# Ensemble methods and random forests

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# Today’s topics

- Ensemble Methods
  - Overview and rationale
  - Boosting
  - Bagging
- Random Forests
  - Overview
  - Some theory and mechanics
  - Practical examples with R

# Ensemble Methods

## Improve classification accuracy by combining classifiers

# Note before we proceed

Our focus will be on explaining the algorithms intuitively

Mathematical proofs and assumptions are left for all of you as an exercise

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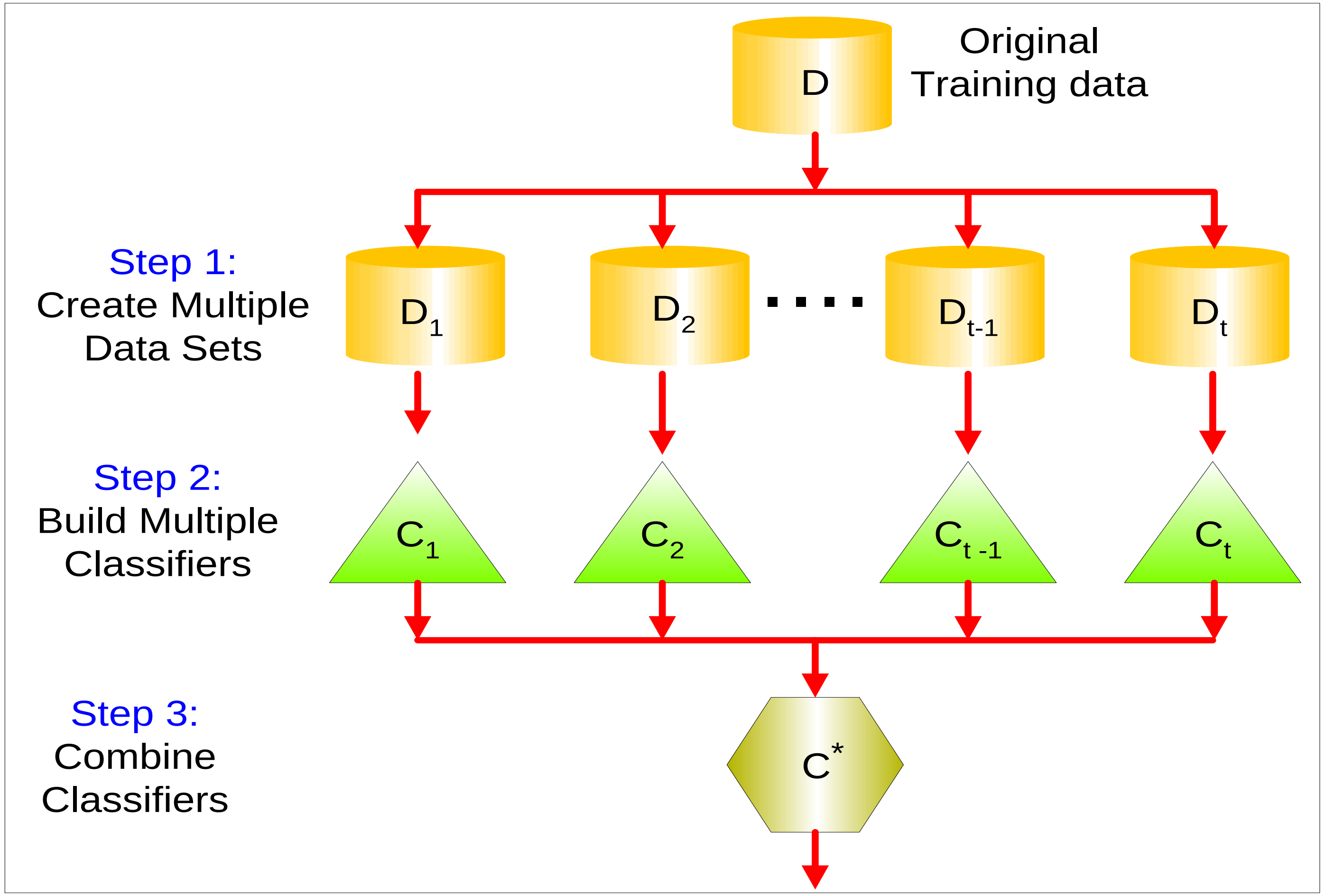
# General Idea of ensemble methods

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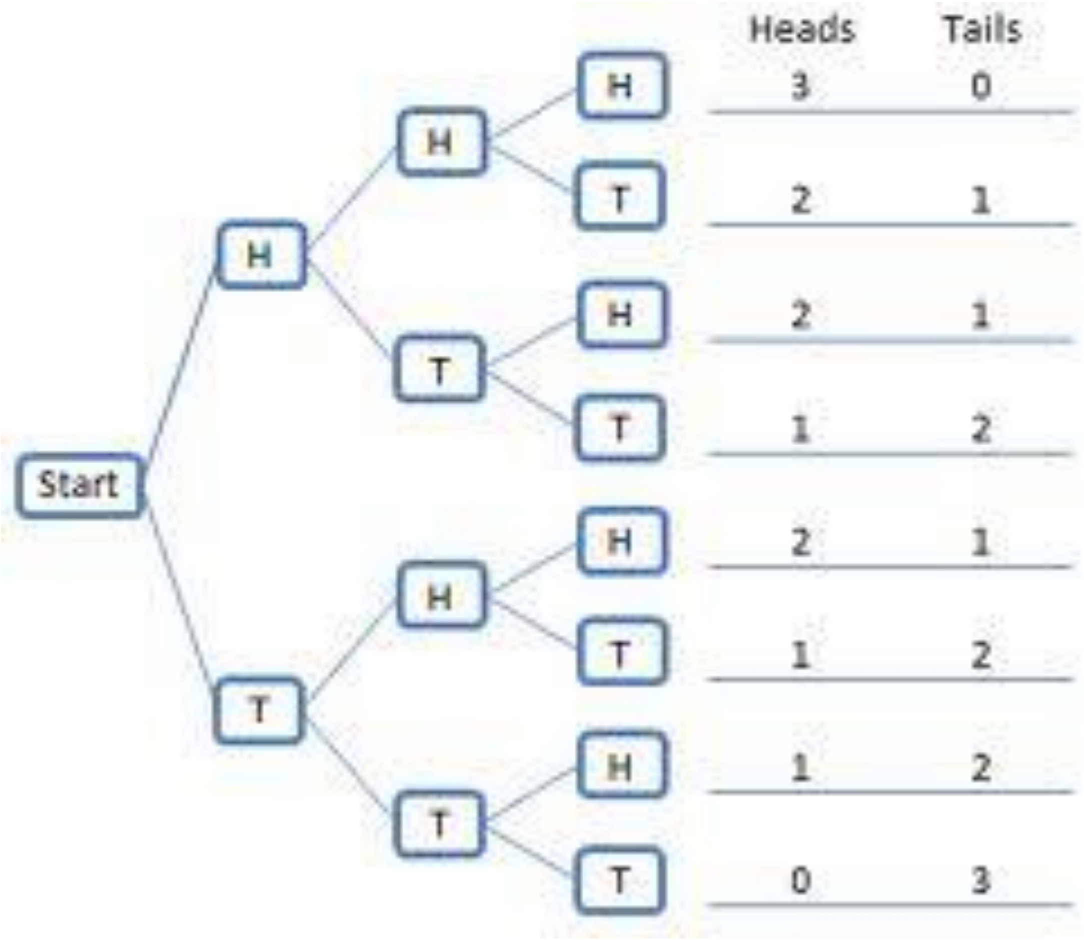
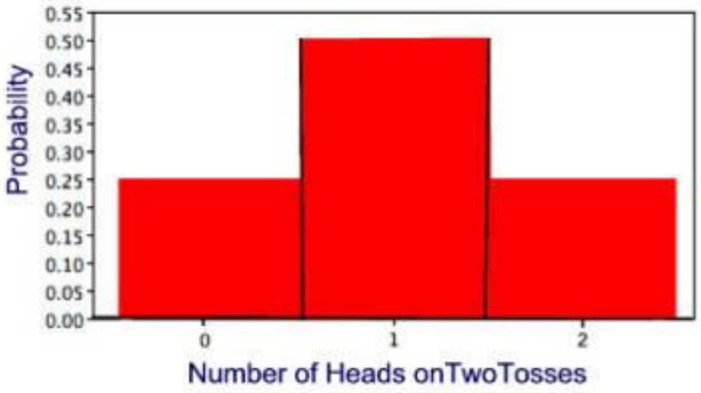
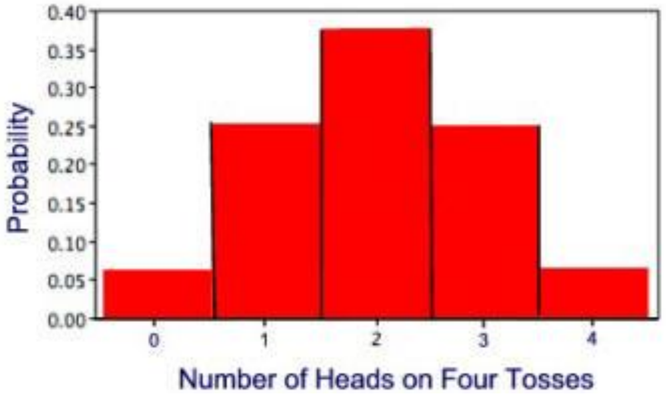
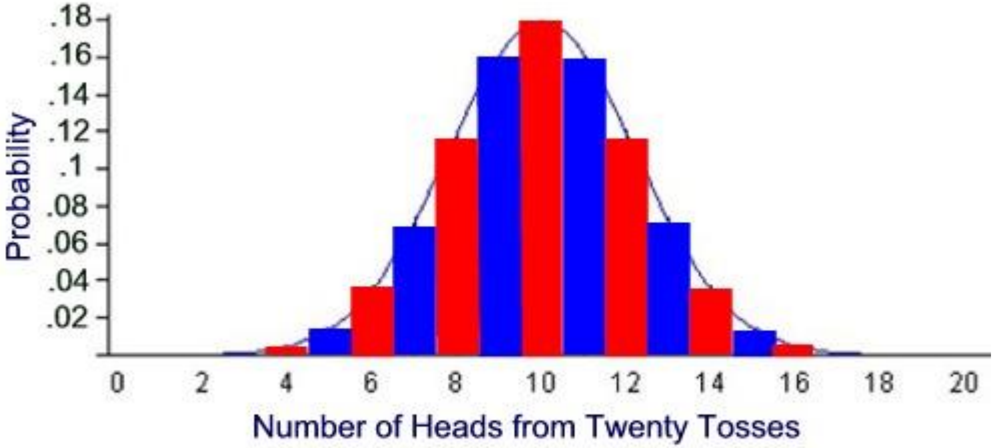
# Digression – Binomial distribution



# Number of heads in n trials

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# Binomial distribution

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

# Tossing a biased coin

What is the probability of 0,1,2,3,4,5,6 heads in six tosses of a biased coin in six tosses total?

n = 6

k = 0,1,2,3,4,5,6

P=0.3 (prob of head)

$$\Pr(0 \text{ heads}) = f(0) = \Pr(X=0) = \binom{6}{0} 0.3^0 (1-0.3)^{6-0} \approx 0.1176$$

$$\Pr(1 \text{ head }) = f(1) = \Pr(X=1) = \binom{6}{1} 0.3^1 (1-0.3)^{6-1} \approx 0.3025$$

$$\Pr(2 \text{ heads}) = f(2) = \Pr(X=2) = \binom{6}{2} 0.3^2 (1-0.3)^{6-2} \approx 0.3241$$

$$\Pr(3 \text{ heads}) = f(3) = \Pr(X=3) = \binom{6}{3} 0.3^3 (1-0.3)^{6-3} \approx 0.1852$$

$$\Pr(4 \text{ heads}) = f(4) = \Pr(X=4) = \binom{6}{4} 0.3^4 (1-0.3)^{6-4} \approx 0.0595$$

$$\Pr(5 \text{ heads}) = f(5) = \Pr(X=5) = \binom{6}{5} 0.3^5 (1-0.3)^{6-5} \approx 0.0102$$

$$\Pr(6 \text{ heads}) = f(6) = \Pr(X=6) = \binom{6}{6} 0.3^6 (1-0.3)^{6-6} \approx 0.0007$$

# Rolling a die

- When rolling a die 100 times, what is the probability of rolling a "4" exactly 25 times?
- Number of trials n = 100
- Number of successes k = 25
- Probability of a ‘4’ in a single roll = 1/6

$$\binom{100}{25}\left(\frac{1}{6}\right)^{25}\left(1-\left(\frac{1}{6}\right)\right)^{100-25}$$

R functions:
dbinom(25,size=100,prob=1/6) = 0.009825882
Pbinom is for calculating cdfs

# Multiple-choice Test

- A test consists of 10 multiple choice questions with five choices for each question. As an experiment, you guess on each and every answer without even reading the questions.
  - What is the probability of getting exactly 6 questions correct on this test?
  - What is the probability of getting at least 6 questions correct on this test?
  - What is the probability of getting less than 6 questions correct on this test?
  - What is the probability of getting all 10 questions correct on this test?

# Solve on whiteboard

# 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, ε = 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

# 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 $1-1/e \sim 0.632$

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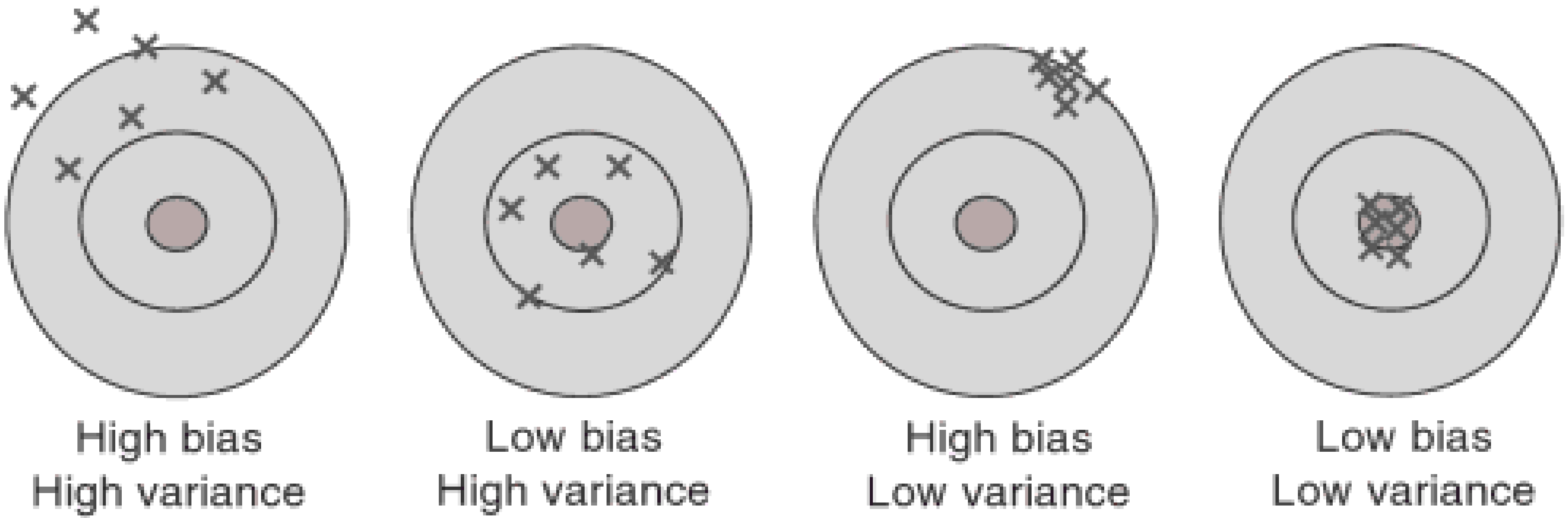
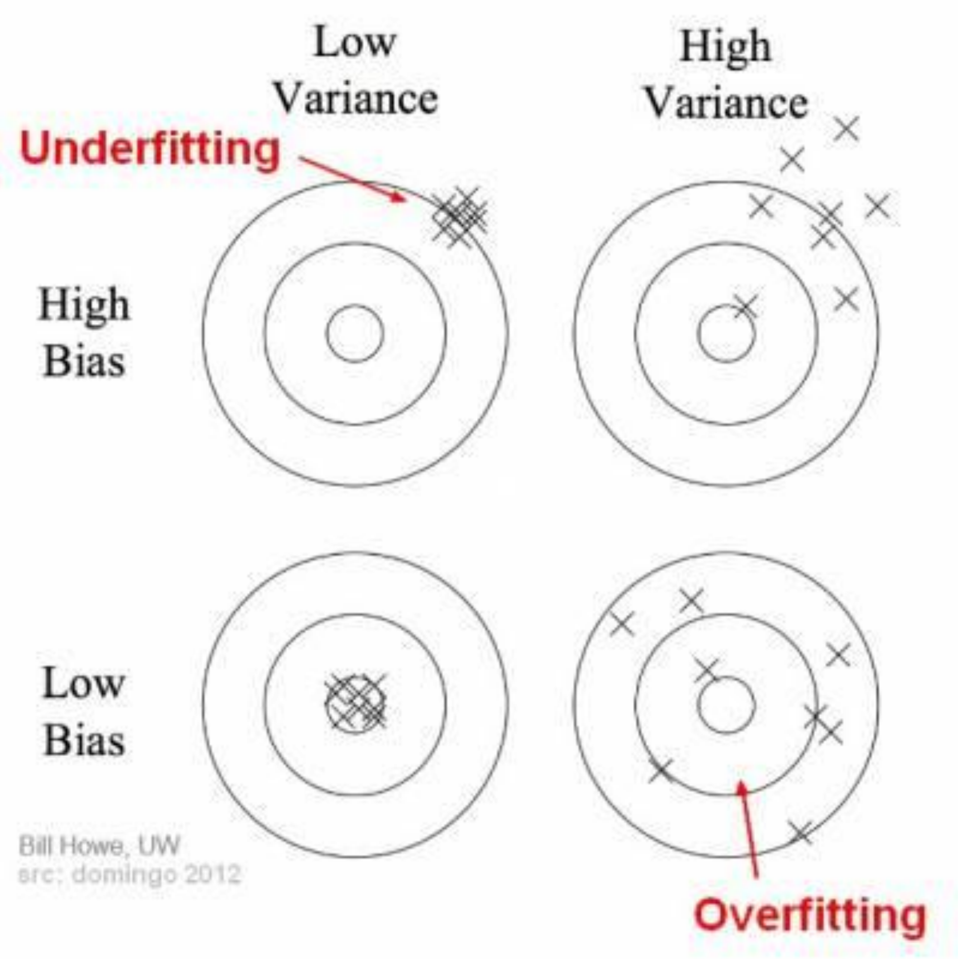
# bagging

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

# UNDERSTANDING BIAS and variance In estimate



# UNDERSTANDING BIAS and variance In estimate

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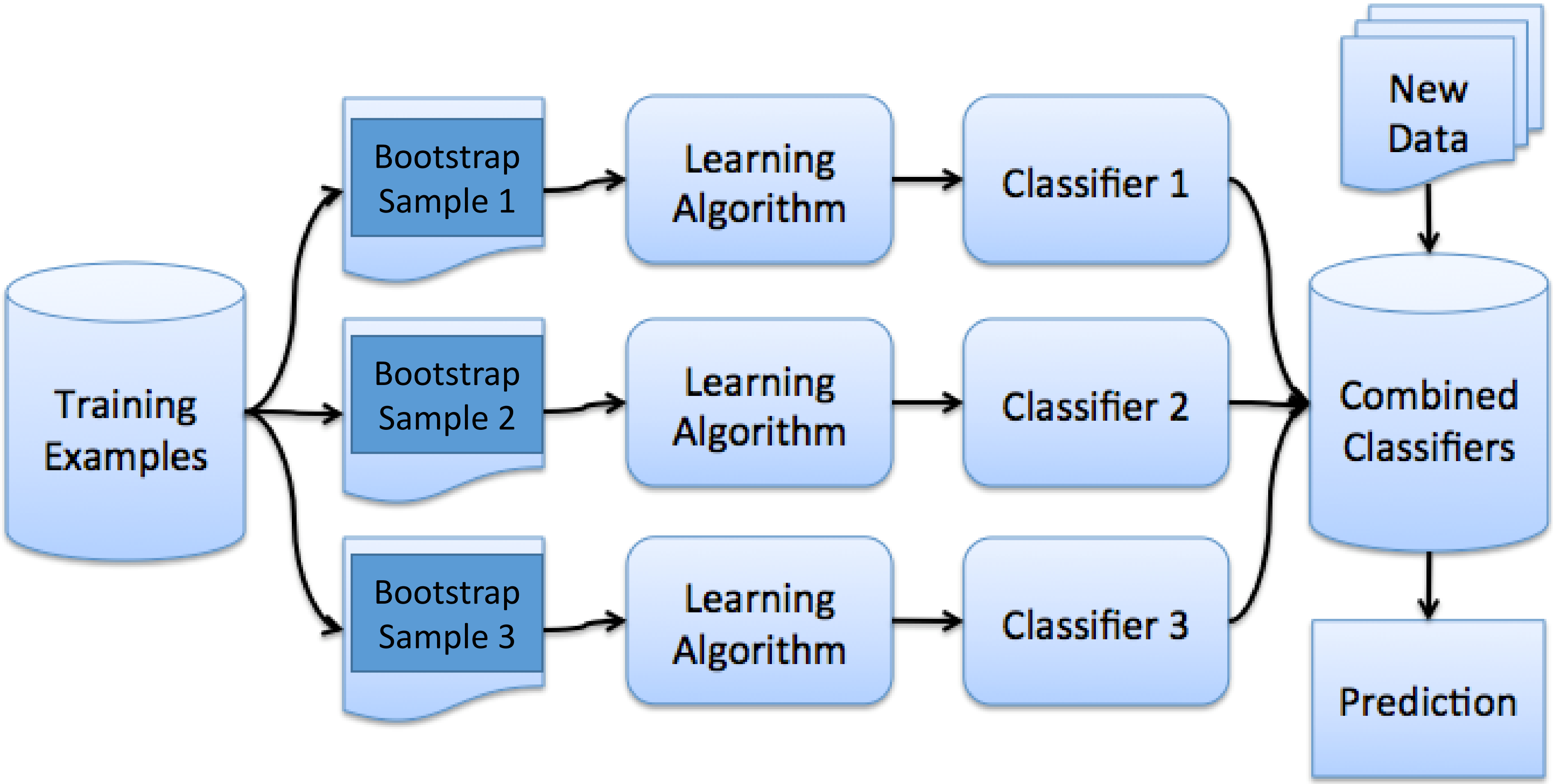
# bagging


Training Examples
Bootstrap Sample 1
Bootstrap Sample 2
Bootstrap Sample 3
Learning Algorithm
Learning Algorithm
Learning Algorithm
Classifier 1
Classifier 2
Classifier 3
New Data
Combined Classifiers
Prediction

# 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

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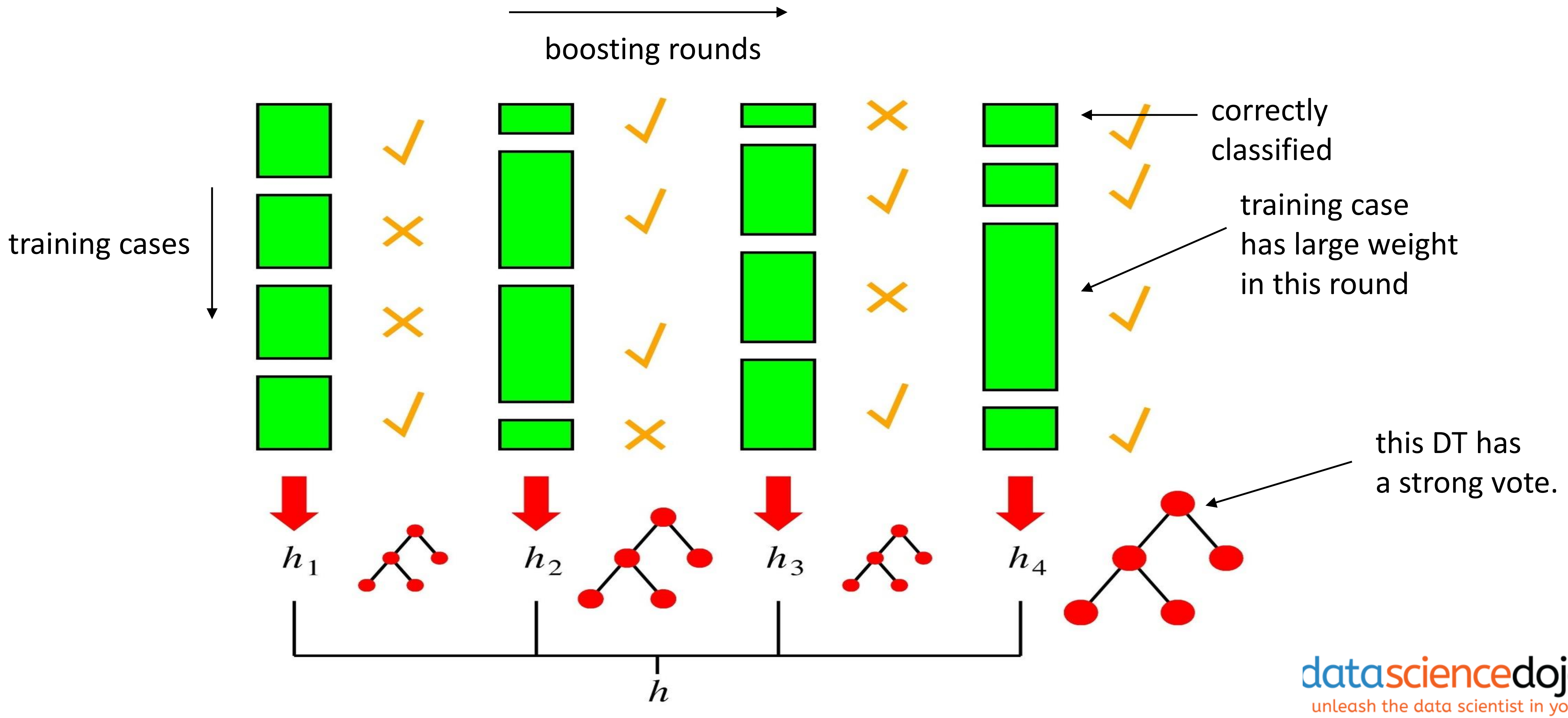
# Boosting Intuition

- We adaptively weigh 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 (cross-validation).

# Boosting in a Picture



# AdaBoost (adaptive Boosting)

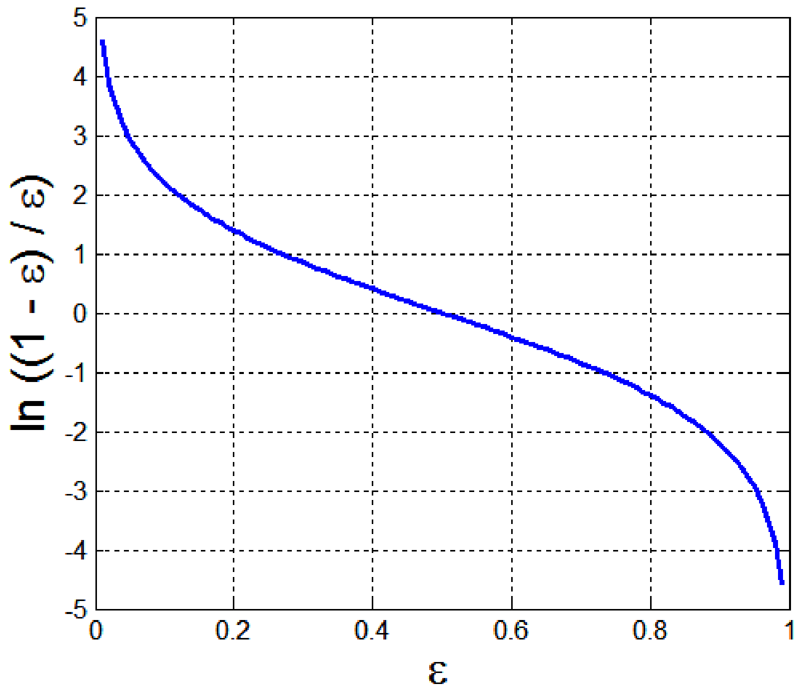
- Base classifiers: $C_1$, $C_2$, ..., $C_T$

- Error rate [Weighted loss function]:

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

- Importance of a classifier:

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



# AdaBoost

- Weight update:

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

$$\textit{where } Z_j \textit{ is the normalization factor}$$

- 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:

$$C^*(x) = \arg\max_y \sum_{j=1}^{T} \alpha_j \delta\left(C_j(x) = y\right)$$

# Random forests classifier

- *Random forests are a combination of tree predicators such that each tree depends on the values of a random vector sampled independently and with same distribution for all trees in the forest.*
- *- Leo Breiman*

# 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 random forests work?

- A different subset of the training data are selected (~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) but lower predictive power (high error rate)

# Rules of thumb

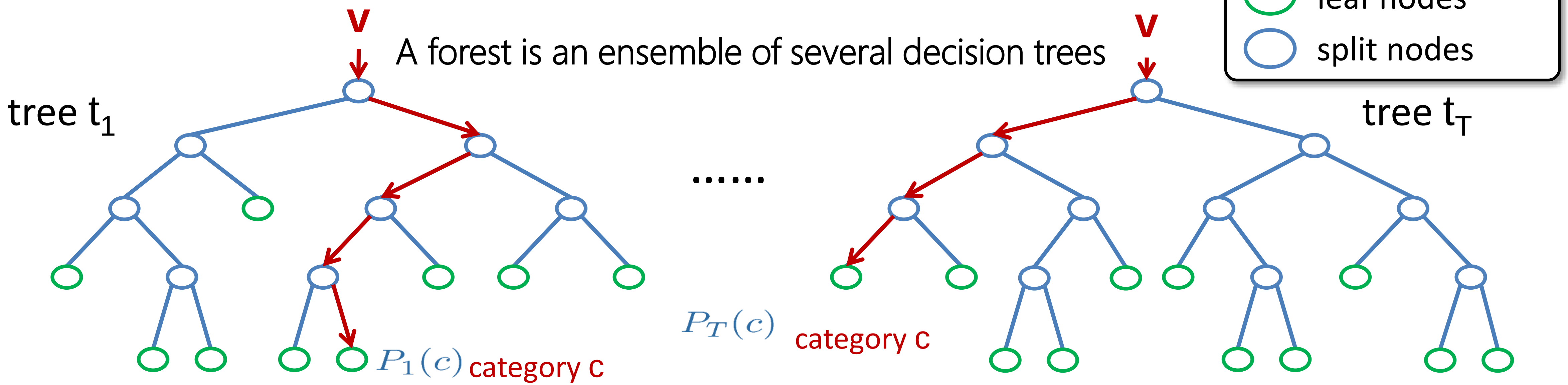
- Given:
- N: Total number of training data points
- M: Number of features in training data
- m: Number of features randomly selected for training each tree

- Sample the data with replacement N times for building the training data for each tree.

- m<<M
- Classification: m = sqrt(M)
- Regression: m = M/3

# A Forest of Trees

- A forest is an ensemble of several decision trees




[Amit & Geman 97]
[Breiman 01]
[Lepetit *et al.* 06]

Classification is $$P(c|\mathbf{v}) = \frac{1}{T}\sum_{t=1}^{T} P_t(c|\mathbf{v})$$

# Learning a Forest

- Dividing training examples into **T** subsets improves generalization
  - Reduces memory requirements & training time
- Train each decision tree **t** on subset $\mathbf{I}_t$
  - 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

# Common pitfall

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

# forest error rate

$$PE^* \leq \rho(1 - s^2) / s^2$$

- The *correlation* between any two trees in the forest. Increasing the correlation increases the forest error rate.
- The *strength* of each individual tree in the forest. A tree with a low error rate is a strong classifier. Increasing the strength of the individual trees decreases the forest error rate.
- Detailed proof: RANDOM FORESTS Leo Breiman

# Random Forest

R package for
Random Forest

# Setting up randomForest

Installation

```
> install.packages('randomForest')
```

Loading in R environment

```
> library(randomForest)
```

Documentation:

http://cran.r-project.org/web/packages/randomForest/randomForest.pdf

# Obtaining the model

```
> iris.rf <- randomForest(
    Species ~ .,
    data=iris,
    importance=TRUE,
    proximity=TRUE
)
```

# Printing the model

```
> print(iris.rf)
```

# Type of random forest: classification                    Number of trees: 500

# No. of variables tried at each split: 2

# OOB estimate of  error rate: 4.67%

# Confusion matrix: setosa versicolor virginica class.error

| | | | | |
|---|---|---|---|---|
| # setosa | 50 | 0 | 0 | 0.00 |
| # versicolor | 0 | 47 | 3 | 0.06 |
| # virginica | 0 | 4 | 46 | 0.08 |

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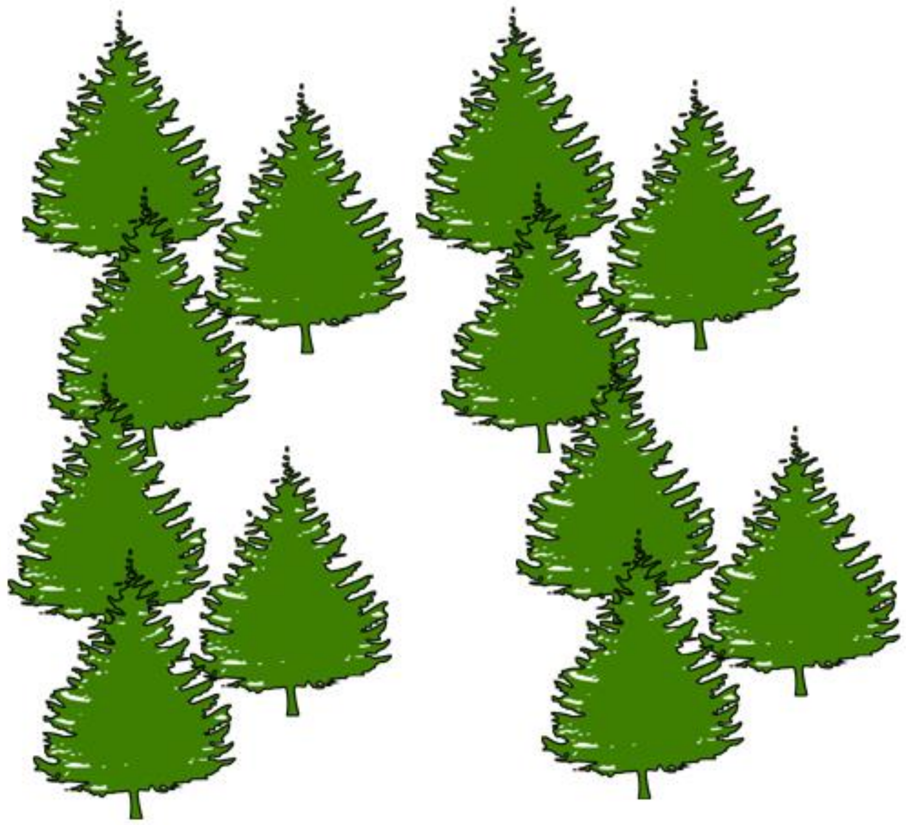
# Restricting Tree Size

# A forest of small trees.
# Specify that you want 30 trees with
# a depth of 4 nodes max each.



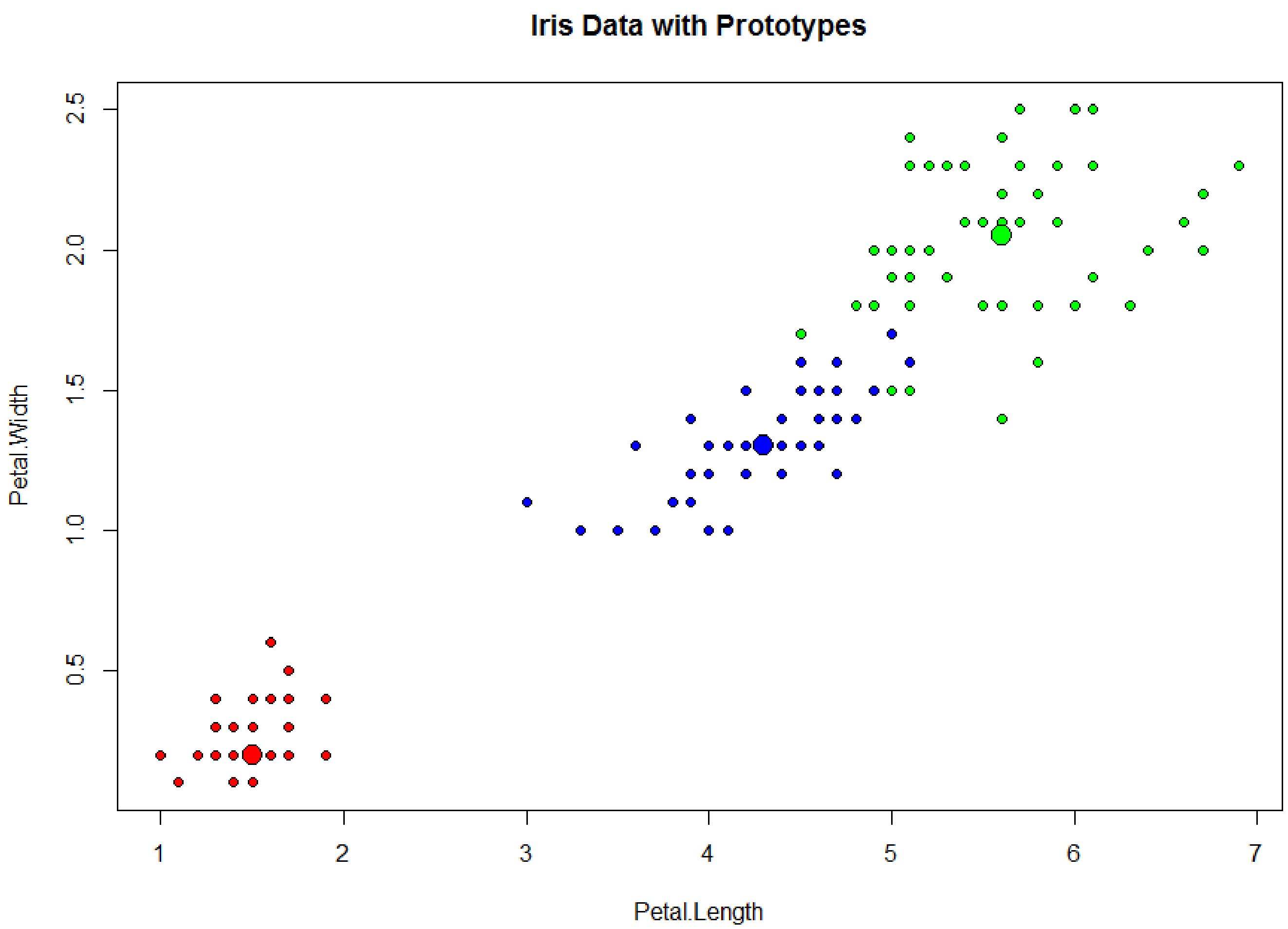
```
(treesize(randomForest(Species ~ ., data=iris,maxnodes=4, ntree=30)))
```

# Finding Class Centers

## classCenter function

```
> data(iris)
> iris.rf <- randomForest(iris[,-5], iris[,5], prox=TRUE)
> iris.p <- classCenter(iris[,-5], iris[,5], iris.rf$prox)
> plot(iris[,3], iris[,4],
      pch=21, xlab=names(iris)[3],ylab=names(iris)[4],
      bg=c("red","blue","green")[as.numeric(factor(iris$Species))],
      main="Iris Data with Prototypes")
> points(iris.p[,3], iris.p[,4], pch=21, cex=2,
      bg=c("red", "blue", "green"))
```

# Finding Class Centers

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# Combining Trees

You can combine two or more random forests into one.
The confusion, err.rate, mse, and rsq components will be NULL

```
> data(iris)
> rf1 <- randomForest(Species ~ ., iris, ntree=50,
norm.votes=FALSE)
> rf2 <- randomForest(Species ~ ., iris, ntree=100,
norm.votes=FALSE)
> rf3 <- randomForest(Species ~ ., iris, ntree=150,mtry=3,
norm.votes=FALSE)
> rf.all <- combine(rf1, rf2, rf3)
> print(rf.all)
```

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# Combining Trees

```
> print(rf.all)
```

Call:

randomForest(formula = Species ~ ., data = iris, ntree = 50, norm.votes = FALSE)

Type of random forest:

classification Number of trees: 150

No. of variables tried at each split: 2

# Variable Importance and Gini Importance

```
> data(iris)
> iris.rf <- randomForest(Species ~., data=iris, importance=TRUE,
      proximity=TRUE)
> round(importance(iris.rf), 2)
```

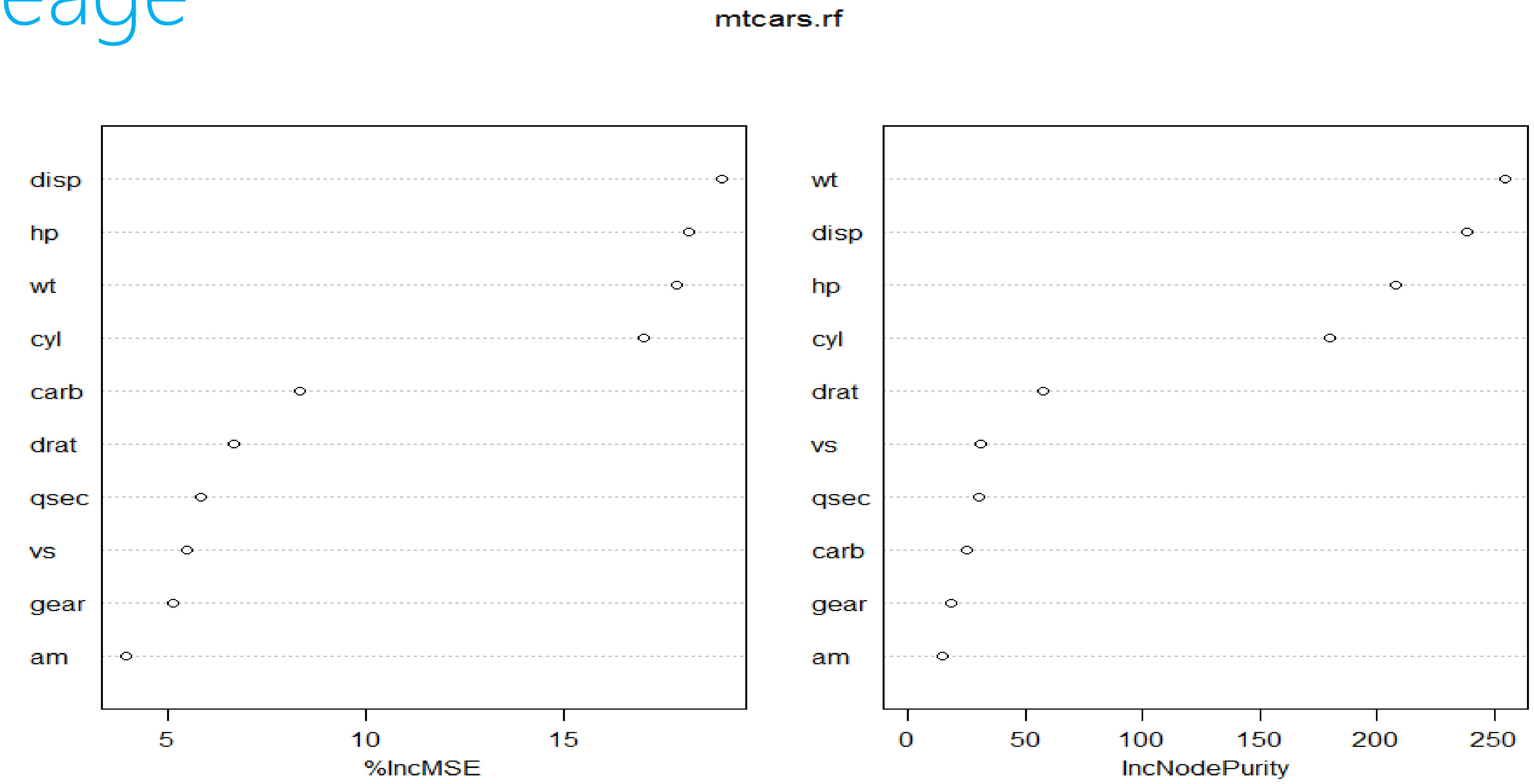
| | setosa | versicolor | virginica | MeanDecreaseAccuracy | MeanDecreaseGini |
|---|---|---|---|---|---|
| Sepal.Length | 6.28 | 8.88 | 7.11 | 10.48 | 9.26 |
| Sepal.Width | 4.87 | 0.77 | 4.85 | 5.17 | 2.33 |
| Petal.Length | 21.48 | 33.88 | 28.44 | 33.95 | 42.97 |
| Petal.Width | 22.96 | 32.47 | 32.10 | 34.60 | 44.65 |

# Important factors in determining car mileage

```
> set.seed(4543)
> data(mtcars)
> mtcars.rf <- randomForest(
    mpg ~ .,
    data=mtcars,
    ntree=1000,
    keep.forest=FALSE,
    importance=TRUE
)
> varImpPlot(mtcars.rf)
```

| Index | Attribute Name | Description |
|---|---|---|
| [, 1] | mpg | Miles/(US) gallon |
| [, 2] | cyl | Number of cylinders |
| [, 3] | disp | Displacement (cu.in.) |
| [, 4] | hp | Gross horsepower |
| [, 5] | drat | Rear axle ratio |
| [, 6] | wt | Weight (lb/1000) |
| [, 7] | qsec | 1/4 mile time |
| [, 8] | vs | V/S |
| [, 9] | am | Transmission (0 = automatic, 1 = manual) |
| [,10] | gear | Number of forward gears |
| [,11] | carb | Number of carburetors |

# Important factors in determining car mileage

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# Regression with random forests

```
> set.seed(131)
> ozone.rf <-
      randomForest(Ozone ~
.,
      data=airquality,
mtry=3,
      importance=TRUE,
      na.action=na.omit)
> print(ozone.rf)
#Impute Missing Values by median/mode.
> ozone.rf <-
      na.roughfix(ozone.rf)
```

| | Ozone | Solar.R | Wind | Temp | Month | Day |
|---|---|---|---|---|---|---|
| 1 | 41 | 190 | 7.4 | 67 | 5 | 1 |
| 2 | 36 | 118 | 8 | 72 | 5 | 2 |
| 3 | 12 | 149 | 12.6 | 74 | 5 | 3 |
| 4 | 18 | 313 | 11.5 | 62 | 5 | 4 |
| 5 | NA | NA | 14.3 | 56 | 5 | 5 |
| 6 | 28 | NA | 14.9 | 66 | 5 | 6 |
| 7 | 23 | 299 | 8.6 | 65 | 5 | 7 |
| 8 | 19 | 99 | 13.8 | 59 | 5 | 8 |
| 9 | 8 | 19 | 20.1 | 61 | 5 | 9 |
| 10 | NA | 194 | 8.6 | 69 | 5 | 10 |
| 11 | 7 | NA | 6.9 | 74 | 5 | 11 |
| 12 | 16 | 256 | 9.7 | 69 | 5 | 12 |
| 13 | 11 | 290 | 9.2 | 66 | 5 | 13 |
| 14 | 14 | 274 | 10.9 | 68 | 5 | 14 |
| 15 | 18 | 65 | 13.2 | 58 | 5 | 15 |

# Prediction

```
> predict(ozone.rf,data=airquality)
```

# RPART – Kyphosis Data

The kyphosis data frame has 81 rows and 4 columns representing data on children who have had corrective spinal surgery.

Kyphosis, a factor with levels absent and present indicating if a kyphosis (a type of deformation) was present after the operation.

Age in months.

Number of vertebrae involved.

Start the number of the first (topmost) vertebra operated on.

| Kyphosis | Age | Number | Start |
|---|---|---|---|
| absent | 71 | 3 | 5 |
| absent | 158 | 3 | 14 |
| present | 128 | 4 | 5 |
| absent | 2 | 5 | 1 |
| absent | 1 | 4 | 15 |
| absent | 1 | 2 | 16 |
| absent | 61 | 2 | 17 |
| absent | 37 | 3 | 16 |

# RPART

```
> install.packages('rpart')
> library(rpart)
```

# RPART

```
> fit <- rpart(Kyphosis ~ Age + Number + Start, data = kyphosis)
> fit2 <- rpart(Kyphosis ~ Age + Number + Start, data = kyphosis,
+     parms = list(prior = c(0.65, 0.35), split = "information"))
> fit3 <- rpart(Kyphosis ~ Age + Number + Start, data=kyphosis,
+     control = rpart.control(cp = 0.05))
> par(mfrow = c(1,2), xpd = TRUE)
> plot(fit)
> text(fit, use.n = TRUE)
> plot(fit2)
> text(fit2, use.n = TRUE)
```

# Resources

Random Forests Homepage

http://www.stat.berkeley.edu/~breiman/RandomForests/cc_home.htm

IRIS Data

IRIS data ships with R. You can learn more about IRIS data here:

http://archive.ics.uci.edu/ml/datasets/Iris