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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

Limitations of classification models

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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 $D_1, D_2, \ldots, D_k$
- Generate models $M_1, M_2, \ldots, M_k$
- 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

Hard voting   Majority of 0/1 decision

Probabilities $\rightarrow$ $[0.21, 0.79]$

Add probabilities $\uparrow$ 0 $\uparrow$ 1

Soft voting

Ensemble models

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- Take this ensemble of models and "average" them
  - For regression, take the mean of the predictions
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- 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

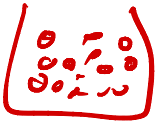
Cross Validation

90% - 10%

$D_i \cap D_j$ overlap on 80%

Bootstrap Aggregating = Bagging

- Training data has N items
  - $TD = \{d_1, d_2, \ldots, d_N\}$
- Pick a random sample with replacement



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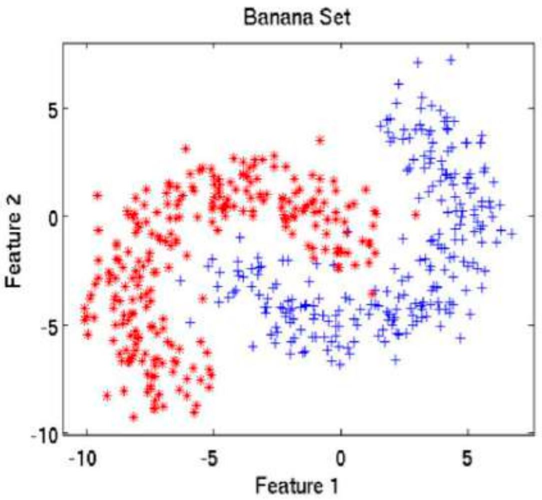
- Some items in the sample will be repeated
- If sample size is same as data size ($K = N$), expected number of distinct items is $(1 - \frac{1}{e}) \cdot N$
  - Approx 63.2%

Bootstrap Aggregating = Bagging

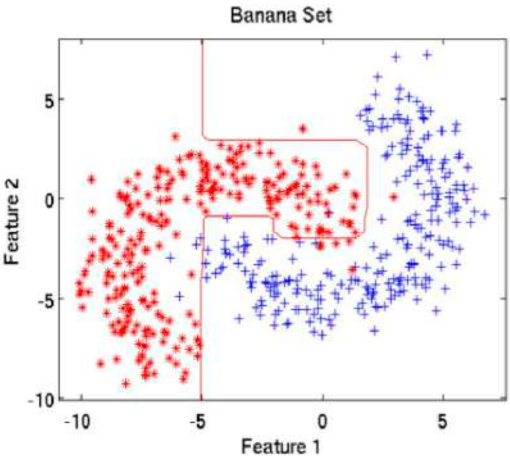
- Sample with replacement of size N : bootstrap sample
  - Approx 2/3 of full training data
- Take k such samples
- Build a model for each sample
  - Models will vary because each uses different training data
- Final classifier: report the majority answer
  - Assumptions: binary classifier, k odd
- Provably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

Bagging with decision trees



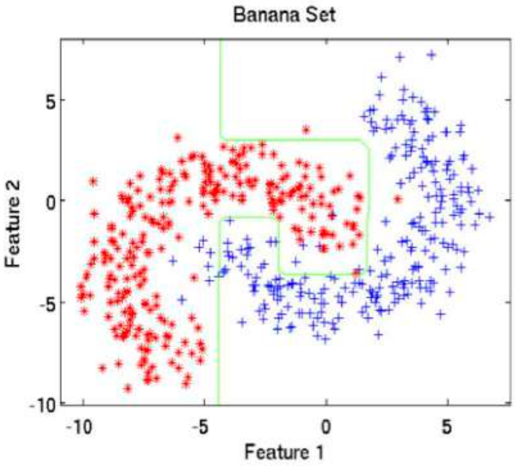
Training data

Bagging with decision trees



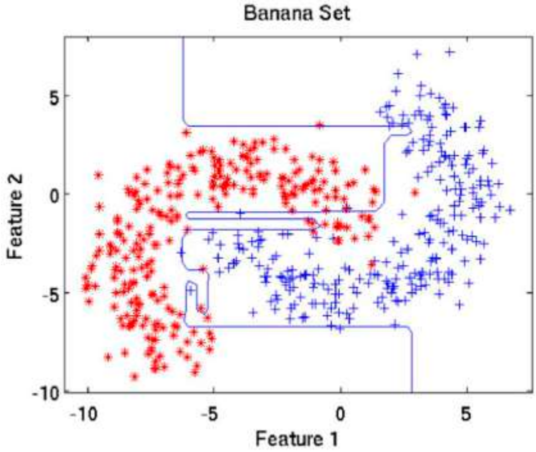
Decision boundary produced by one tree

Bagging with decision trees



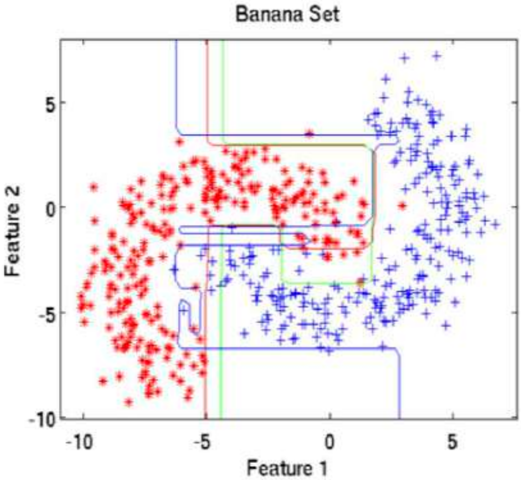
Decision boundary produced by a second tree

Bagging with decision trees



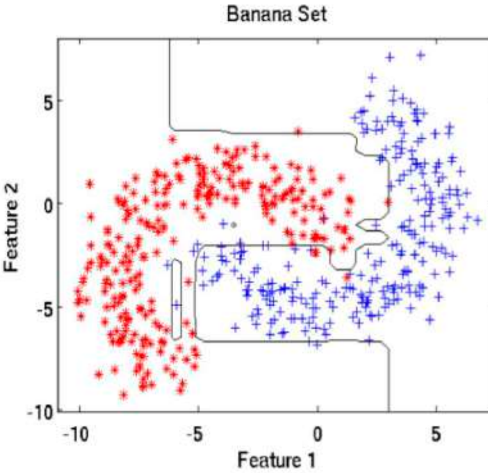
Decision boundary produced by a third tree

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

Bagging produces

$D_1, D_2, \ldots, D_k$

$\downarrow \quad \downarrow \quad \downarrow$

$M_1 \quad M_2 \quad M_k$

~~Deterministic~~

Randomized

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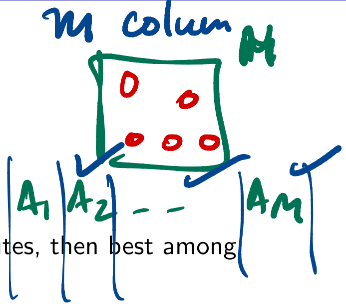
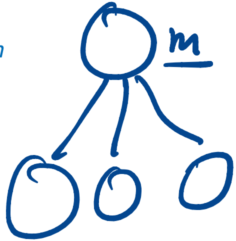
  - Normally, choose maximum impurity gain among M attributes, then best among remaining $M - 1, \ldots$
  - Instead, fix a small limit $m < M$ — say $m = \log_2 M + 1$
  - At each level, choose a random subset of available attributes of size m
  - Evaluate only these m attributes to choose next query





Choose m

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  - 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 $T_1, T_2, \ldots, T_k$

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

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- Reducing m, the number of attributes examined at each level, reduces correlation and strength
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- Increasing m increases both correlation and strength
- Search for a value of m that optimizes overall error rate

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k trees

$\frac{2}{3}k$ use d

$\frac{1}{3}k$ do not use d

d does not influence M

Out of bag error estimate

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- 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

Ask M_i for its verdict on d

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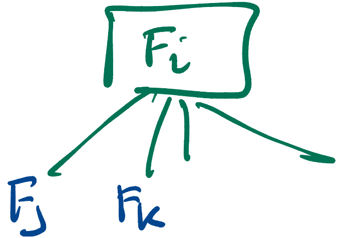
- Hence, each data item is omitted by about $1/3$ of the samples
- If data item d does not appear in bootstrap sample D_i, d is out of bag (oob) for D_i
- Oob classification — for each d, vote only among those T_i where d is oob for D_i
- Use oob samples to validate the model
  - Estimate generalization 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?

Features are ordered in importance by sequence in which they are chosen



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- 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

High Variance → Bagging → Random Forest

High Bias ?

- OOB error
- Feature importance