

Statistical Machine Learning

Hilary Term 2019

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Slide credits and other course material can be found at:

<http://www.stats.ox.ac.uk/~palamara/SML19.html>

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Model Complexity

- When should a regression tree growing be stopped?
- As for classification, can use pruning (early stopping or post-pruning)
- In general, can also use a regularized objective

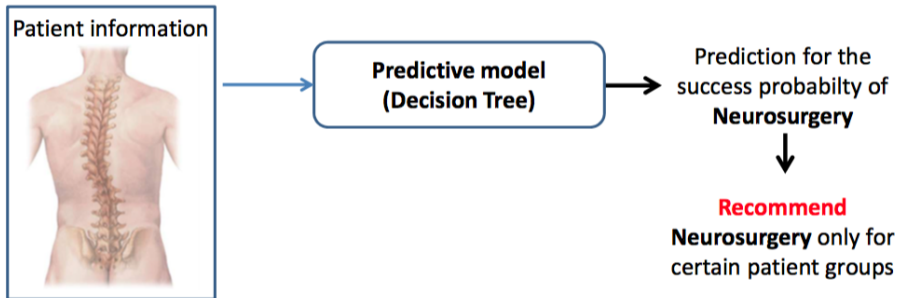
$$R^{\text{emp}}(T) + C \times \text{size}(T)$$

- Early stopping: row the tree from scratch and stop once the criterion objective starts to increase.
- Pruning: first grow the full tree and prune nodes (starting at leaves), until the objective starts to increase.
- Pruning is preferred as the choice of tree is less sensitive to “wrong” choices of split points and variables to split on in the first stages of tree fitting.
- Use cross-validation to determine optimal C .

Possible decision tree pruning rules

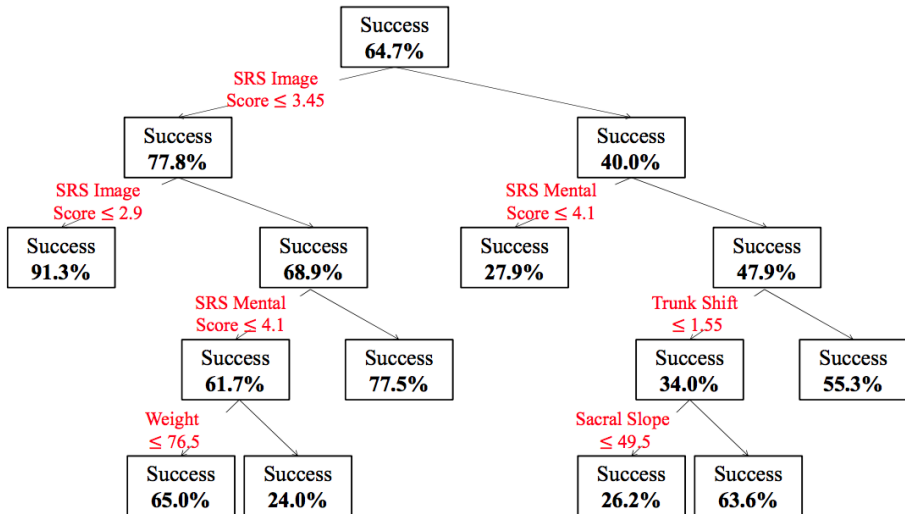
- Stop when the number of leaves is more than a threshold
- Stop when the leaf's error is less than a threshold
- Stop when the number of instances in each leaf is less than a threshold
- Stop when the p-value between two divided leafs is smaller than a certain threshold (e.g. 0.05 or 0.01) based on chosen statistical tests.

Example: Neurosurgery

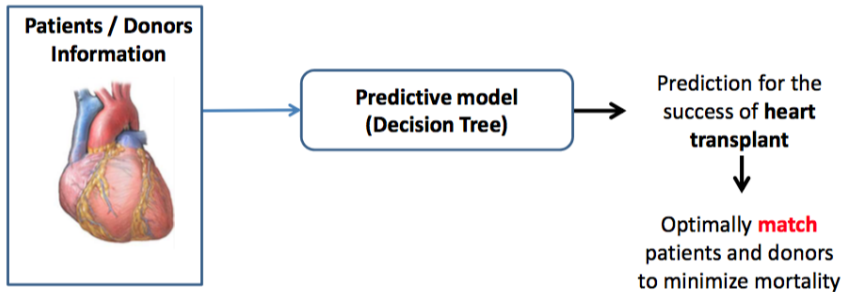


Type	Explanation	Note
Patient	1,449 patients with neurosurgery	2 year follow-up
Feature	91 Features (61 Continuous / 30 Binary)	
Label	MCID 1: 938 Patients (64.7%) MCID 0: 511 Patients (35.3%)	

Example: Neurosurgery

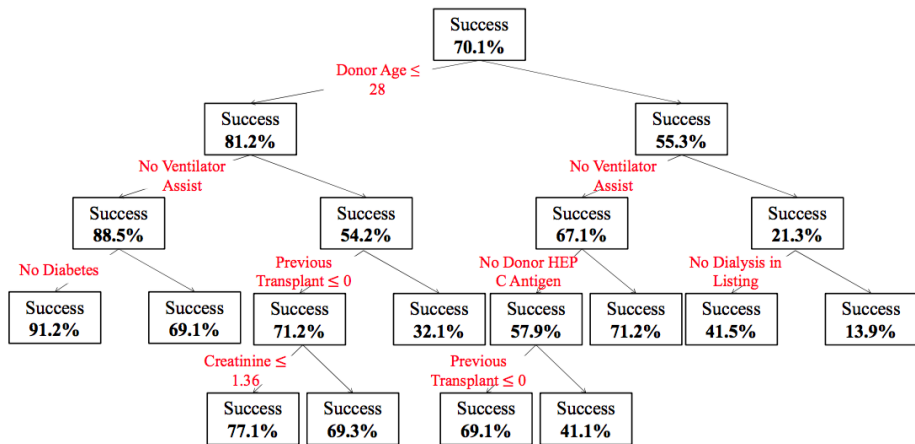


Example: Heart Transplant



Type	Explanation	Note
Patient	56,716 patients (heart transplant patients)	follow-up until they died
Feature	141 Features (84 Continuous / 57 Binary)	From 1986 to 2015
Label	Dead: 16,986 Patients (29.95%) Alive: 39,730 Patients (70.05%)	

Example: Heart Transplant

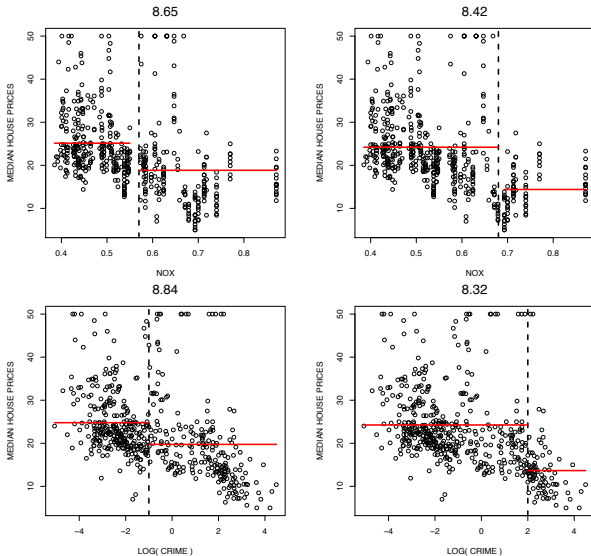


Example: Boston Housing Data

```
crim    per capita crime rate by town
nox     nitric oxides concentration (parts per 10 million)
rm      average number of rooms per dwelling
dis     weighted distances to five Boston employment centres
lstat   percentage of lower status of the population
... (6 more features)
```

- Predict median house value.

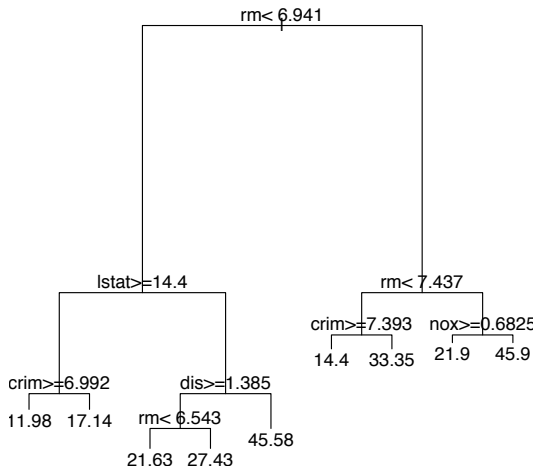
Example: Boston Housing Data



Different possible splits (features and thresholds) result in different quality measures.

Example: Boston Housing Data

- Overall, the best first split is on variable `rm`, average number of rooms per dwelling.
- Final tree contains predictions in leaf nodes.



Example: Pima Indians Diabetes Dataset

Goal: predict whether or not a patient has diabetes.

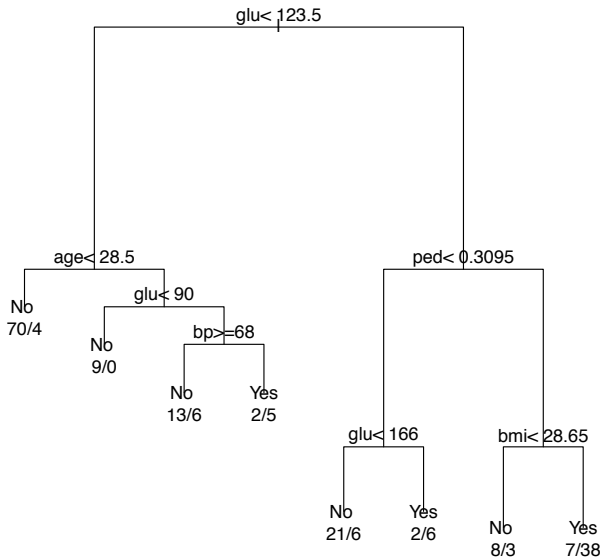
```
> library(rpart)
> library(MASS)
> data(Pima.tr)
> rp <- rpart(Pima.tr[,8] ~ ., data=Pima.tr[, -8])
> rp
n= 200

node), split, n, loss, yval, (yprob)
* denotes terminal node

1) root 200 68 No (0.66000000 0.34000000)
 2) glu< 123.5 109 15 No (0.86238532 0.13761468)
   4) age< 28.5 74 4 No (0.94594595 0.05405405) *
   5) age>=28.5 35 11 No (0.68571429 0.31428571)
     10) glu< 90 9 0 No (1.00000000 0.00000000) *
     11) glu>=90 26 11 No (0.57692308 0.42307692)
       22) bp>=68 19 6 No (0.68421053 0.31578947) *
       23) bp< 68 7 2 Yes (0.28571429 0.71428571) *
 3) glu>=123.5 91 38 Yes (0.41758242 0.58241758)
   6) ped< 0.3095 35 12 No (0.65714286 0.34285714)
     12) glu< 166 27 6 No (0.77777778 0.22222222) *
     13) glu>=166 8 2 Yes (0.25000000 0.75000000) *
 7) ped>=0.3095 56 15 Yes (0.26785714 0.73214286)
   14) bmi< 28.65 11 3 No (0.72727273 0.27272727) *
   15) bmi>=28.65 45 7 Yes (0.15555556 0.84444444) *
```

Example: Pima Indians Diabetes Dataset

```
> plot(rp,margin=0.1); text(rp,use.n=T)
```



Bagging

Model Variability



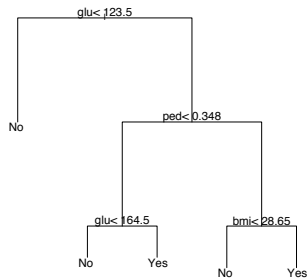
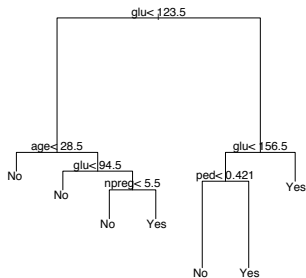
- Is the tree 'stable' if training data were slightly different?

Bootstrap for Classification Trees

- The **bootstrap** is a way to assess the variance of estimators.
- Fit multiple trees, each on a **bootstrapped sample**. This is a data set obtained by **sampling with replacement** n times from training set.

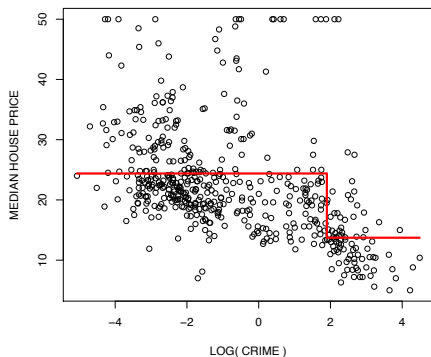
```
> n <- nrow(Pima.tr)
> bss <- sample(1:n, n , replace=TRUE)
> sort(bss)
[1]  2 4 4 5 6 7 9 10 11 12 12 12 12 13 13 15 15 20 ...

> tree_boot <- rpart(Pima.tr[bss,8] ~ ., data=Pima.tr[bss,-8],
                    control=rpart.control(xval=10)) ## 10-fold CV
```



Bootstrap for Regression Trees

- Regression for Boston housing data.
- Predict median house prices based only on crime rate.
- Use decision **stump**—the simplest tree with a single split at root.

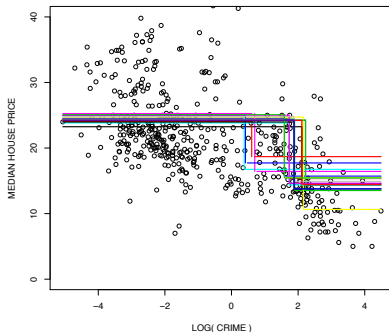
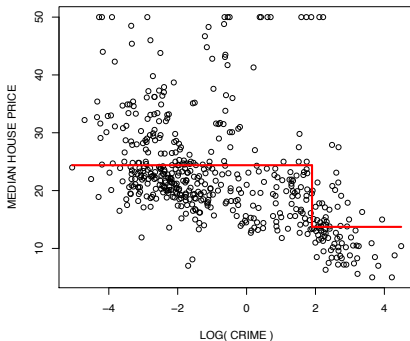


Bootstrap for Regression Trees

- We fit a predictor $\hat{f}(x)$ on the data $\{(x_i, y_i)\}_{i=1}^n$.
- Assess the variance of $\hat{f}(x)$ by taking $B = 20$ bootstrap samples of the original data, and obtaining bootstrap estimators

$$\hat{f}^b(x), \quad b = 1, \dots, B$$

- Each tree \hat{f}^b is fitted on the resampled data $(x_{j_i}, y_{j_i})_{i=1}^n$ where each j_i is chosen randomly from $\{1, \dots, n\}$ with replacement.



Bagging

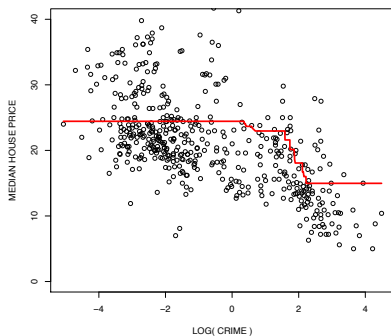
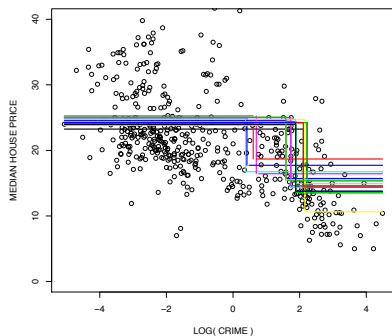
- **Bagging (Bootstrap Aggregation)**: average across all B trees fitted on different bootstrap samples.
- ① For $b = 1, \dots, B$:
 - ① Draw indices (j_1, \dots, j_n) from the set $\{1, \dots, n\}$ with replacement.
 - ② Fit the model, and form predictor $\hat{f}^b(x)$ based on bootstrap sample

$$(x_{j_1}, y_{j_1}), \dots, (x_{j_n}, y_{j_n})$$

- ② Form bagged estimator

$$\hat{f}_{Bag}(x) = \frac{1}{B} \sum_{b=1}^B \hat{f}^b(x)$$

Bagging



- Bagging smooths out the drop in the estimate of median house prices.
- Bagging reduces the variance of predictions, i.e. when taking expectations over a random dataset \mathcal{D} :

$$\mathbb{E}_{\mathcal{D}}[(\hat{f}(x) - \mathbb{E}_{\mathcal{D}}[\hat{f}(x)])^2] \geq \mathbb{E}_{\mathcal{D}}[(\hat{f}_{Bag}(x) - \mathbb{E}_{\mathcal{D}}[\hat{f}_{Bag}(x)])^2]$$

Variance Reduction in Bagging

- Suppose, in an ideal world, our estimators \hat{f}^b are each based on different independent datasets of size n from the true joint distribution of X, Y .
- The aggregated estimator would then be

$$\hat{f}_{ag}(x) = \frac{1}{B} \sum_{b=1}^B \hat{f}^b(x) \rightarrow \bar{f}(x) = \mathbb{E}_{\mathcal{D}}[\hat{f}(x)] \quad \text{as } B \rightarrow \infty$$

where expectation is with respect to datasets of size n .

- The squared-loss is:

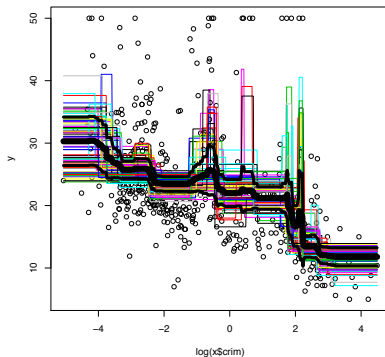
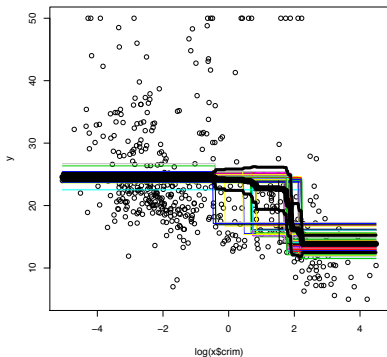
$$\begin{aligned} \mathbb{E}_{\mathcal{D}}[(Y - \hat{f}_{ag}(X))^2 | X = x] &= \\ &= \mathbb{E}_{\mathcal{D}}[(Y - \bar{f}(X))^2 | X = x] + \mathbb{E}_{\mathcal{D}}[(\bar{f}(X) - \hat{f}_{ag}(X))^2 | X = x] \\ &\rightarrow \mathbb{E}_{\mathcal{D}}[(Y - \bar{f}(X))^2 | X = x] \quad \text{as } B \rightarrow \infty. \end{aligned}$$

Aggregation reduces the squared loss by eliminating variance of $\hat{f}(x)$.

- In bagging, variance reduction still applies at the cost of a **small increase in bias**.
- Bagging is most useful for **flexible estimators with high variance** (and low bias).

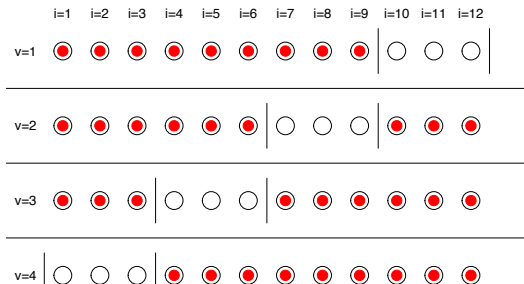
Variance Reduction in Bagging

- Deeper trees have higher complexity and variance.
- Compare bagging trees of depth 1 and 3.



Out-of-bag Test Error Estimation

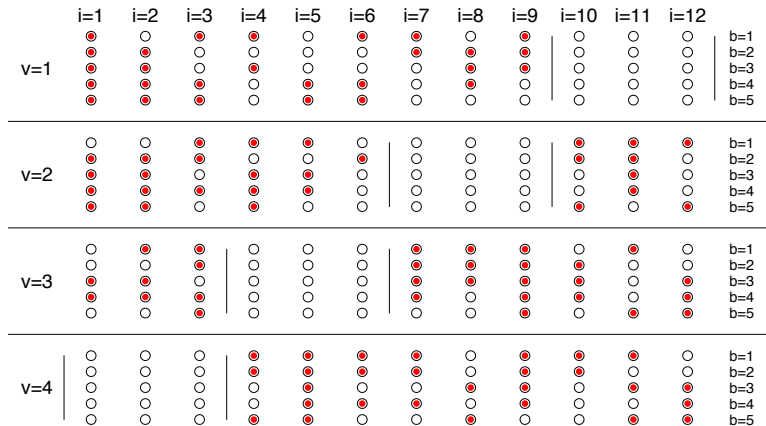
- How well does bagging to? Can we estimate generalization performance, and tune hyperparameters?
- Answer 1: cross-validation.



- For each $v = 1, \dots, V$,
 - fit \hat{f}_{Bag} on the training samples.
 - predict on validation set.
- Compute the CV error by averaging the loss across all test observations.

Out-of-bag Test Error Estimation

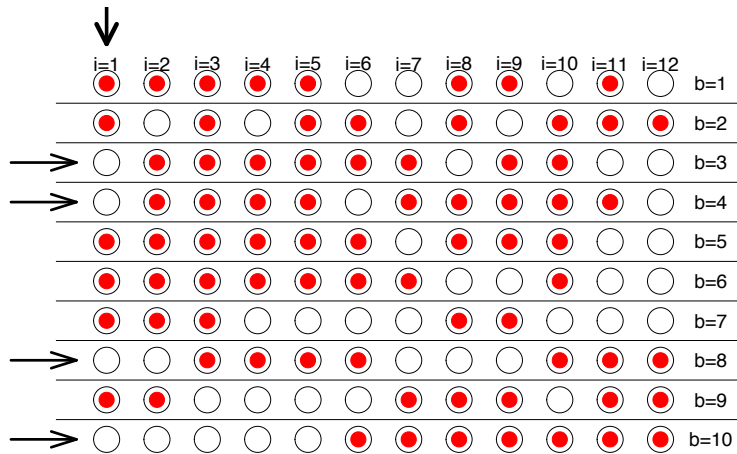
- But to fit \hat{f}_{Bag} on the training set for each $v = 1, \dots, V$, we have to train on B bootstrap samples!



- Answer 2: **Out-of-bag** test error estimation.

Out-of-bag Test Error Estimation

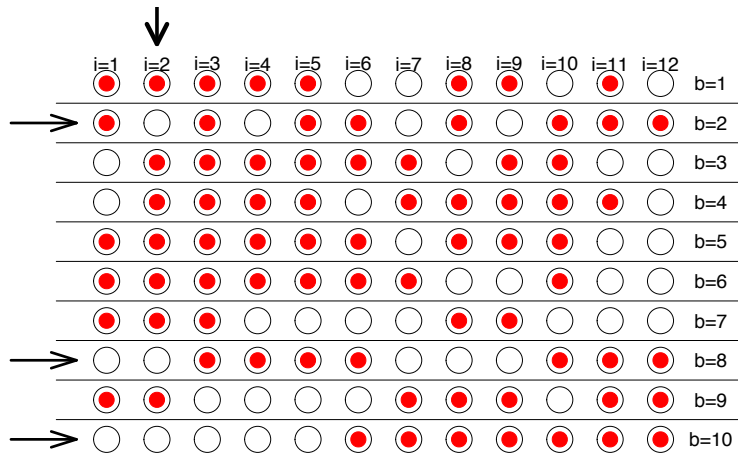
- Idea: test on the “unused” data points in each bootstrap iteration to estimate the test error.



$$\hat{f}^{\text{oob}}(x_1) = \frac{1}{4} \sum_{b \in \{3, 4, 8, 10\}} \hat{f}^b(x_1)$$

Out-of-bag Test Error Estimation

- Idea: test on the “unused” data points in each bootstrap iteration to estimate the test error.



$$\hat{f}^{\text{oob}}(x_2) = \frac{1}{3} \sum_{b \in \{2, 8, 10\}} \hat{f}^b(x_2)$$

Out-of-bag Test Error Estimation

- For each $i = 1, \dots, n$, the out-of-bag sample is:

$$\tilde{B}_i = \{b : x_i \text{ is not in training set}\} \subseteq \{1, \dots, B\}.$$

- Construct the out-of-bag estimate at x_i :

$$\hat{f}^{\text{oob}}(x_i) = \frac{1}{|\tilde{B}_i|} \sum_{b \in \tilde{B}_i} \hat{f}^b(x_i)$$

- Out-of-bag risk:

$$R^{\text{oob}} = \frac{1}{n} \sum_{i=1}^n L(y_i, \hat{f}^{\text{oob}}(x_i))$$

Out-of-bag Test Error Estimation

- We need $|\tilde{B}_i|$ to be reasonably large for all $i = 1, \dots, n$.
- The probability π^{oob} of an observation NOT being included in a bootstrap sample (j_1, \dots, j_n) (and hence being 'out-of-bag') is:

$$\pi^{\text{oob}} = \prod_{i=1}^n \left(1 - \frac{1}{n}\right) \xrightarrow{n \rightarrow \infty} \frac{1}{e} \approx 0.367.$$

- Hence $\mathbb{E}[|\tilde{B}_i|] \approx 0.367B$
- In practice, number of bootstrap samples B is typically between 200 and 1000, meaning that the number $|\tilde{B}_i|$ of out-of-bag samples will be approximately in the range 70 – 350.
- The obtained test error estimate is asymptotically unbiased for large number B of bootstrap samples and large sample size n .

Example: Boston Housing Dataset

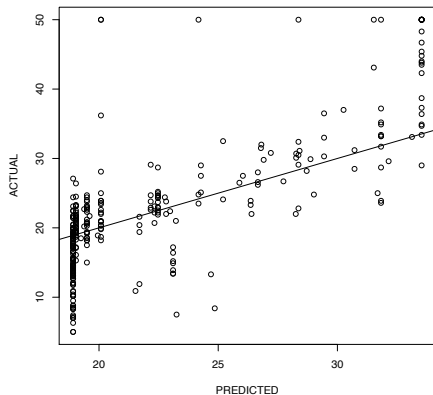
- Apply out of bag test error estimation to select optimal tree depth and assess performance of bagged trees for Boston Housing data.
- Use the entire dataset with $p = 13$ predictor variables.

```
n <- nrow(BostonHousing)    ## n samples
X <- BostonHousing[,-14]
Y <- BostonHousing[,14]
B <- 100
maxdepth <- 3
prediction_oob <- rep(0,length(Y))    ## vector with oob predictions
numbertrees_oob <- rep(0,length(Y))   ## number of oob trees
for (b in 1:B) {                  ## loop over bootstrap samples
  subsample <- sample(1:n,n,replace=TRUE)    ## "in-bag" samples
  outofbag <- (1:n)[-subsample]             ## "out-of-bag" samples
                                          ## fit tree on "in-bag" samples
  treeboot <- rpart(Y ~ ., data=X, subset=subsample,
                    control=rpart.control(maxdepth=maxdepth,minsplitlevel=2))
                                          ## predict on oob-samples
  prediction_oob[outofbag] <- prediction_oob[outofbag] +
    predict(treeboot, newdata=X[outofbag,])
  numbertrees_oob[outofbag] <- numbertrees_oob[outofbag] + 1
}
## final oob-prediction is average across all "out-of-bag" trees
prediction_oob <- prediction_oob / numbertrees_oob
```

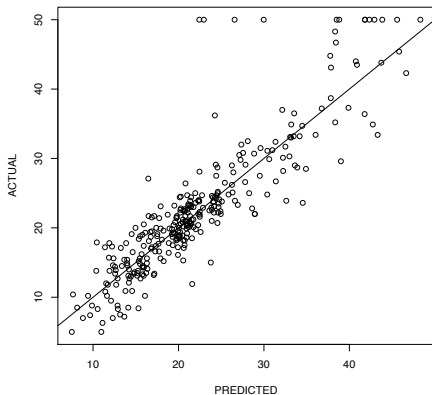
Example: Boston Housing Dataset

```
plot(prediction_oob, Y, xlab="PREDICTED", ylab="ACTUAL")
```

For depth $d = 1$.



For depth $d = 10$.



Example: Boston Housing Dataset

- Out-of-bag error as a function of tree depth d :

tree depth d	1	2	3	4	5	10	30
single tree \hat{f}	60.7	44.8	32.8	31.2	27.7	26.5	27.3
bagged trees \hat{f}_{Bag}	43.4	27.0	22.8	21.5	20.7	20.1	20.1

- Without bagging, the optimal tree depth seems to be $d = 10$.
- With bagging, we could also take the depth up to $d = 30$.

Summary:

- Bagging reduces variance and prevents overfitting
- Often improves accuracy in practice.
- Bagged trees cannot be displayed as nicely as single trees and some of the interpretability of trees is lost.

Random Forests

Random Forests and Extremely Randomized Trees

- **Random forests** are similar to bagged decision trees with a few key differences:
 - For each split point, the search is not over all p variables but just over $mtry$ randomly chosen ones (where e.g. $mtry = \lfloor p/3 \rfloor$)
 - No pruning necessary. Trees can be grown until each node contains just very few observations (1 or 5).
 - Random forests tend to produce better predictions than bagging.
 - Results often not sensitive to the only tuning parameter $mtry$.
 - Implemented in `randomForest` library.
- Even more random methods, e.g. **extremely randomized trees**:
 - For each split point, sample $mtry$ variables each with a **random value to split on**, and pick the best one.
 - Often works even when $mtry$ equals 1!
- Often produce state-of-the-art results, and top performing methods in machine learning competitions.

Random Forests

TABLE 2
Test set misclassification error (%)

Data set	Forest	Single tree
Breast cancer	2.9	5.9
Ionosphere	5.5	11.2
Diabetes	24.2	25.3
Glass	22.0	30.4
Soybean	5.7	8.6
Letters	3.4	12.4
Satellite	8.6	14.8
Shuttle $\times 10^3$	7.0	62.0
DNA	3.9	6.2
Digit	6.2	17.1

From [Breiman, Statistical Modelling: the two cultures, 2001.](#)

Random Forests

Comparison of 179 classifiers on 121 datasets. Random forests come top with SVMs close behind.

Rank	Acc.	κ	Classifier
32.9	82.0	63.5	parRF_t (RF)
33.1	82.3	63.6	rf_t (RF)
36.8	81.8	62.2	svm_C (SVM)
38.0	81.2	60.1	svmPoly_t (SVM)
39.4	81.9	62.5	rforest_R (RF)
39.6	82.0	62.0	elm_kernel_m (NNET)
40.3	81.4	61.1	svmRadialCost_t (SVM)
42.5	81.0	60.0	svmRadial_t (SVM)
42.9	80.6	61.0	C5.0_t (BST)
44.1	79.4	60.5	avNNet_t (NNET)

From [Delgado et al, 2014](#)

Looking at the Boston Housing data again (and at the help page for `randomForest` first).

```
library(randomForest)
library(MASS)
data(Boston)

y <- Boston[,14]
x <- Boston[,1:13]

?randomForest
```

```
> randomForest          package:randomForest          R Documentation
```

```
Classification and Regression with Random Forest
```

Description:

'randomForest' implements Breiman's random forest algorithm (based on Breiman and Cutler's original Fortran code) for classification and regression. It can also be used in unsupervised mode for assessing proximities among data points.

Usage:

```
## S3 method for class 'formula':
randomForest(formula, data=NULL, ..., subset, na.action=na.fail)
## Default S3 method:
randomForest(x, y=NULL, xtest=NULL, ytest=NULL, ntree=500,
             mtry=if (!is.null(y) && !is.factor(y))
                 max(floor(ncol(x)/3), 1) else floor(sqrt(ncol(x))),
             replace=TRUE, classwt=NULL, cutoff, strata,
             sampsize = if (replace) nrow(x) else ceiling(.632*nrow(x))
             nodesize = if (!is.null(y) && !is.factor(y)) 5 else 1,
             importance=FALSE, localImp=FALSE, nPerm=1,
             proximity=FALSE, oob.prox=proximity,
             norm.votes=TRUE, do.trace=FALSE,
             keep.forest=!is.null(y) && is.null(xtest), corr.bias=FALSE,
             keep.inbag=FALSE, ...)
```



```
> rf <- randomForest(x,y)
> print(rf)
>
Call:
randomForest(x = x, y = y)
      Type of random forest: regression
      Number of trees: 500
No. of variables tried at each split: 4

      Mean of squared residuals: 10.26161
      % Var explained: 87.84
```

Can plot the predicted values (out-of-bag estimation) vs. true values by

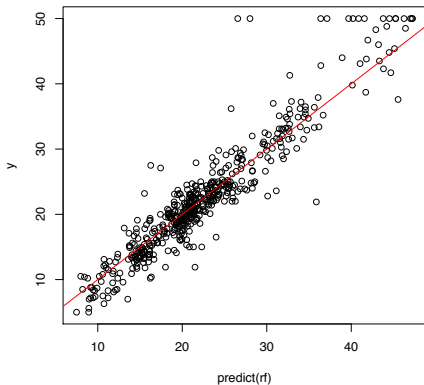
```
> plot(predict(rf), y)
> abline(c(0,1),col=2)
```

Same if treating the training data as new data

```
> plot(predict(rf,newdata=x), y)
```

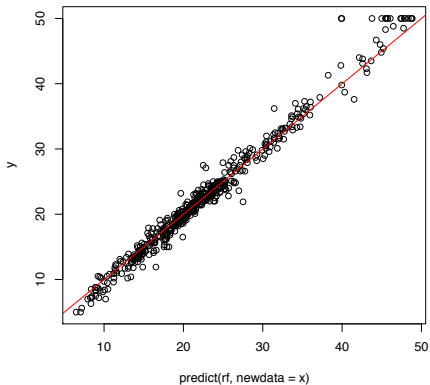
Out-of-bag error.

```
> plot( predict(rf), y)
> abline(c(0,1), col=2)
```



Training error.

```
> plot( predict(rf,newdata=x), y)
> abline(c(0,1), col=2)
```



Try mtry 2

```
> (rf <- randomForest(x,y,mtry=2))
Call:
randomForest(x = x, y = y, mtry = 2)
      Type of random forest: regression
      Number of trees: 500
No. of variables tried at each split: 2

      Mean of squared residuals: 12.17176
      % Var explained: 85.58
```

Try mtry 4

```
> (rf <- randomForest(x,y,mtry=4))
Call:
randomForest(x = x, y = y, mtry = 4)
      Type of random forest: regression
      Number of trees: 500
No. of variables tried at each split: 4

      Mean of squared residuals: 10.01574
      % Var explained: 88.14
```

And `mtry` 8 and 10.

```
> (rf <- randomForest(x,y,mtry=8))
Call:
randomForest(x = x, y = y, mtry = 8)
      Type of random forest: regression
      Number of trees: 500
No. of variables tried at each split: 8

      Mean of squared residuals: 9.552806
      % Var explained: 88.68
```

```
> > (rf <- randomForest(x,y,mtry=10))
Call:
randomForest(x = x, y = y, mtry = 10)
      Type of random forest: regression
      Number of trees: 500
No. of variables tried at each split: 10

      Mean of squared residuals: 9.774435
      % Var explained: 88.42
```

`mtry` is the only real tuning parameter and typically performance not sensitive to its choice (can use `tuneRF` to select it automatically).

Variable “Importance”

- Tree ensembles have better performance, but decision trees are more interpretable.
- How to interpret a forest of trees ?

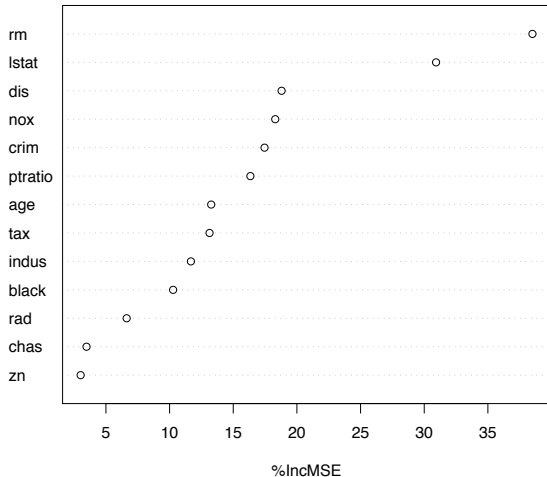
Idea: denote by \hat{e} the out-of bag estimate of the loss when using the original data samples. For each variable $k \in \{1, \dots, p\}$,

- permute randomly the k -th predictor variable to generate a new set of samples $(\tilde{X}_1, Y_1), \dots, (\tilde{X}_n, Y_n)$, i.e., $\tilde{X}_i^{(k)} = X_{\tau(i)}^{(k)}$, for a permutation τ .
- compute the out-of-bag estimate \hat{e}_k of the prediction error with these new samples.

A measure of importance of variable k is then $\hat{e}_k - \hat{e}$, the increase in error rate due to a random permutation of the k -th variable.

Example for Boston Housing data.

```
rf <- randomForest(x,y,importance=TRUE)  
varImpPlot(rf)
```



Ensemble Methods

- Bagging and random forests are examples of **ensemble methods**, where predictions are based on an ensemble of many individual predictors.
- Many other ensemble learning methods: boosting, stacking, mixture of experts, Bayesian model combination, Bayesian model averaging etc.
- Often gives significant boost to predictive performance.

Microsoft Kinect Pose Recognition

Kinect algorithm CVPR Paper

Video