## Supplemental – Ensemble Methods And Random Forests



# Why Does Ensembling Work?

- Suppose there are 25 base classifiers
  - Each classifier has error rate,  $\varepsilon = 0.35$
  - Assume classifiers are independent
  - Probability that the ensemble classifier makes a wrong prediction:

$$\sum_{i=13}^{25} {25 \choose i} \varepsilon^i (1-\varepsilon)^{25-i} = 0.06$$



#### Binomial Theorem on Model Error

$$\sum_{k=n^*0.51}^n \binom{n}{k} p^k (1-p)^{n-k} \ \frac{n}{k} \ \ \frac{n}{k} \$$

#### **Example: assume a 3 model ensemble:**

| Accuracy of each Model | On Paper  | In R                                     |
|------------------------|---|--|
| .5                     | $\binom{3}{2} \times .50^2 \times (150)^{3-2} \approx .5$     | 1-pbinom(1, size=3, prob=0.50) = 0.5     |
| .51                    | $\binom{3}{2} \times .49^2 \times (149)^{3-2} \approx .48500$ | 1-pbinom(1, size=3, prob=0.49) = 0.48500 |
| .65                    | $\binom{3}{2} \times .35^2 \times (135)^{3-2} \approx .28175$ | 1-pbinom(1, size=3, prob=0.35) = 0.28175 |

Ensemble amplifies general performance of individual trees.



# **Adding More Trees**

#### **Example: assume all classifiers have an accuracy of 65%**

| # of Models | On Paper   | In R  |
|-------------|--|---|
| 3           | $\binom{3}{2} \times .35^2 \times (135)^{3-2} \approx 0.28175$                       | 1 - pbinom(1, size=3, prob=0.35) = 0.28175      |
| 12          | $\binom{12}{7} \times .35^2 \times (135)^{12 - 7} \approx 0.21273$                   | 1 - pbinom(7, size=12, prob=0.35) = 0.21273     |
| 25          | $\binom{25}{13} \times .35^2 \times (135)^{25 - 13} \approx 0.06044$                 | 1 - pbinom(12, size=25, prob=0.35) = 0.06045    |
| 100         | $\binom{100}{51} \times .35^2 \times (135)^{100 - 51} \approx 0.00145$               | 1 - pbinom(49, size=100, prob=0.35) = 0.00145   |
| 500         | $\binom{500}{251} \times .35^2 \times (135)^{500 - 251} \approx 4.3 \times 10^{-13}$ | 1 - pbinom(249, size=500, prob=0.35) = 4.38e-12 |

Error rate decreases as the number of (independent) models increases.

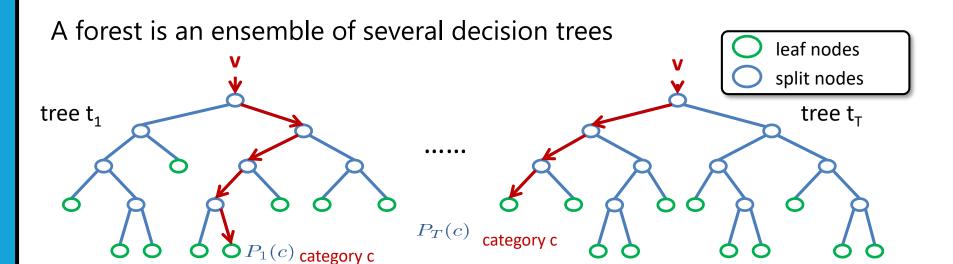


## **Bagging in Random Forests**

- 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



#### A Forest of Trees



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

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



#### **Learning a Forest – GPU Performance**

- Dividing training examples into T subsets improves generalization
  - Reduces memory requirements & training time
- Train each decision tree t on subset I<sub>t</sub>
  - 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



#### **Forest Error Rate**

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

- 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



#### randomForest

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
)</pre>
```



# 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
                                0.00
# versicolor 0 47 3
                                0.06
# virginica 0 4
                         46
                                0.08
```



# Restricting Tree Size

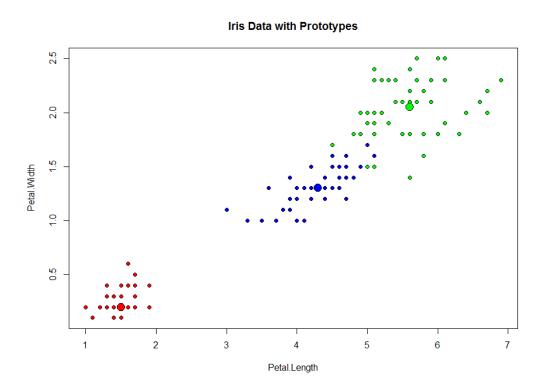


## Finding Class Centers

#### classCenter function



# **Finding Class Centers**





# **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)
```



# **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

|              | 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            |



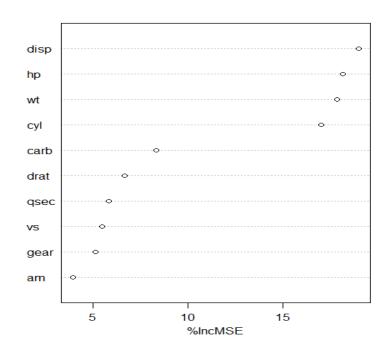
Important Factors In Determining Car Mileage

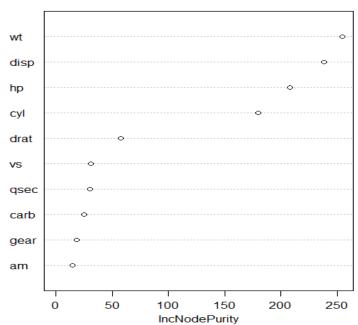
```
> set.seed(4543)
> data(mtcars)
> mtcars.rf <- randomForest(</pre>
    mpq \sim .,
    data=mtcars,
    ntree=1000,
    keep.forest=FALSE,
    importance=TRUE
> varImpPlot(mtcars.rf)
```

| 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 mtcars.rf







### Regression With Random Forests

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



#### 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

