

Lecture 11: 13 May, 2021

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Data Mining and Machine Learning
April–July 2021

Limitations of classification models

- **Bias** : Expressiveness of model limits classification
 - For instance, linear separators
- **Variance**: Variation in model based on sample of training data
 - Shape of a decision tree varies with distribution of training inputs

Models with high variance are expressive but **unstable**

- In principle, a decision tree can capture an arbitrarily complex classification criterion
- Actual structure of the tree depends on impurity calculation
- Danger of overfitting: model tied too closely to training set
- Is there an alternative to pruning?

Ensemble models

- Sequence of independent training data sets D_1, D_2, \dots, D_k
- Generate models M_1, M_2, \dots, M_k
- Take this **ensemble** of models and “average” them
 - For regression, take the mean of the predictions
 - For classification, take a vote among the results and choose the most popular one
- **Challenge:** Infeasible to get large number of independent training samples
- Can we build independent models from a single training data set?
 - Strategy to build the model is fixed
 - Same data will produce same model

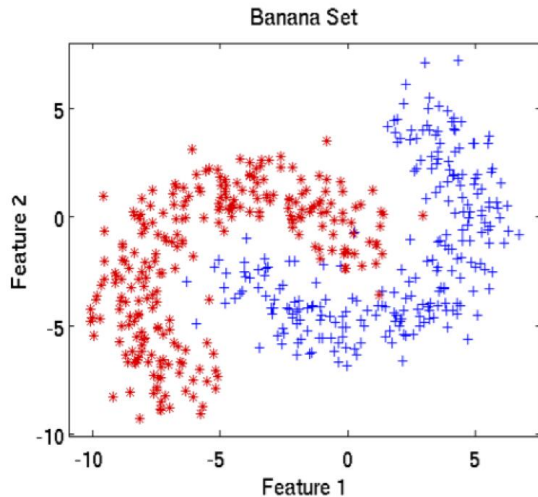
Bootstrap Aggregating = Bagging

- Training data has N items
 - $TD = \{d_1, d_2, \dots, d_N\}$
- Pick a random sample **with replacement**
 - Pick an item at random (probability $\frac{1}{N}$)
 - Put it back into the set
 - Repeat K times
- Some items in the sample will be repeated
- If sample size is same as data size ($K = N$), expected number of distinct items is $(1 - \frac{1}{e}) \cdot N$
 - Approx 63.2%

Bootstrap Aggregating = Bagging

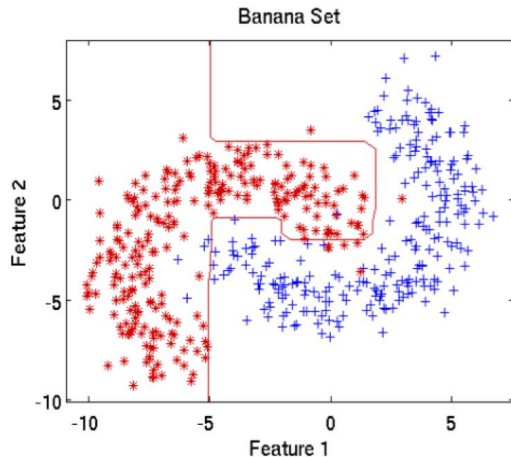
- Sample with replacement of size N : bootstrap sample
 - Approx 2/3 of full training data
- Take k such samples
- Build a model for each sample
 - Models will vary because each uses different training data
- Final classifier: report the majority answer
 - Assumptions: binary classifier, k odd
- Provably reduces variance

Bagging with decision trees



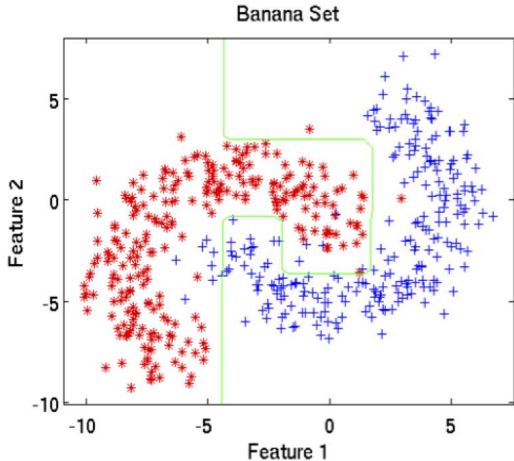
Training data

Bagging with decision trees



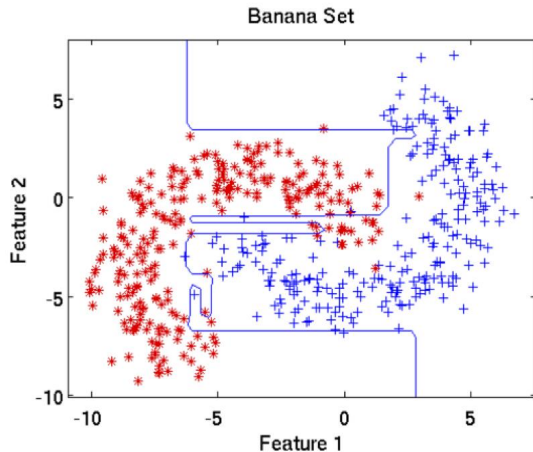
Decision boundary produced
by one tree

Bagging with decision trees



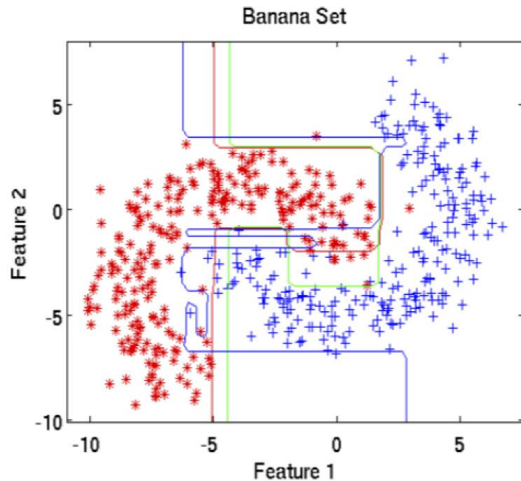
Decision boundary produced by a second tree

Bagging with decision trees



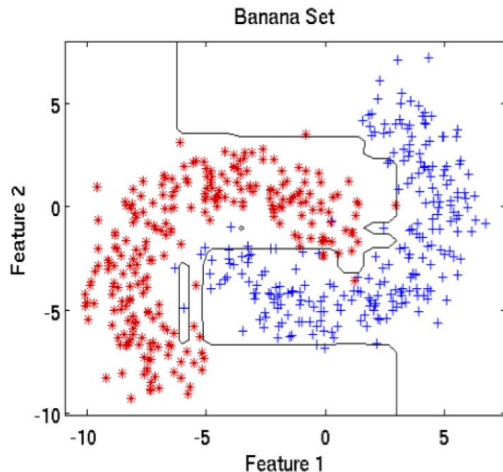
Decision boundary produced by a third tree

Bagging with decision trees



Three trees and final boundary
overlaid

Bagging with decision trees



Final result from bagging all trees.

When to use bagging

- Bagging improves performance when there is high variance
 - Independent samples produce sufficiently different models
- A model with low variance will not show improvement
 - **k-nearest neighbour** classifier
 - Given an unknown input, find k nearest neighbours and choose majority
 - Across different subsets of training data, variation in k nearest neighbours is relatively small
 - Bootstrap samples will produce similar models

Random Forest

- Applying bagging to decision trees with a further twist
- As before, k bootstrap samples D_1, D_2, \dots, D_k
- For each D_i , build decision tree T_i as follows
 - Each data item has M attributes
 - Normally, choose maximum impurity gain among M attributes, then best among remaining $M - 1, \dots$
 - Instead, fix a small limit $m < M$ — say $m = \log_2 M + 1$
 - At each level, choose a random subset of available attributes of size m
 - Evaluate only these m attributes to choose next query
 - No pruning — build each tree to the maximum
- Final classifier: vote on the results returned by T_1, T_2, \dots, T_k

Random Forest ...

- Theoretically, overall error rate depends on two factors
 - **Correlation** between pairs of trees — higher correlation results in higher overall error rate
 - **Strength (accuracy)** of each tree — higher strength of individual trees results in lower overall error rate
- Reducing m , the number of attributes examined at each level, reduces correlation and strength
 - Both changes influence the error rate in opposite directions
- Increasing m increases both correlation and strength
- Search for a value of m that optimizes overall error rate

Out of bag error estimate

- Each bootstrap sample omits about $1/3$ of the data items
- Hence, each data item is omitted by about $1/3$ of the samples
- If data item d does not appear in bootstrap sample D_i , d is **out of bag (oob)** for D_i
- **Oob classification** — for each d , vote only among those T_i where d is oob for D_i
- Use oob samples to validate the model
 - Estimate generalization error rate of overall model based on error rate of oob classification
 - Do not require a separate test data set

Feature importance

- What is the impurity gain of a feature across trees in ensemble?
- Variation due to randomness of samples
- Even greater variation in a random forest
- Compute weighted average of impurity gain
 - Weight is given by number of training samples at the node