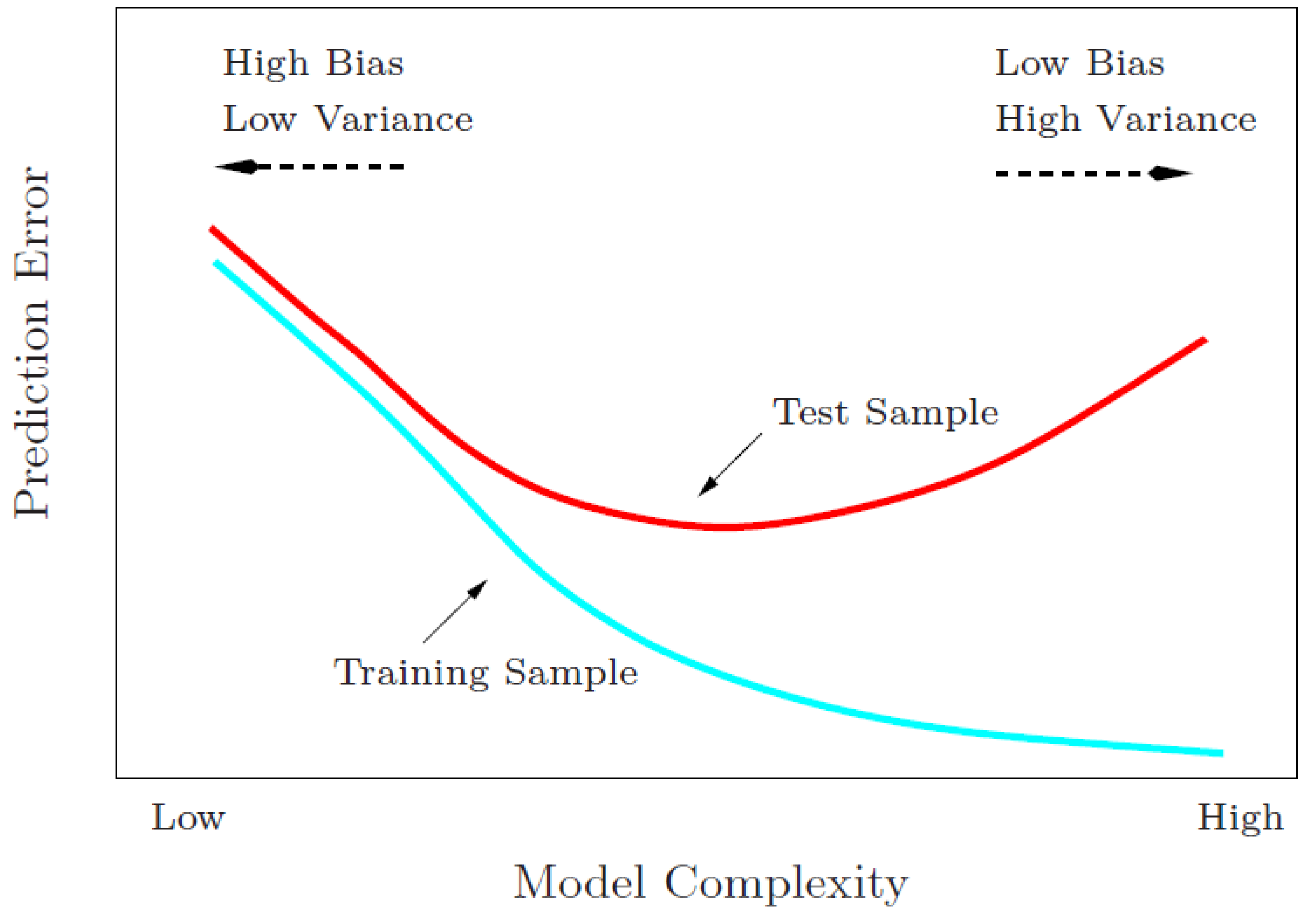
Supplementary Materials of Lecture 15

Bias/Variance Tradeoff



Hastie, Tibshirani, Friedman "Elements of Statistical Learning" 2001

Reduce Variance Without Increasing Bias

- Averaging reduces variance:

$$Var(\bar{X}) = \frac{Var(X)}{N}$$

(when predictions are **independent**)

Average models to reduce model variance

One problem:

only one training set

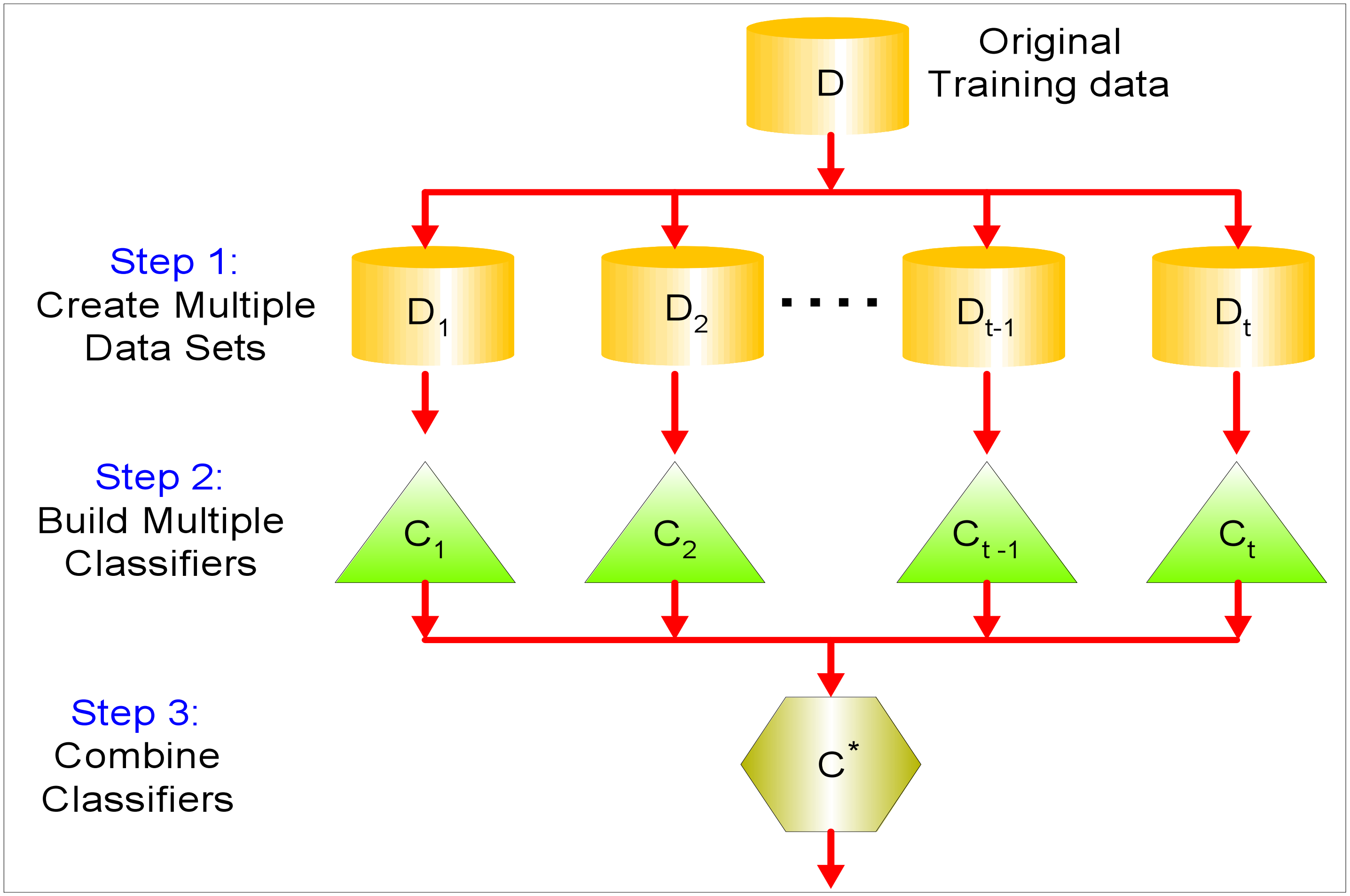
where do multiple models come from?

Bagging: Bootstrap Aggregation

- Leo Breiman (1994)
- Take repeated bootstrap samples from training set D
- *Bootstrap sampling*: Given set D containing N training examples, create D' by drawing N examples at random with replacement from D.

- Bagging:
  - Create k bootstrap samples $D_1 \ldots D_k$.
  - Train distinct classifier on each D_i.
  - Classify new instance by majority vote / average.

General Idea



Bagging

- Sampling with replacement

Training Data

Data ID

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
- Each data point has probability $(1 – 1/n)^n$ of not being selected as training data
- Training data = 1- $(1 – 1/n)^n$ of the original data

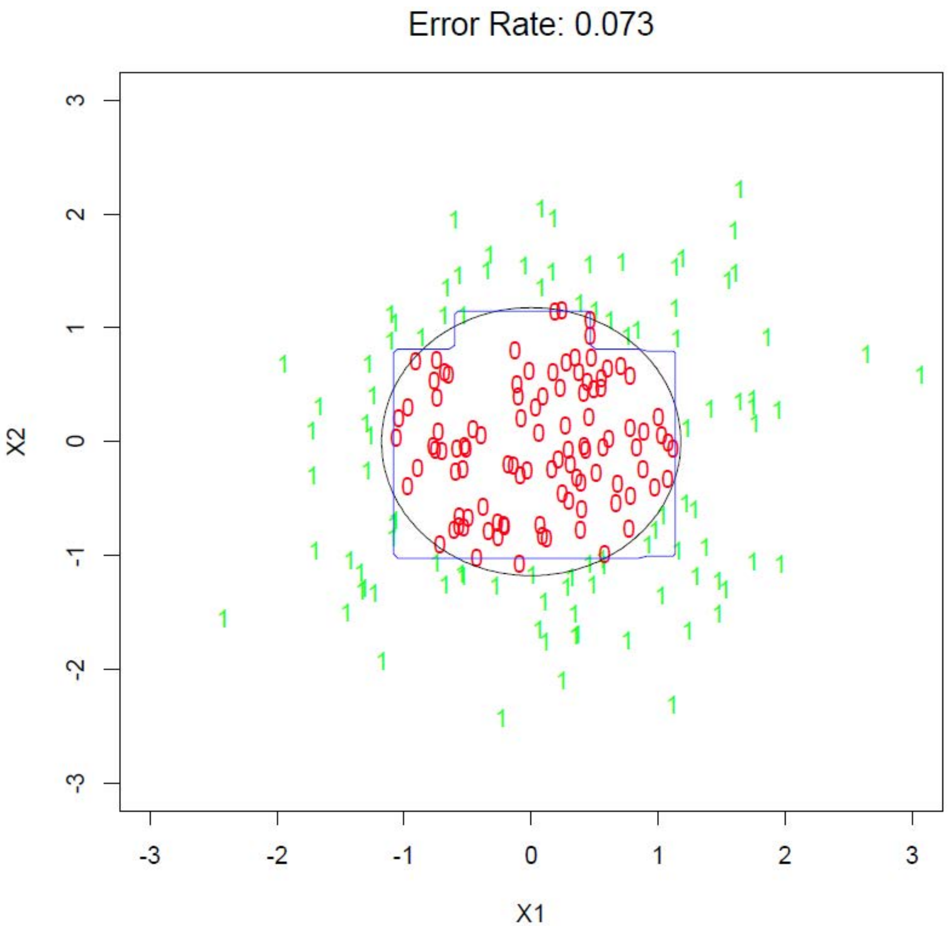
The 0.632 bootstrap

- This method is also called the *0.632 bootstrap*
  - A particular training data has a probability of 1-1/*n* of *not* being picked
  - Thus its probability of ending up in the test data (not selected) is:

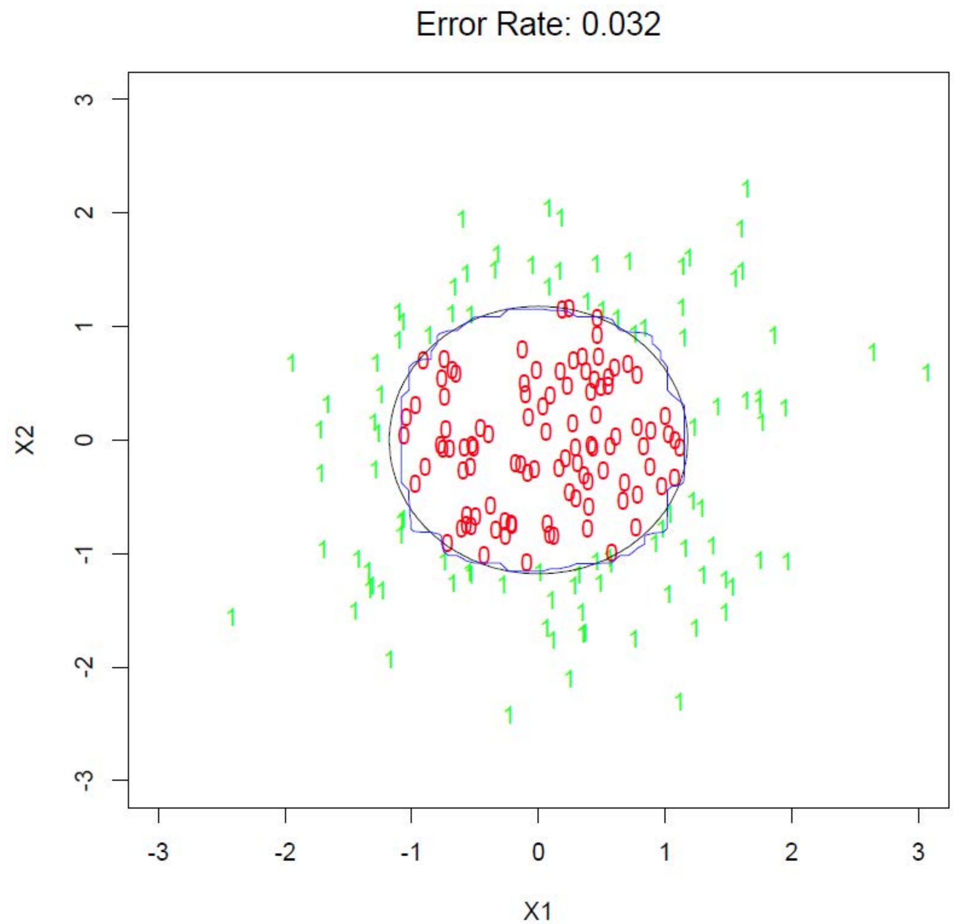
$$\left(1-\frac{1}{n}\right)^{n} \approx e^{-1} = 0.368$$

  - This means the training data will contain approximately 63.2% of the instances

Comparison on Decision Boundaries



Single decision tree



Bagging (decision tree)

Bagging produces smoother decision boundary

Random Forests

- Ensemble method specifically designed for decision tree classifiers
- Introduce two sources of randomness: "Bagging" and "Random input vectors"
  - Bagging method: each tree is grown using a bootstrap sample of training data
  - Random vector method: At each node, best split is chosen from a random sample of *m* attributes instead of all attributes

Random Forests

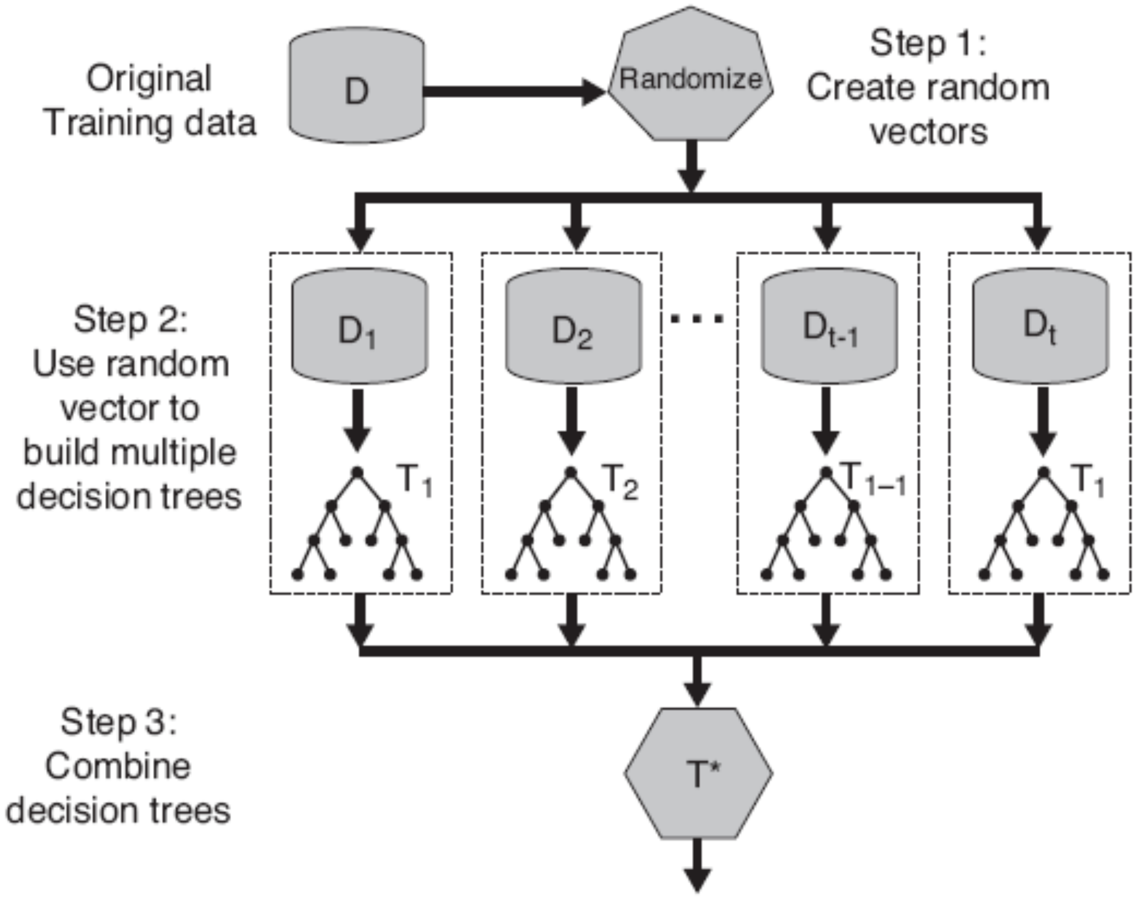


Figure 5.40. Random forests.

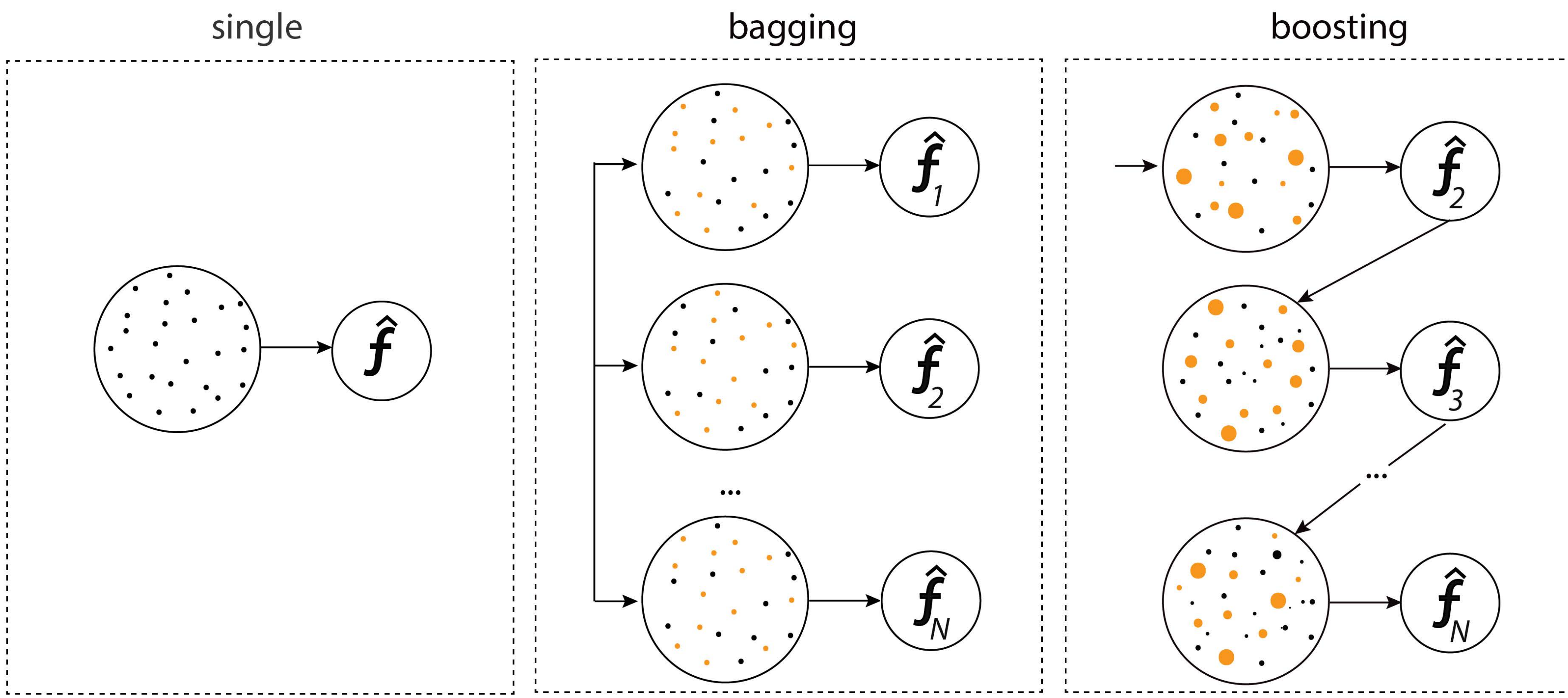
Reduce Bias^2 and Decrease Variance?

- Bagging reduces variance by averaging
- Bagging has little effect on bias
- Can we average *and* reduce bias?
- Yes:

- Boosting

In general, Boosting > Bagging > Base learner
(In performance)

Bagging versus Boosting



Parallel

Sequential