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(slides by Madhavan Mukund)

Data Mining and Machine Learning
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Limitations of classification models

- Bias : Expressiveness of model-family limits classification
  - leads to a gap in predictions vs true values; no matter how much training data we have
  - High bias leads to Underfitting
  - e.g. linear separators fitting a quadratic curve
- Variance: Variation in constructed model due to small changes in the training data
  - *Overfitting* by learning the random noise in training data
  - High Variance leads to overfitting and poor generalization to unseen data
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Bias-Variance Tradeoff:

- If the model-family is too simple, bias is low, but we underfit
- If the model-family is complex, variance is high and we overfit
- Need to choose the model-family to balance these two constraints.

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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
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  - 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

Bootstrap Aggregating = Bagging

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  - $TD = \{d_1, d_2, \ldots, d_N\}$
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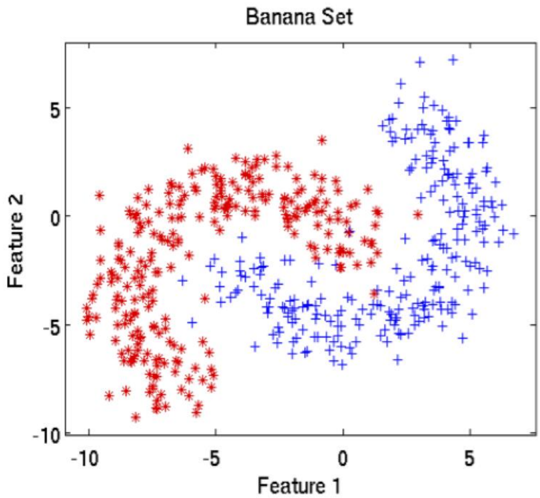
- If sample size is same as data size ($K = N$), expected number of distinct items is $(1 - \frac{1}{e}) \cdot N$
  - Approx 63.2%

Bootstrap Aggregating = Bagging

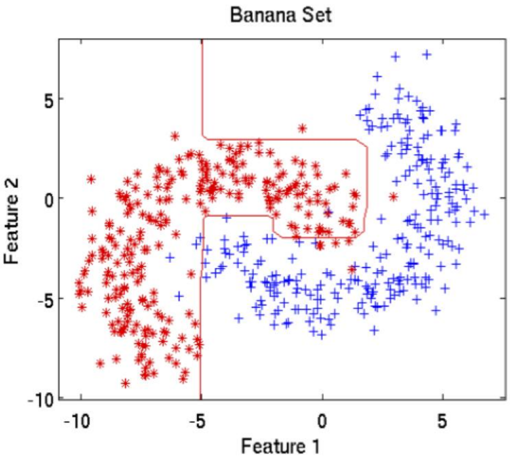
- Sample with replacement of size N : bootstrap sample
  - Approx 2/3 of full training data
- Take k such samples
- Build a model for each sample
  - Models will vary because each uses different training data
- Final classifier: report the majority answer
  - Assumptions: binary classifier, k odd
- Provably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

Bagging with decision trees



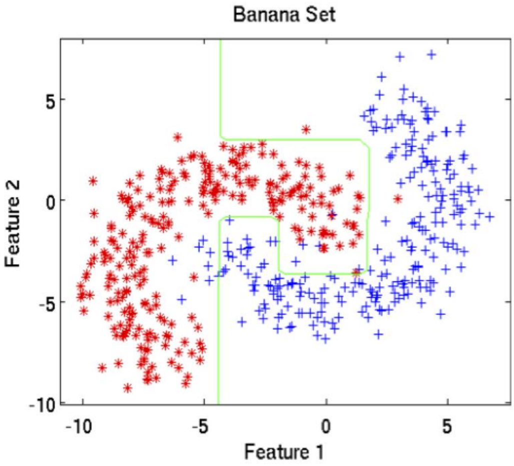
Training data

Bagging with decision trees



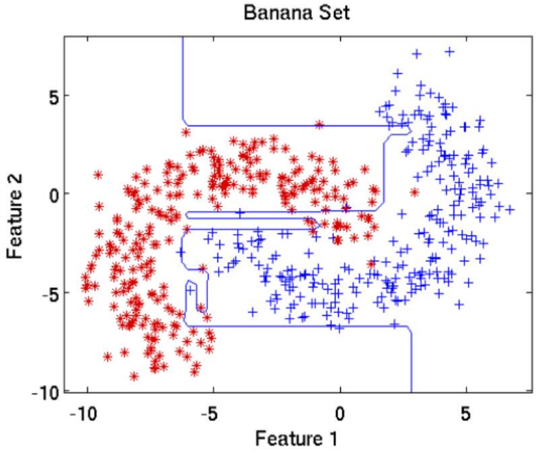
Decision boundary produced by one tree

Bagging with decision trees



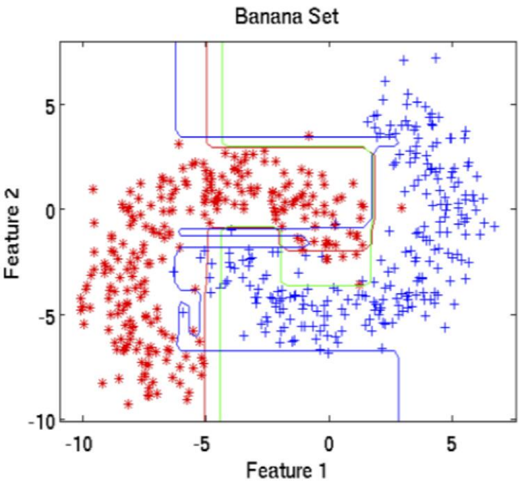
Decision boundary produced by a second tree

Bagging with decision trees



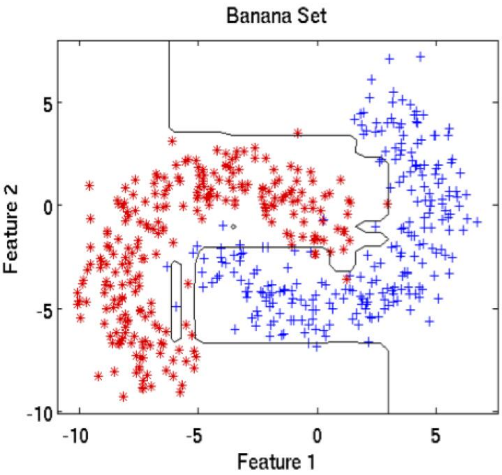
Decision boundary produced by a third tree

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

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  - 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 . . .

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  - Correlation between pairs of trees — higher correlation results in higher overall error rate
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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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- 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

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- Even greater variation in a random forest
- Compute weighted average of impurity gain
  - Weight is given by number of training samples at the node