Random forests

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Outline

boston dataset

- Trees versus linear models
- Bootstrap aggregation: bagging
- Random forests
- Revisiting the spam dataset
- Simulation exercise
- Revisiting the motorcycle data
- The ALS data
- Additional references

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boston dataset

Boston Housing data, Harrison and Rubinfeld $(1978)^1$

The data consist of 14 characteristics of 506 census tracts in the Boston area.

The response is the logged median value of owner occupied homes in each tract.

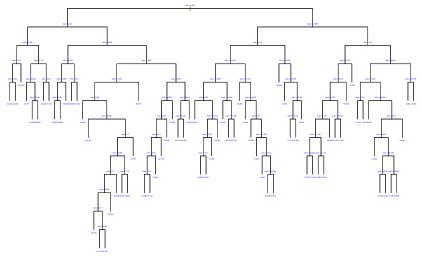
Name	Description		Max
CRIM	per capita crime rate by town	0.006	88.976
ZN	proportion of residential land zoned for lots over 25,000 sq.ft.	0.000	100.000
INDUS	proportion of non-retail business acres per town	0.460	27.740
CHAS	Charles River dummy variable (=1 if tract bounds river; 0 otherwise)	0.000	1.000
NOX	nitric oxides concentration (parts per 10 million)	0.385	0.871
RM	average number of rooms per dwelling	3.561	8.780
AGE	proportion of owner-occupied units built prior to 1940	2.900	100.000
DIS	weighted distances to five Boston employment centres	1.130	12.126
RAD	index of accessibility to radial highways	1.000	24.000
TAX	full-value property-tax rate per \$10,000	187.000	711.000
PTRATIO	pupil-teacher ratio by town	12.600	22.000
В	$1000(Bk - 0.63)^2$ where Bk is the proportion of blacks by town	0.320	396.900
LSTAT	% lower status of the population	1.730	37.970
MEDV	Log Median value of owner-occupied homes in \$1000's	1.609	3.912

Table 1. Variables in the Boston dataset.

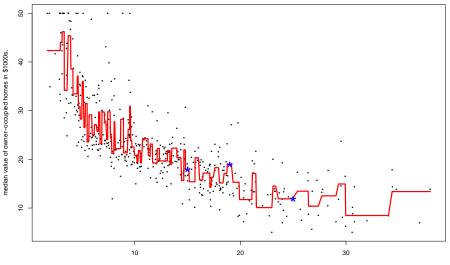
¹Harrison and Rubinfeld (1978) Hedonic prices and the demand for clean air. *Journal of Environmental Economic and Management*, 5, 81-102.

Let us try p = 1

lstat: lower status of the population (percent)

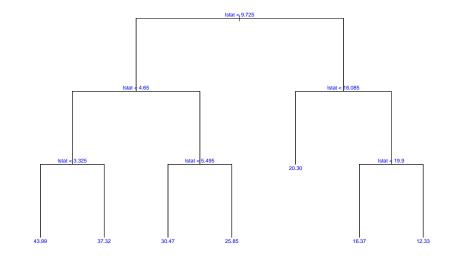


Fitted model

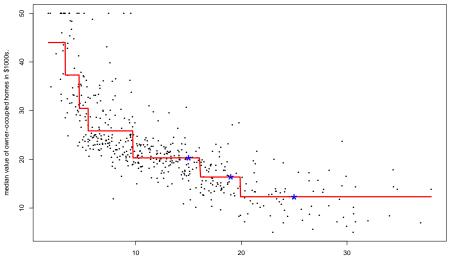


lower status of the population (percent)

Pruned tree



Fitted model



lower status of the population (percent)

R code

install.packages("tree")
library(tree)
library(MASS)
attach(Boston)

Fitting a large tree

```
temp.tree = tree(medv~lstat,data=Boston,mindev=.0001)
plot(temp.tree,type="uniform")
text(temp.tree,col="blue",label=c("yval"),cex=.3)
```

```
temp.fit = predict(temp.tree)
oo=order(lstat)
preddf = data.frame(lstat=c(15,19,25))
yhat = predict(temp.tree,preddf)
```

```
plot(lstat,medv,cex=.5,pch=16)
lines(lstat[oo],temp.fit[oo],col="red",lwd=3)
points(preddf$lstat,yhat,col="blue",pch="*",cex=3)
```

Pruning the large tree

```
# ------
```

```
boston.tree=prune.tree(temp.tree,best=7)
plot(boston.tree,type="uniform")
text(boston.tree,col="blue",label=c("yval"),cex=.8)
```

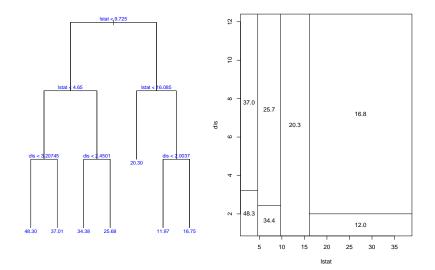
```
boston.fit = predict(boston.tree)
oo=order(lstat)
preddf = data.frame(lstat=c(15,19,25))
yhat = predict(boston.tree,preddf)
```

```
plot(lstat,medv,cex=.5,pch=16)
lines(lstat[oo],boston.fit[oo],col="red",lwd=3)
points(preddf$lstat,yhat,col="blue",pch="*",cex=3)
```

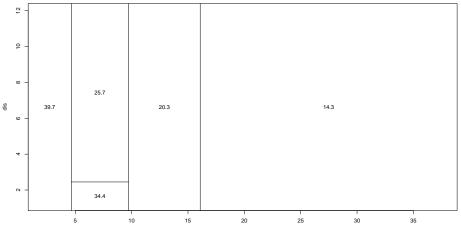
Let us try p = 2

lstat: lower status of the population (percent)

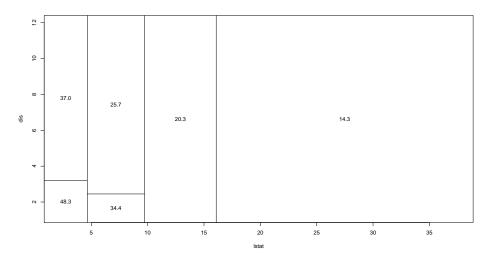
dis: weighted mean of distances to five Boston employment centres.



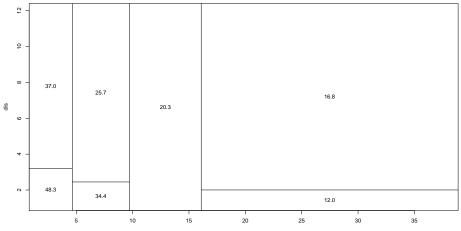
10/71



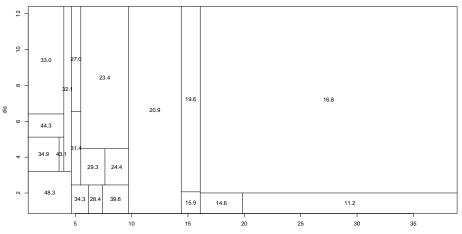
Istat



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Istat



Istat

R code

```
df2=Boston[,c(8,13,14)]
```

```
temp.tree = tree(medv~.,df2,mindev=.0001)
```

```
boston.tree=prune.tree(temp.tree,best=7)
```

```
par(mfrow=c(1,2))
```

```
plot(boston.tree,type="u")
```

```
text(boston.tree,col="blue",label=c("yval"),cex=.8)
```

partition.tree(boston.tree)

Comparing in-sample fits

boston.fit2 = predict(boston.tree)

fmat = cbind(medv,boston.fit,boston.fit2)

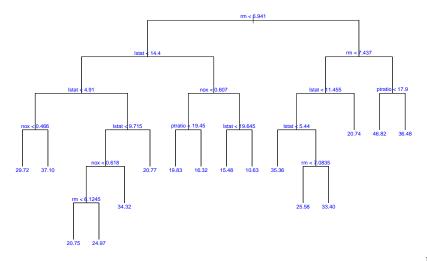
```
colnames(fmat)=c("y=medv","treel","treeld")
```

```
print(cor(fmat))
```

y=medv treel treeld y=medv 1.0000000 0.8338431 0.8560183 treel 0.8338431 1.0000000 0.9364702 treeld 0.8560183 0.9364702 1.0000000

Let us try p = 4

nox: nitrogen oxides concentration (parts per 10 million)
rm: average number of rooms per dwelling
ptratio: pupil-teacher ratio by town
lstat: lower status of the population (percent)



R code

```
df4=Boston[,c(5,6,11,13,14)]
temp = tree(medv~.,df4,mindev=.0001)
boston.tree4=prune.tree(temp,best=15)
```

```
par(mfrow=c(1,1))
plot(boston.tree4,type="u")
text(boston.tree4,col="blue",label=c("yval"),cex=.8)
```

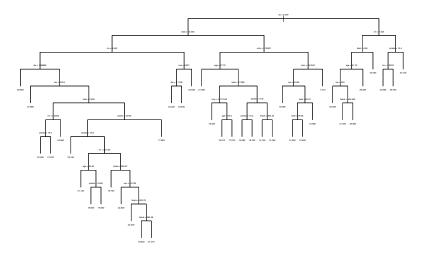
```
fmat4=cbind(fmat,predict(boston.tree4))
colnames(fmat4)[4]="tree4"
```

```
print(cor(fmat4))
```

y=medv treel treeld tree4 y=medv 1.0000000 0.8338431 0.8560183 0.9266955 treel 0.8338431 1.0000000 0.9364702 0.8783099 treeld 0.8560183 0.9364702 1.0000000 0.8830659 tree4 0.9266955 0.8783099 0.8830659 1.0000000

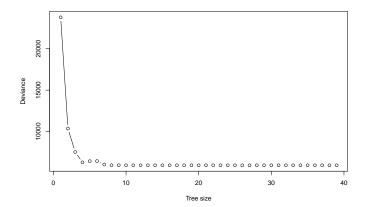
Tree with all p = 13 predictors

library (MASS)
sst.seed (31415)
train = ssmple (1: nrow(Boston), nrow(Boston)/2)
tree.boston = tree(medv⁻.,Boston ,subset =train,mindev=.0001)
plot(tree.boston,pret^u")
text(tree.boston,pret^u"o,cx=0.3)



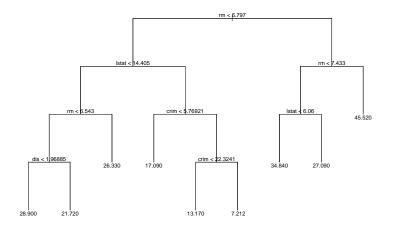
Cross-validation

```
cv.boston = cv.tree(tree.boston)
plot(cv.boston$size,cv.boston$dev,type="b")
```



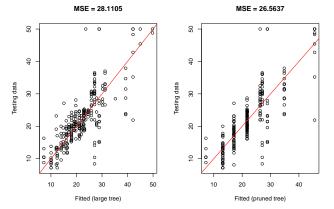
Pruned tree

prune.boston = prune.tree(tree.boston,best=9)
plot(prune.boston,type="u")
text(prune.boston,pretty=0)



Large and pruned trees

```
y = Boston[-train,"medv"]
yhat = predict(tree.boston,mewdata=Boston[-train,])
yhat1 = predict(prume.boston,mewdata=Boston[-train,])
corr(y,yhat) = 0.798, corr(y,yhat1) = 0.806, corr(yhat,yhat1) = 0.946
par(mfrow=c(1,2))
plot(yhat,boston.test,xlab="Fitted (large tree)",ylab="Testing data")
title(paste("MSE = ",round(mean((yhat-y)^2),4),sep=""))
abline(0,1,col=2)
plot(yhat1,boston.test,xlab="Fitted (prumed tree)",ylab="Testing data")
title(paste("MSE = ",round(mean((yhat1-y)^2),4),sep=""))
abline(0,1,col=2)
plot(yhat1,col=2)
```



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Trees versus linear models²

Regression and classification trees have a very different flavor from the more classical approaches for regression and classification.

In particular, linear regression assumes a model of the form

$$f(x) = \sum_{j=1}^{p} \beta_j x_j$$

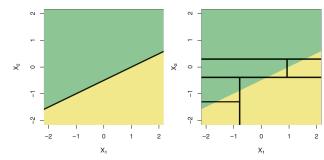
whereas regression trees assume a model of the form

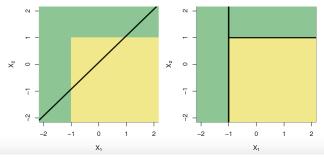
$$f(x) = \sum_{m=1}^{M} c_m \mathbb{1}_{x \in R_m}$$

where R_1, \ldots, R_m represent a partition of feature space.

²ISLR, Section 8.1.3

Trees versus linear models





Advantages of trees³

- Trees are very easy to explain to people. In fact, they are even easier to explain than linear regression!
- Some people believe that decision trees more closely mirror human decision-making than do the regression and classification approaches.
- Trees can be displayed graphically, and are easily interpreted even by a non-expert (especially if they are small).
- Trees can easily handle qualitative predictors without the need to create dummy variables.

Disadvantages of trees

- Unfortunately, trees generally do not have the same level of predictive accuracy as some of the other regression and classification approaches.
- Additionally, trees can be very non-robust. In other words, a small change in the data can cause a large change in the final estimated tree.

Bagging, random forests and boosting

However, by aggregating many decision trees, using methods like bagging, random forests, and boosting, the predictive performance of trees can be substantially improved.

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Bootstrap aggregation: bagging⁴

Bootstrap aggregation, or bagging, is a general-purpose procedure for reducing the variance of a statistical learning method.

A natural way to reduce the variance and hence increase the prediction accuracy of a statistical learning method is to take many training sets from the population, build a separate prediction model using each training set, and average the resulting predictions. In other words, we could calculate

$$\hat{f}^1(x), \hat{f}^2(x), \ldots, \hat{f}^B(x)$$

using B separate training sets, and average them in order to obtain a single low-variance statistical learning model given by

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

Bagging

Of course, this is not practical because we generally do not have access to multiple training sets.

Instead, we can bootstrap, by taking repeated samples from the (single) training data set.

In this approach we generate B different bootstrapped training data sets.

We then train our method on the *b*th bootstrapped training set in order to get $\hat{f}^{*b}(x)$, and finally average all the predictions, to obtain

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

This is called bagging.

Bagging for regression trees

Construct B regression trees using B bootstrapped training sets, and average the resulting predictions.

These trees are grown deep, and are not pruned.

Hence each individual tree has high variance, but low bias.

Averaging these B trees reduces the variance.

Bagging has been demonstrated to give impressive improvements in accuracy by combining together hundreds or even thousands of trees into a single procedure.

Bagging the boston data

bag.boston = randomForest(medv~.,data=Boston,subset=train,mtry=13,importance=TRUE)

Type of random forest: regression Number of trees: 500 No. of variables tried at each split: 13

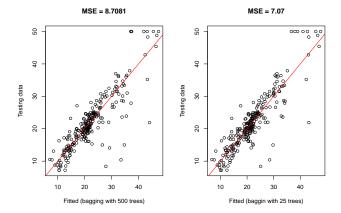
> Mean of squared residuals: 15.33724 % Var explained: 83.59

bag.boston = randomForest(medv~.,data=Boston,subset=train,mtry=13,ntree=25)

Type of random forest: regression Number of trees: 25 No. of variables tried at each split: 13

> Mean of squared residuals: 16.46512 % Var explained: 82.38

Fitted models



cor(cbind(boston.test,yhat,yhat1,yhat.bag,yhat.bag1))

	boston.test	yhat	yhat1	yhat.bag	yhat.bag1
boston.test	1.0000000	0.7982040	0.8057710	0.8686673	0.8932177
yhat	0.7982040	1.0000000	0.9461125	0.9317866	0.9363935
yhat1	0.8057710	0.9461125	1.0000000	0.9357755	0.9395889
yhat.bag	0.8686673	0.9317866	0.9357755	1.0000000	0.9893311
yhat.bag1	0.8932177	0.9363935	0.9395889	0.9893311	1.0000000

R code

library(randomForest)

```
set.seed(31415)
bag.boston = randomForest(medv~.,data=Boston,subset=train,mtry=13,importance=TRUE)
bag.boston
bag.boston = randomForest(medv~..data=Boston.subset=train.mtrv=13.ntree=25)
bag.boston
yhat.bag = predict (bag.boston ,newdata =Boston [-train ,])
yhat.bag1 = predict (bag.boston ,newdata =Boston [-train ,])
par(mfrow=c(1,2))
plot(yhat.bag,boston.test,xlab="Fitted (bagging 1)",ylab="Testing data")
title(paste("MSE = ",round(mean((vhat-vhat.bag)^2).4).sep=""))
abline(0.1.col=2)
plot(vhat.bag1.boston.test.xlab="Fitted (pruned tree)".vlab="Testing data")
title(paste("MSE = ",round(mean((yhat1-yhat.bag1)^2),4),sep=""))
abline(0,1,col=2)
```

cor(cbind(boston.test,yhat,yhat1,yhat.bag,yhat.bag1))

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Random forests⁵

Random forests provide an improvement over bagged trees by way of a random small tweak that decorrelates the trees.

As in bagging, we build a number forest of decision trees on bootstrapped training samples.

But when building these decision trees, each time a split in a tree is considered, a random sample of m predictors is chosen as split candidates from the full set of p predictors.

The split is allowed to use only one of those m predictors. A fresh sample of m predictors is taken at each split, and typically we choose $m \approx \sqrt{p}$.

⁵ISLR, Section 8.2.2

When does random forests beat bagging?

One very strong predictor + many moderately strong predictors.

Bagging:

- Most or all of the trees will use this strong predictor in the top split.
- ► All of the bagged trees will look quite similar to each other.
- The predictions from the bagged trees will be highly correlated.
- Averaging many highly correlated quantities does not reduce the variance.

Random forests:

- ▶ Random forests forces each split to consider only *m* predictors.
- On average (p m)/p of the splits will not consider the strong predictor.
- Other predictors will have more of a chance.
- This process decorrelates the trees.
- ► The average of the resulting trees less variable and hence more reliable.

Random Forest for Regression or Classification⁶

Algorithm 15.1 Random Forest for Regression or Classification.

- 1. For b = 1 to B:
 - (a) Draw a bootstrap sample \mathbf{Z}^* of size N from the training data.
 - (b) Grow a random-forest tree T_b to the bootstrapped data, by recursively repeating the following steps for each terminal node of the tree, until the minimum node size n_{min} is reached.
 - i. Select m variables at random from the p variables.
 - ii. Pick the best variable/split-point among the m.
 - iii. Split the node into two daughter nodes.
- 2. Output the ensemble of trees $\{T_b\}_1^B$.

To make a prediction at a new point x:

Regression:
$$\hat{f}_{rf}^B(x) = \frac{1}{B} \sum_{b=1}^B T_b(x).$$

Classification: Let $\hat{C}_b(x)$ be the class prediction of the *b*th random-forest tree. Then $\hat{C}^B_{\rm rf}(x) = majority \ vote \ \{\hat{C}_b(x)\}_1^B$.

⁶Hastie, Tibshirani and Friedman (2008) *The Elements of Statistical Learning: Data Mining, Inference, and Prediction, 2nd Edition*, page 588.

Out-of-bag error⁷

The out-of-bag (OOB) estimate, for response observation y_i in the training data, is obtained by averaging those $T_b(x_i)$ for which observation *i* was NOT in the bootstrap sample:

$$\hat{f}_{rf}^{(i)} = \frac{1}{B_i} \sum_{b: i \notin \mathbb{Z}_b^*} T_b(x_i),$$

where B_i is the number of times observation *i* was not in the bootstrap sample.

The overall out-of-bag (OOB) error estimate is

$$\operatorname{err}_{OOB} = \frac{1}{N} \sum_{i=1}^{N} L[y_i, \hat{f}_{rf}^{(i)}]$$

Random forests deliver cross-validated error estimates at virtually no extra cost.

▶ If *B* is sufficiently large (about three times the number needed for the random forest to stabilize), we can see that the OOB error estimate is equivalent to leave-one-out cross-validation error.

⁷Efron and Hastie (2016) *Computer Age Statistical Inference: Algorithms, Evidence, and Data Science*, page 327-330.

Adele Cutler's Random Forests page⁸

Random Forests Leo Breiman and Adele Cutler

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classification/clustering regression survival analysis

graphics

Statistical Methods for Prediction and Understanding.



Phil Cutler

⁸http://www.math.usu.edu/~adele/forests

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Revisiting the spam dataset

Overall misclassification erros: 9.3% (tree) vs 5.7% (lasso with interactions)

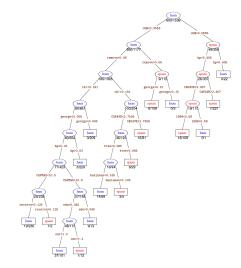


Figure 17.1 Regression tree fit to the binary spam data, a bigger version of Figure 8.7. The initial trained tree was far bushier than the one displayed; it was then *optimally* pruned using 10-fold cross-validation.

Test error

Random Forest on the Spam Data

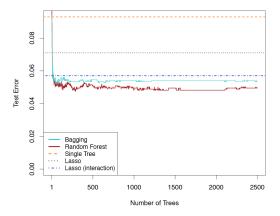


Figure 17.2 Test misclassification error of random forests on the spam data, as a function of the number of trees. The red curve selects m = 7 of the p = 57 features at random as candidates for the split variable, each time a split is made. The blue curve uses m = 57, and hence amounts to bagging. Both bagging and random forests outperform the lasso methods, and a single tree.

OOB error

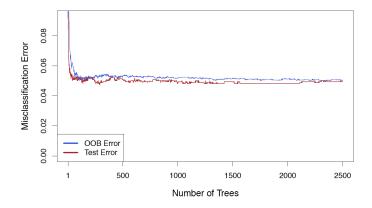


Figure 17.3 Out-of-bag misclassification error estimate for the spam data (blue) versus the test error (red), as a function of the number of trees.

Variable-importance plots

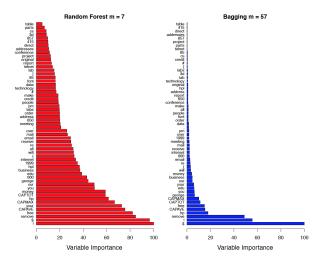
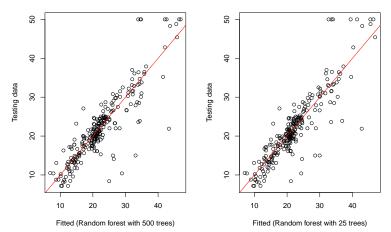


Figure 17.5 Variable-importance plots for random forests fit to the spam data. On the left we have the m = 7 random forest; due to the split-variable randomization, it spreads the importance among the variables. On the right is the m = 57 random forest or bagging, which focuses on a smaller subset of the variables.

Random forest: the boston data

randomForest() defaults: m = p/3 variables (regression trees) $m = \sqrt{p}$ variables (classification trees)



MSE = 7.8471

MSE = 7.5677

R code

```
set.seed(31415)
rf.boston = randomForest(medv~..data=Boston.subset=train.mtrv=10.importance=TRUE)
rf.boston
yhat.rf = predict (rf.boston ,newdata =Boston [-train ,])
rf.boston = randomForest(medv<sup>~</sup>.,data=Boston,subset=train,mtry=10,ntree=25,importance=TRUE)
rf.boston
vhat.rf1 = predict (rf.boston .newdata =Boston [-train .])
par(mfrow=c(1,2))
plot(yhat.rf,boston.test,xlab="Fitted (Random forest with 500 trees)",ylab="Testing data")
title(paste("MSE = ",round(mean((yhat-yhat.rf)^2),4),sep=""))
abline(0.1.col=2)
plot(yhat.rf1,boston.test,xlab="Fitted (Random forest with 25 trees)",ylab="Testing data")
title(paste("MSE = ".round(mean((vhat1-vhat.rf1)^2).4).sep=""))
abline(0,1,col=2)
round(cor(cbind(boston.test,yhat,yhat1,yhat.bag,yhat.bag1,yhat.rf,yhat.rf1)),4)
           boston.test yhat yhat1 yhat.bag yhat.bag1 yhat.rf yhat.rf1
boston test
               1.0000 0.7982 0.8058 0.8687 0.8932 0.8801 0.8754
               0.7982 1.0000 0.9461 0.9318 0.9364 0.9367 0.9306
yhat
              0.8058 0.9461 1.0000 0.9358 0.9396 0.9431 0.9401
vhat1
vhat.bag 0.8687 0.9318 0.9358 1.0000 0.9893 0.9963 0.9874
yhat.bag1 0.8932 0.9364 0.9396 0.9893 1.0000 0.9902
                                                               0.9802
         0.8801 0.9367 0.9431 0.9963 0.9902 1.0000
vhat.rf
                                                               0.9939
vhat.rf1
            0.8754 0.9306 0.9401 0.9874 0.9802 0.9939 1.0000
```

```
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```

IncNodePurity

"IncNodePurity is a measure of the total decrease in node impurity that results from splits over that variable, averaged over all trees. In the case of regression trees, the node impurity is measured by the training RSS, and for classification trees by the deviance." (ISLR, page 330)

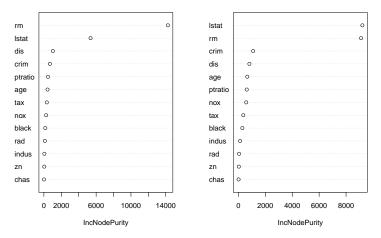
cbind(importance(bag.boston),importance(rf.boston))

	IncNodePurity	IncNodePurity
crim	686.54263	1096.69409
zn	42.13764	34.86653
indus	59.16361	126.10467
chas	12.19279	15.02267
nox	255.99583	582.10465
rm	14242.36653	9118.38936
age	416.35425	661.10425
dis	1032.03573	818.34677
rad	113.72632	49.43791
tax	335.51800	367.36610
ptratio	471.69760	623.26081
black	165.22122	295.30598
lstat	5357.56649	9214.00802

Variable importance

Bagging

Random forest



"The results indicate that across all of the trees considered in the random forest, the wealth level of the community (lstat) and the house size (rm) are by far the two most important variables." (ISLR, page 330)

Outline

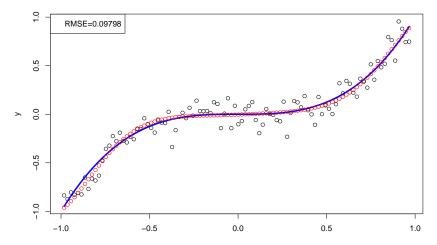
boston dataset

- Trees versus linear models
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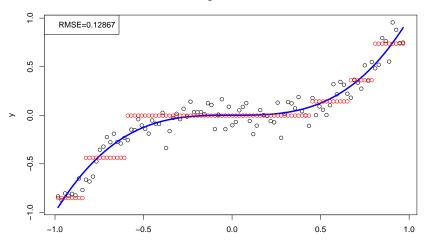
Simulated exercise

$$\begin{split} n &= 200 \; (100 \; \text{for training and } 100 \; \text{for testing}) \\ x_i &\sim U(-1,1) \\ y_i &\sim N(x_i^3,0.1^2) \end{split}$$

OLS – polynomial regression

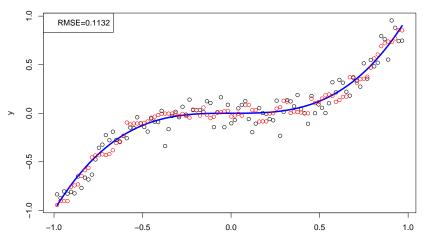


Regression tree



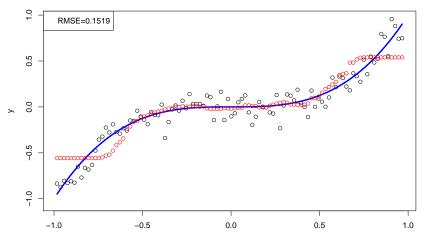
Regression tree

Bagging regression trees



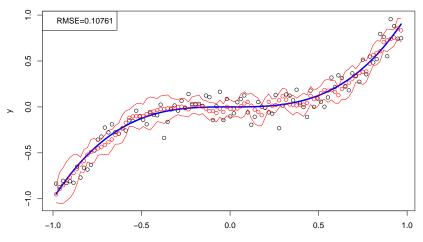
Bagging regression trees

Boosting regression trees



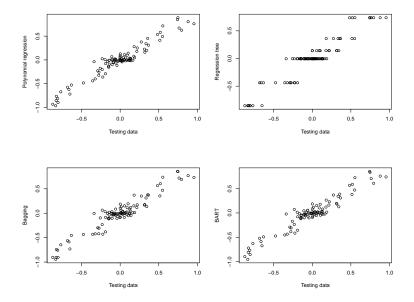
Boosting regression trees

Bayesian additive regression trees



Bayesian additive regression trees

True versus fitted

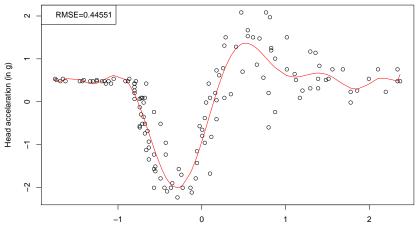


Outline

boston dataset

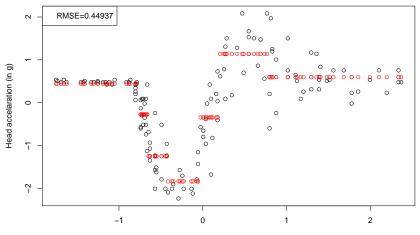
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Revisiting the motorcycle data



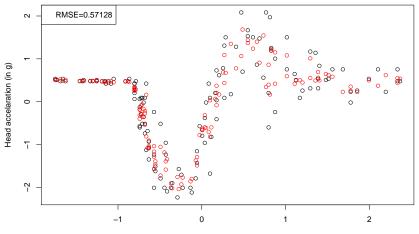
OLS - polynomial regression

Regression tree



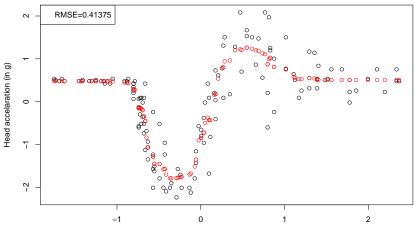
Regression tree

Bagging regression tree



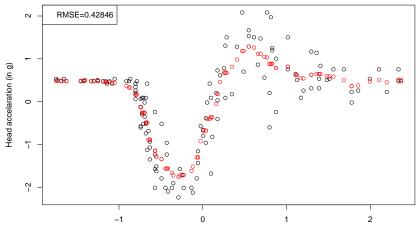
Bagging regression tree

Boosting



Boosting

BART



Bayesian additive regression trees

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The ALS data

Additional references

The ALS data⁹

These data represent measurements on patients with amyotrophic lateral sclerosis (Lou Gehrig's disease). The goal is to predict the rate of progression of an ALS functional rating score (FRS). There are 1197 training measurements on 369 predictors and the response, with a corresponding test set of size 625 observations.

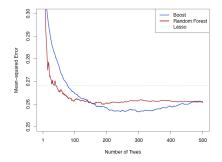


Figure 17.6 Test performance of a boosted regression-tree model fit to the ALS training data, with n = 1197 and p = 369. Shown is the mean-squared error on the 625 designated test observations, as a function of the number of trees. Here the depth d = 4 and $\epsilon = 0.02$. Boosting achieves a lower test MSE than a random forest. We see that as the number of trees *B* gets large, the test error for boosting achieves a lower test MSE than a random voerfitting. The random forest does not overfit. The dotted blue horizontal line shows the best performance of a linear model, fit by the lasso. The differences are less dramatic than they appear, since the vertical scale does not extend to zero.

⁹Computer Age Statistical Inference, pages 334-337.

Variable-importance plot

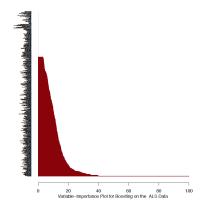


Figure 17.7 Variable importance plot for the ALS data. Here 267 of the 369 variables were used in the ensemble. There are too many variables for the labels to be visible, so this plot serves as a visual guide. Variable Onset. Delta has relative importance 100 (the lowest red bar), more than double the next two at around 40 (last.slope.weight and alsfrs.score.slope). However, the importances drop off slowly, suggesting that the model requires a significant fraction of the variables.

Only 267 of the 369 variables were ever used, with one variable **Onset.Delta** standing out ahead of the others. This measures the amount of time that has elapsed since the patient was first diagnosed with ALS, and hence a larger value will indicate a slower progression rate.

The DREAM challenge¹⁰

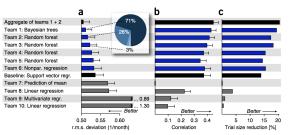
The ALS data were kindly provided by Lester Mackey and Lilly Fang, who won the DREAM challenge prediction prize in 2012 (Kuffner et al., 2015). It includes some additional variables created by them. Their winning entry used Bayesian trees, not too different from random forests.

Model	Our RMSD (Test)	Our RMSD (Validation)
Lasso Regression	0.5006	0.5287
Random Forests	0.5052	0.5120
Boosted Trees	0.4940	0.5118
BART	0.4860	0.5109

¹⁰https://web.stanford.edu/ lmackey/papers/alsprize4life-slides.pdf

The DREAM challenge¹¹

Figure 2 Performance of methods, (a,b) We compared the approaches of the ten teams that submitted executable R code in the final phase of the challenge and a baseline approach designed by the challenge organizers. All the solvers' algorithms had to be compatible with R version 2.13.1. The teams are numbered according to their ranking in r.m.s. deviation performance (a) or Pearson Correlation (b). They are colored blue if they performed better than, and gray if they performed worse than, the baseline. In addition, an aggregate of the predictions of teams 1 and 2 is shown. Whiskers indicate bootstrapped s.d. (inset). The frequency with which methods were ranked first is estimated across different bootstrap samples



of patients. Teams 1 and 2 were ranked first in 71% and 26%, respectively, of the bootstrap samples (percentage rounded to the nearest integer). (d) By simulation, we estimated to what extent clinical trials can be reduced in size by each of the participating approaches corresponding to their improved prediction of disease progression.

Küffner, Zach, Norel, Hawe, Schoenfeld, Wang, Li, Fang, Mackey, Hardiman, Cudkowicz, Sherman, Ertaylan, Grosse-Wentrup, Hothorn, van Ligtenberg, Macke, Meyer, Schölkopf, Tran, Vaughan, Stolovitzky and Leitner (2014) Crowdsourced analysis of clinical trial data to predict amyotrophic lateral sclerosis progression. *Journal Nature Biotechnology*, 33, 51.

¹¹http://neurology.arizona.edu/sites/default/files/dr_scherer-nbt_3051.pdf

Institutions

1 Institute of Bioinformatics and Systems Biology, German Research Center for Environmental Health, Munich, Germany, 2 Department of Informatics, Ludwig-Maximilians-University, Munich, Germany, 3 Prize4Life, Tel Aviv, Israel and Cambridge, Massachusetts, USA. 4 IBM T.J. Watson Research Center, Yorktown Heights, New York, USA, 5 MGH Biostatistics Center, Massachusetts General Hospital, Boston, Massachusetts, USA. 6 Harvard Medical School, Charlestown, Massachusetts, USA, 7 Sentrana Inc., Washington, DC, USA. 8 Latham&Watkins LLP. Silicon Valley, California, USA. 9 Department of Statistics, Stanford University, Stanford, California, USA, 10 Department of Neuroscience, Beaumont Hospital and Trinity College Dublin, Dublin, Ireland. 11 Neurological Clinical Research Institute, Massachusetts General Hospital, Charlestown, Massachusetts, USA. 12 Luxembourg Centre for Systems Biomedicine, University of Luxembourg, Esch/Alzette, Luxembourg. 13 Max Planck Institute for Intelligent Systems, Tübingen, Germany, 14 Institute of Social- and Preventive Medicine, University of Zirich, Zürich, Switzerland. 15 Orca XL Problem Solvers, Amsterdam, the Netherlands. 16 Max Planck Institute for Biological Cybernetics and Bernstein Center for Computational Neuroscience, Tübingen, Germany, 17 Berkeley School of Public Health, University of California, Berkeley, California, USA.

18 ALS Innovation Hub, Biogen Idec, Cambridge, Massachusetts, USA.

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Bibliographic Notes¹²

Random forests as described here were introduced by Breiman (2001), although many of the ideas had cropped up earlier in the literature in different forms.

Notably Ho (1995) introduced the term "random forest," and used a consensus of trees grown in random subspaces of the features.

The idea of using stochastic perturbation and averaging to avoid overfitting was introduced by Kleinberg (1990), and later in Kleinberg (1996).

Amit and Geman (1997) used randomized trees grown on image features for image classification problems.

Breiman (1996) introduced bagging, a precursor to his version of random forests.

Dietterich (2000) also proposed an improvement on bagging using additional randomization. His approach was to rank the top 20 candidate splits at each node, and then select from the list at random. He showed through simulations and real examples that this additional randomization improved over the performance of bagging.

Friedman and Hall (2007) showed that sub-sampling (without replacement) is an effective alternative to bagging. They showed that growing and averaging trees on samples of size N/2 is approximately equivalent (in terms bias/variance considerations) to bagging, while using smaller fractions of N reduces the variance even further (through decorrelation).

¹²ESL, page 602.

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