Consider...

- Flipping a coin 3 times in a row
- Each coin flip is considered **independent**
- A fair coin has a 50% rate of heads and tails

Properties of a binomial distribution:

- Well studied statistical property
- You cannot tell how each individual coin toss session will behave or their individual outcomes (such as HHH or HTH)
- However you can tell and **predict** the behavior of the aggregations of many coin toss sessions

Binomial Distribution

$$f(k; n, p) = \Pr(X = k) = \binom{n}{k} p^k (1 - p)^{n-k}$$

Exercises

Applications

- Number of life insurance holders who will claim in a given period
- Number of loan holders who will default in a certain period
- Number of false starts of a car in n attempts
- Number of faulty items in n samples from a production line
- **AND** Ensemble Methods

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:

$$\sum_{i=13}^{25} \binom{25}{i} \varepsilon^i (1-\varepsilon)^{25-i} = 0.06$$

Examples of Ensemble Methods

Bagging

- All classifiers are created equal

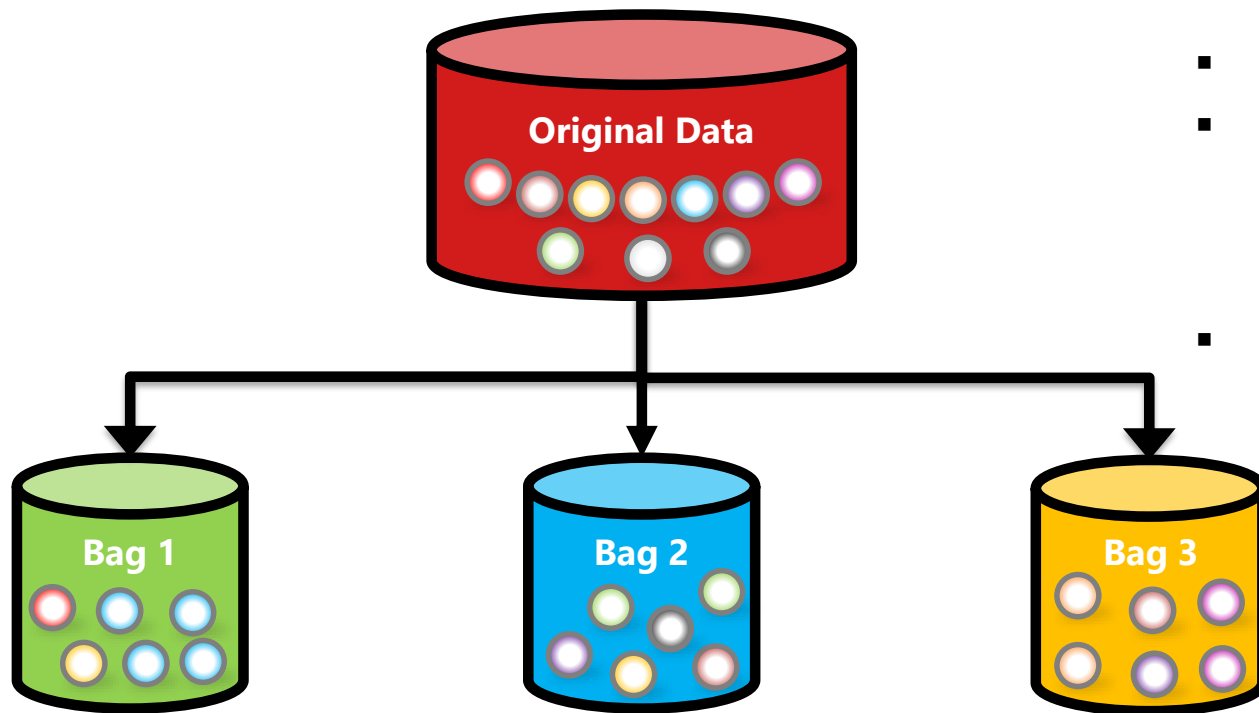
Boosting

- **Not** all classifiers are created equal

Ensemble Methods

- Overview and rationale
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- **Bagging**
- Random Forests
- Boosting
- AdaBoost

Bagging Samples (rows)



- Sampling with replacement
- Build a projection of the data based upon the original distribution of the data
- Each tree will now see a different dataset, which will spawn **different** trees

Bagging

- Sampling with replacement

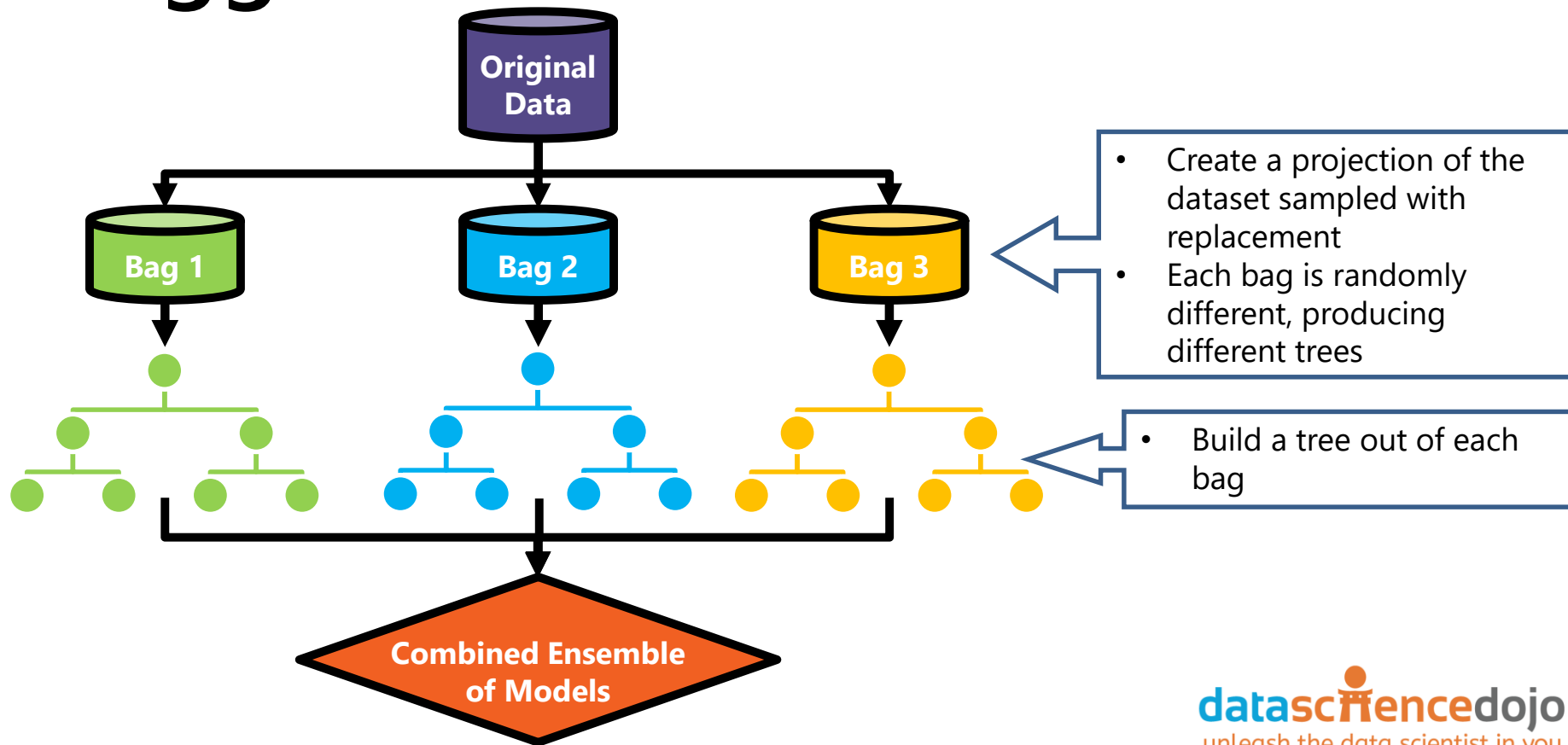
Original Data	1	2	3	4	5	6	7	8	9	10
Bagging (Round 1)	7	8	10	8	2	5	10	10	5	9
Bagging (Round 2)	1	4	9	1	2	3	2	7	3	2
Bagging (Round 3)	1	8	5	10	5	5	9	6	3	7

- Build classifier on each bootstrap sample
- For a training data of size n , each sample has probability $[1 - (1 - 1/n)^n]$ of being selected
- If n is large, this approximates to $1 - 1/e \sim 0.632$

Bagging

- Reduces variance in estimate
- Prevents overfitting
- Robust to outliers

Bagged Decision Forest



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What Is A Random Forest?

- An ensemble classifier using many decision tree models
- Can be used for classification or regression
- Accuracy and variable importance information is built-in

How Do Random Forests Work?

- A different subset of the training data are selected ($\sim 2/3$), with replacement, to train each tree
- Remaining training data (aka out-of-bag data or simply OOB) is used to estimate error and variable importance
- Class assignment is made by the number of votes from all of the trees, and for regression, the average of the results is used

Which Features Are Used For Learning?

- A randomly selected subset of variables is used to split each node
- The number of variables used is decided by the user (mtry parameter in R)
- A smaller subset produces less correlation (lower error rate)

Rules of Thumb

- Given:
 - **N**: Total number of training data points
 - **M**: Number of features in training data
 - **m**: Number of features randomly selected for training each node
- Sample the data with replacement N times for building the training data for each tree.
- $m \ll M$
- Classification: $m = \sqrt{M}$
- Regression: $m = M/3$

Learning a Forest

- Dividing training examples into T subsets improves generalization
 - Reduces memory requirements & training time
- Train each decision tree t on subset I_t
 - Same decision tree learning as before
- Multi-core friendly (GPU implementation)

Implementation Details

- How many features and thresholds to try?
 - Just one = “extremely randomized” [Geurts *et al.* 06]
 - Few → fast training, may under-fit, may be too deep
 - Many → slower training, may over-fit
- When to stop growing the tree?
 - Maximum depth
 - Minimum entropy gain
 - Delta class distribution
 - Pruning

Random Forest: R Exercise

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Boosting

- An iterative procedure to adaptively change distribution of training data by focusing more on previously misclassified records
 - Initially, all N records are assigned equal weights
 - Unlike bagging, weights may change at the end of boosting round

Boosting

- Records that are wrongly classified will have their weights increased
- Records that are classified correctly will have their weights decreased

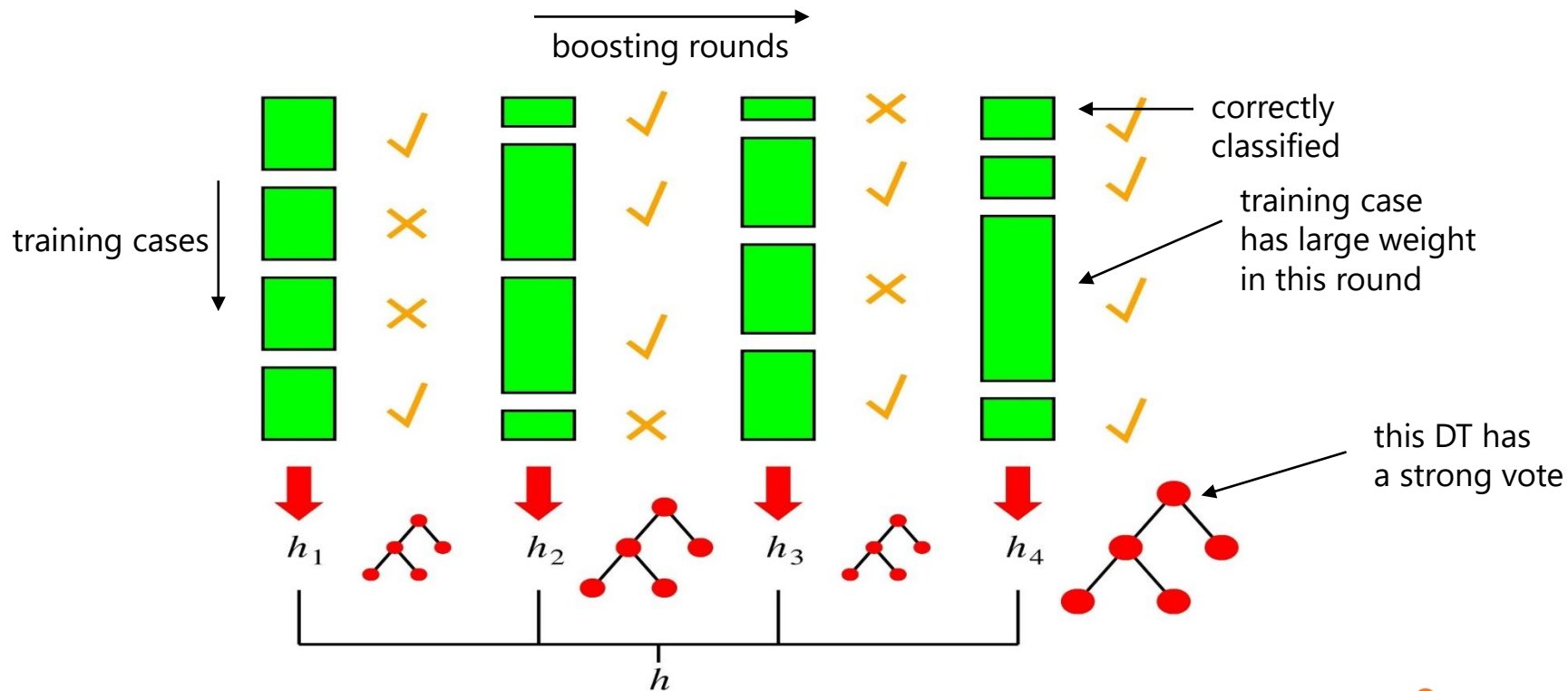
Original Data	1	2	3	4	5	6	7	8	9	10
Boosting (Round 1)	7	3	2	8	7	9	4	10	6	3
Boosting (Round 2)	5	4	9	4	2	5	1	7	4	2
Boosting (Round 3)	4	4	8	10	4	5	4	6	3	4

- Example 4 is hard to classify
- Its weight is increased, therefore it is more likely to be chosen again in subsequent rounds

Boosting Intuition

- We adaptively weight each data case.
- Data cases which are wrongly classified get high weight (the algorithm will focus on them).
- Each boosting round learns a new (simple) classifier on the weighed dataset.
- These classifiers are weighed to combine them into a single powerful classifier.
- Classifiers that obtain low training error rate have high weight.
- We stop by monitoring a hold out set.

Boosting in a Picture



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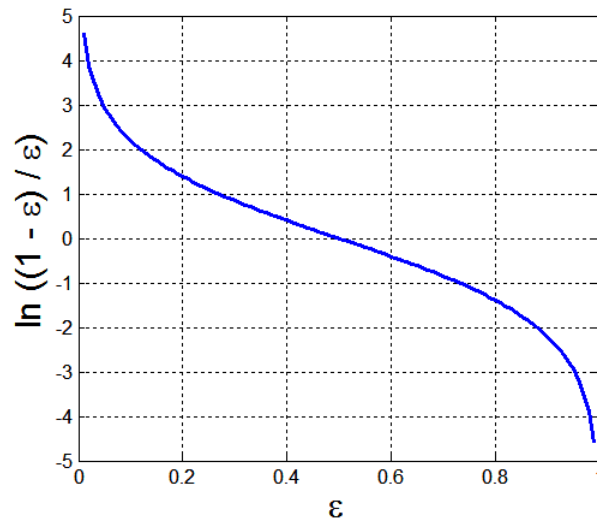
AdaBoost (Adaptive Boosting)

- Base classifiers: C_1, C_2, \dots, C_T
- Error rate [Weighted loss function]:

$$\varepsilon_i = \frac{1}{N} \sum_{j=1}^N w_j \delta(C_i(x_j) \neq y_j)$$

- Importance of a classifier:

$$\alpha_i = \frac{1}{2} \ln \left(\frac{1 - \varepsilon_i}{\varepsilon_i} \right)$$



AdaBoost

- Weight update:

$$w_i^{(j+1)} = \frac{w_i^{(j)}}{Z_j} \begin{cases} \exp^{-\alpha_j} & \text{if } C_j(x_i) = y_i \\ \exp^{\alpha_j} & \text{if } C_j(x_i) \neq y_i \end{cases}$$

where Z_j is the normalization factor

- If any intermediate rounds produce error rate higher than 50%, the weights are reverted back to $1/n$ and the resampling procedure is repeated.
- Classification: $C^*(x) = \arg \max_y \sum_{j=1}^T \alpha_j \delta(C_j(x) = y)$

Common Pitfall

A Random Forest and a Boosted Decision Tree
are **not** the same

QUESTIONS