Statistical Machine Learning
Hilary Term 2020

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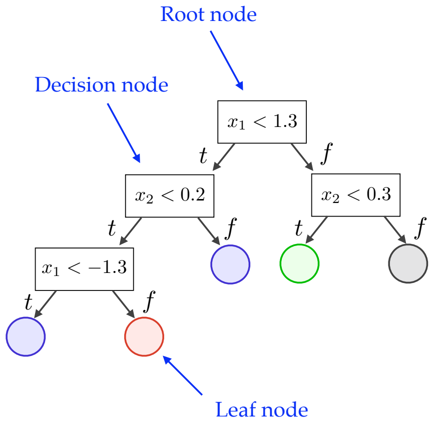
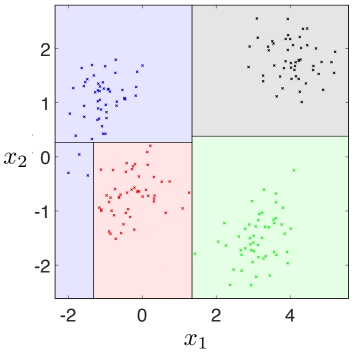
Slide credits and other course material can be found at:
http://www.stats.ox.ac.uk/~palamara/SML20.html

March 10, 2020

Recap: Decision Trees





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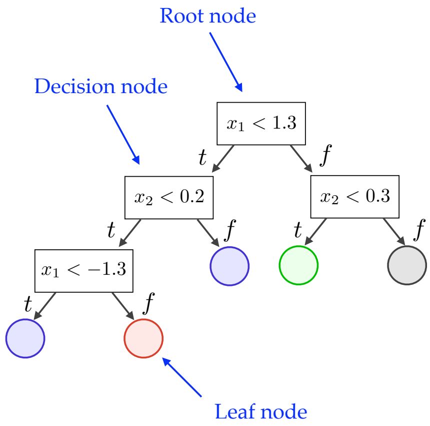

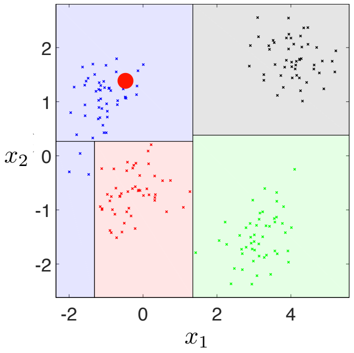

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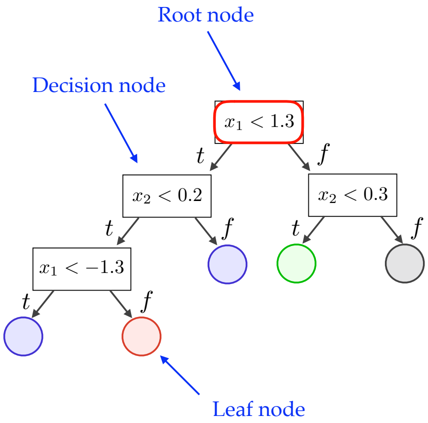

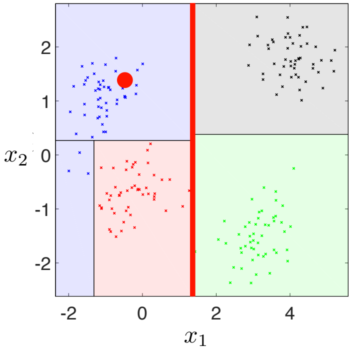

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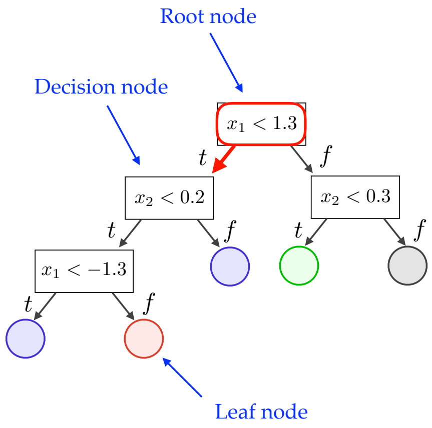

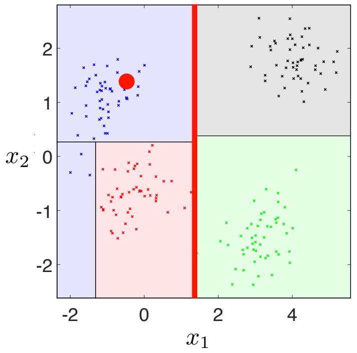

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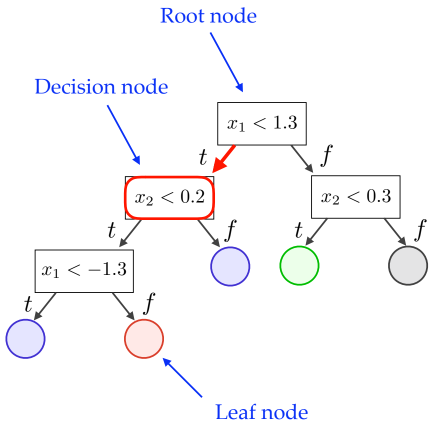

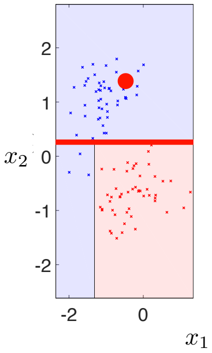

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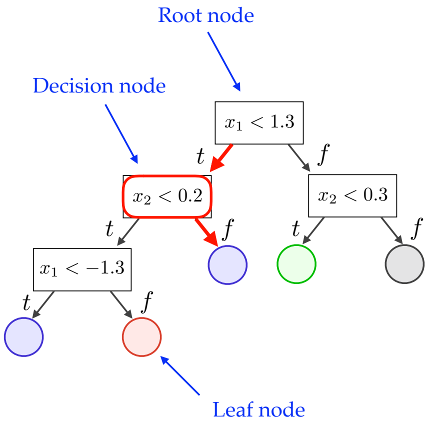

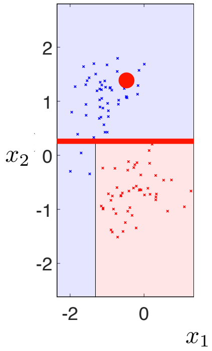

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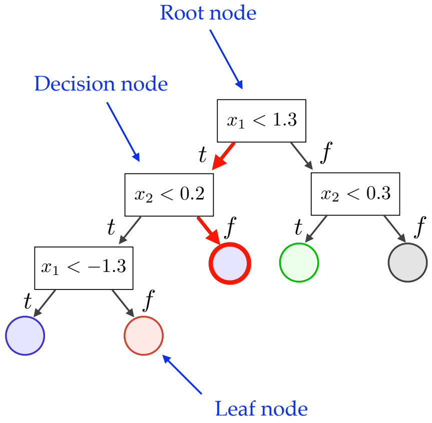
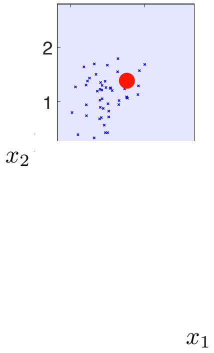
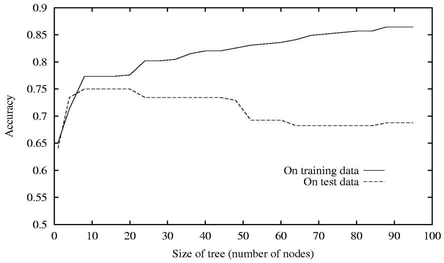
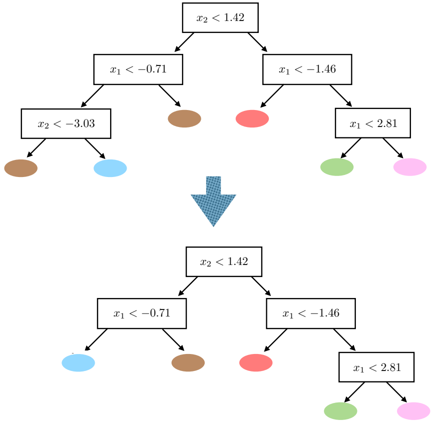




Recap: Regularization for Decision Trees

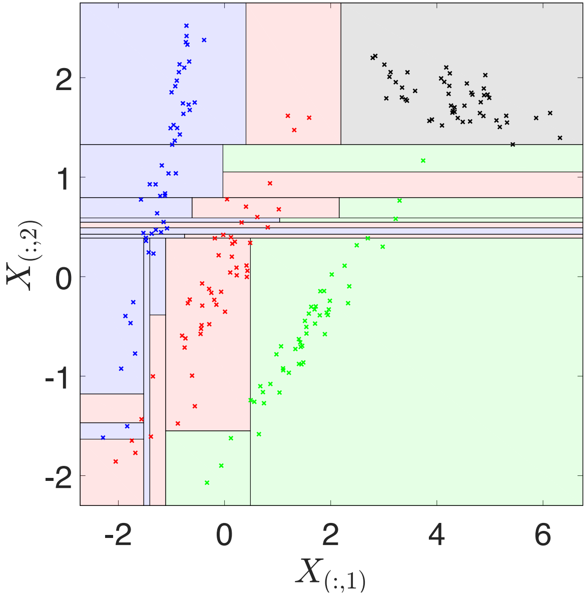
Trees can overfit if they are too large so we usually look to regularize or prune them



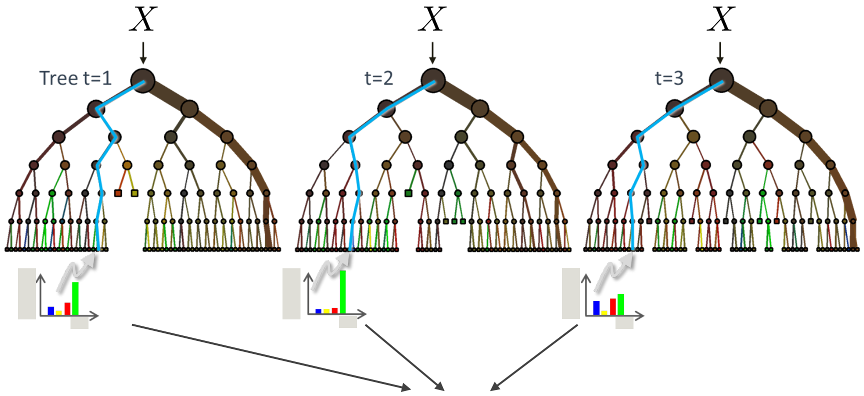


Ensembles: Bootstrapping, Bagging, and Random Forests

Individual Trees are Not Good Predictive Models

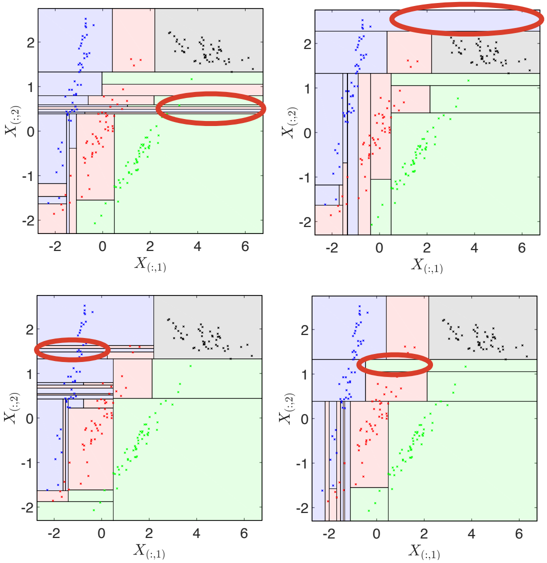


Learn Multiple Trees and Average Their Predictions Instead



$$p(Y|X) = \frac{1}{L}\sum_{t}^{L} p_t(Y|X)$$

Different Trees will Make Different Errors: Averaging Can Cancel Errors Out



Decision Ensembles are More Powerful Models

Decision **ensembles** (also known as **forests**) are fundamentally more powerful models than individual trees

- They can have more complex decision boundaries
- They reduce the variation on predictions: we can average away the errors as not all trees will make the same “mistakes”
- They are less prone to overfitting
- No need to prune

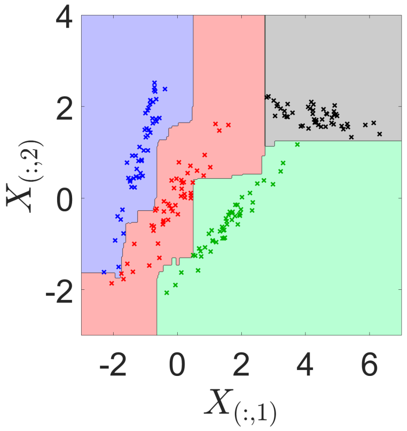
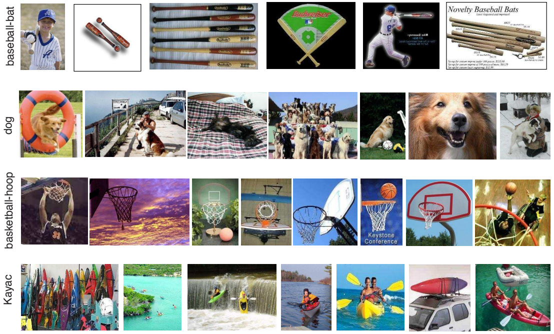


Figure: Decision surface for a random forest

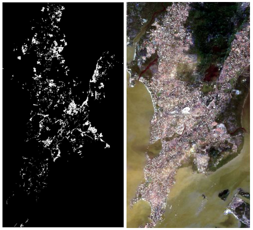
Forests have a huge number of applications

Image Classification



Motion Detection

Processing Satellite Images



[Image Credits: Bosch et al and Gram-Hansen et al]

Microsoft Kinect Pose Recognition

https://youtu.be/lntbRsi8lU8?t=41
https://www.microsoft.com/en-us/research/wp-content/uploads/2016/02/BodyPartRecognition.pdf

Forests are extremely easy to use

$$\begin{array}{c}\text{Number of trees (bigger the better)}\\ \downarrow\end{array}$$

```
RF = TreeBagger(200,XTrain,YTrain); % Training
preds = predict(RF,XTest); % Predict
```

- Applicable to wide range of problems and data types
- Extremely fast

Average Rank

Average Error (%)

Random forests and their extensions give **spectacular out-of-the box performance**: 7 out of the top 20 classifiers from a survey of 180 classifiers on 82 datasets are based on them

Classifier	R	E
CCF	**28.87**	**14.08**
svmPoly (SVM)	31.53	15.73
svmRadialCost (SVM)	31.84	15.33
svm_C (SVM)	32	15.67
elm_kernel (NNET)	32.19	15.20
parRF (RF)	33.03	15.54
svmRadial (SVM)	33.77	15.68
rf_caret (RF)	34.48	15.56
rforest_R (RF)	40.70	15.82
TreeBagger (RF)	40.91	15.75
Bag_LibSVM (Bag)	42.28	16.65
C50_t (BST)	42.61	16.85
nnet_t (NNET)	42.87	18.74
avNNet_t (NNET)	43.26	18.77
RotationForest	44.62	16.64
pcaNNet_t (NNET)	45.86	19.28
mlp_t (NNET)	46.06	17.38
LibSVM (SVM)	46.50	16.65
MB_LibSVM (BST)	46.90	16.82
RRF_t (RF)	49.56	16.71

[Rainforth, Tom, and Frank Wood. "Canonical correlation forests." *arXiv preprint arXiv:1507.05444* (2015).]

[Fernández-Delgado, Manuel, Eva Cernadas, Senén Barro, and Dinani Amorim. "Do we need hundreds of classifiers to solve real world classification problems?." *The Journal of Machine Learning Research* 15, no. 1 (2014): 3133-3181.]

Ensembling

- **Ensembling** is much more general than just the concept of decision tree ensembles
- We can take almost any machine learning model and convert it into an ensemble (e.g. we might also construct an ensemble of neural networks)
- General idea is always the same: train multiple instances of the model and then combine their predictions to a single prediction (usually by averaging)
- To ensure that we do not just end up with the same predictions as a single model, we need to introduce some form of randomness into the training process.
- To construct a good ensemble we need to ensure we get a good balance between the **diversity** of the constituent models (i.e. how correlated the errors they make are) and their **individual predictive power**
- Ensembling almost always improves the performance compared to a single model at the expense of increased cost
    - Machine learning “competitions” (e.g. Kaggle) are usually won by some sort of ensemble method, often an ensemble of neural network

Key Questions

- How should be introduce randomness into the training process?
  - Though this can vary depending on the base model, our focus will be on a universally applicable method called bagging and some additional methods that are specific to decision trees
- How can we control the diversity vs predictive power trade-off?
  - This will effectively boil down to controlling how much randomness we instill.

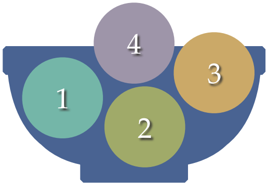
Bootstrapping

Model Variability

- To have an effective ensemble, our individual models need to make different errors in their predictions: we need diversity
- Some algorithms have **instability** in their training such that small changes in data can lead to large differences in the learned model
- Decision trees and neural networks are unstable algorithms, k-nearest neighbors are stable
- **Bootstrapping** allows us to exploit instabilities to produce a diverse set of models by training each on a slightly different dataset

Bootstrap Sampling

- Samples a new dataset from the old dataset by **resampling with replacement**
- Each new sample is drawn independently from the full old dataset



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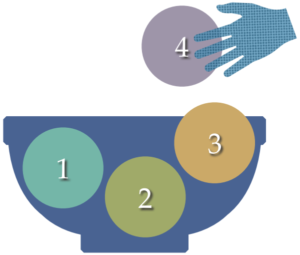

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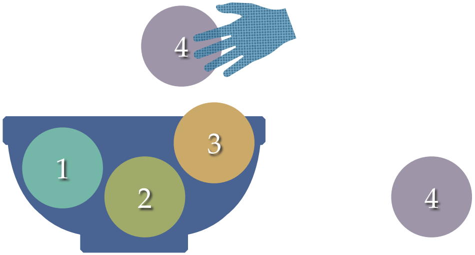

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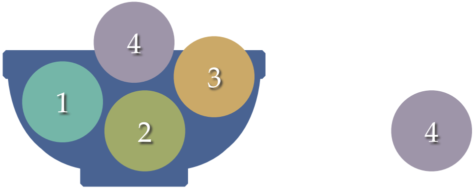

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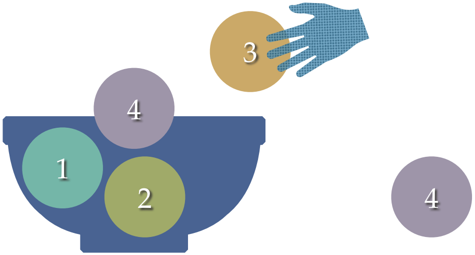

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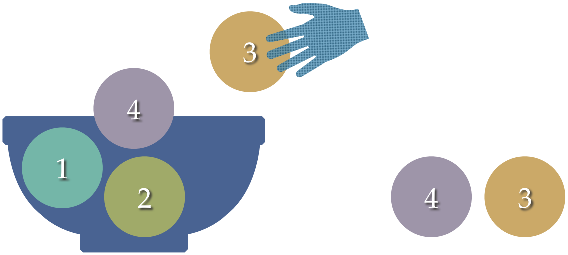

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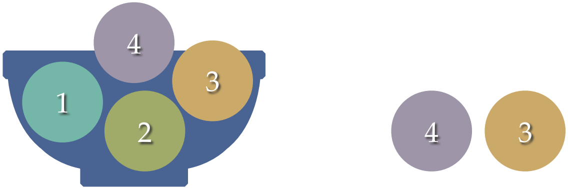

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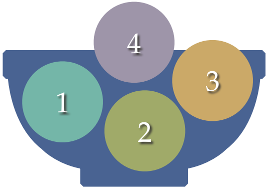
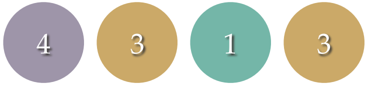
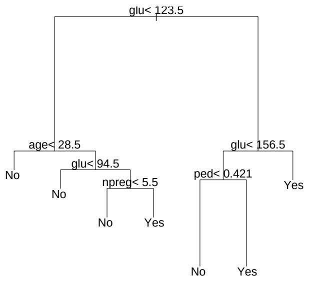


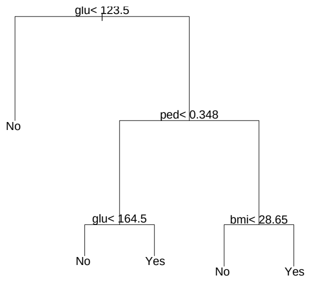


Bootstrap for Decision Trees

- The **bootstrap** is itself a way to assess the variance of estimators.
- Fit multiple trees, each on a **bootstrapped sample**.

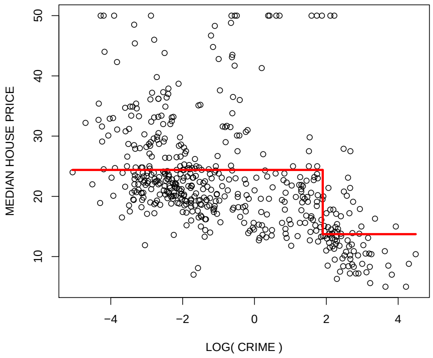
```
> n <- nrow(Pima.tr)
> bss <- sample(1:n, n , replace=TRUE)
> sort(bss)
[1]  2 4 4 5 6 7 9 10 11 12 12 12 12 13 13 15 15 20 ...

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

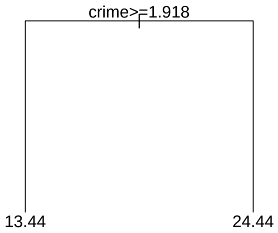




Example: Bootstrap for Regression Trees

- 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 (note this for the purposes of the example on not good practice in general)



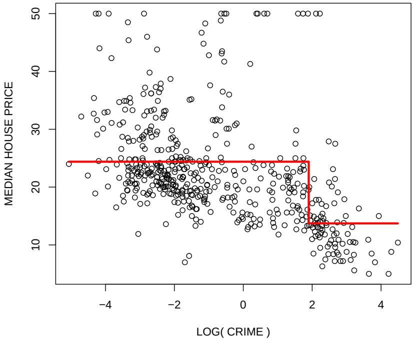


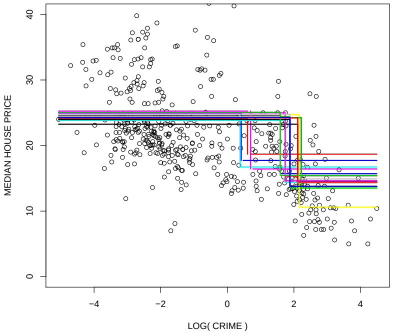
Example: Bootstrap for Regression Trees

- We are aiming to fit a predictor $\hat{f}(x)$ and have 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

$$\hat{f}^b(x), \qquad b = 1, \ldots, B$$

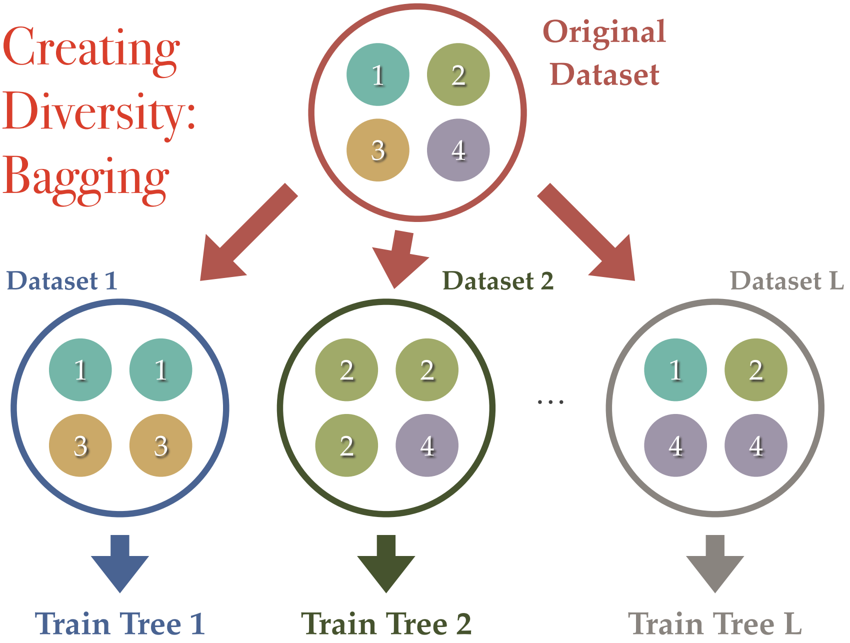
- Each tree $\hat{f}^b$ is fitted on the resampled data $(x_{j_i}, y_{j_i})_{i=1}^n$ where each j_i is chosen randomly from $\{1, \ldots, n\}$ with replacement.



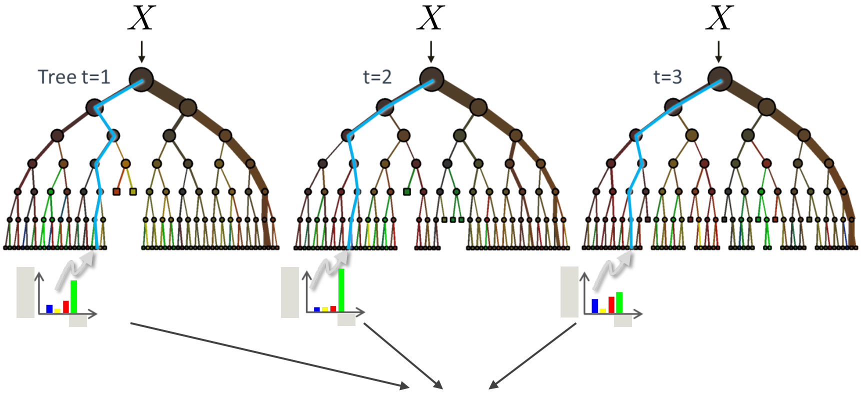


Bagging

Creating Diversity: Bagging



Average Predictions over Trees



$$p(Y|X) = \frac{1}{L}\sum_{t}^{L} p_t(Y|X)$$

Bagging

- **Bagging** (**B**ootstrap **Agg**regation): average across all B predictive models (e.g. trees) fitted on different bootstrap samples.

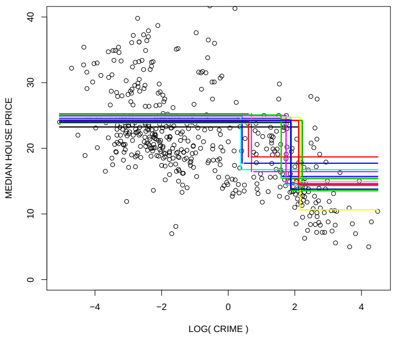
1. For $b = 1, \ldots, B$:
    1. Draw indices $(j_1, \ldots, j_n)$ from the set $\{1, \ldots, n\}$ with replacement.
    2. Fit the model, and form predictor $\hat{f}^b(x)$ based on bootstrap sample

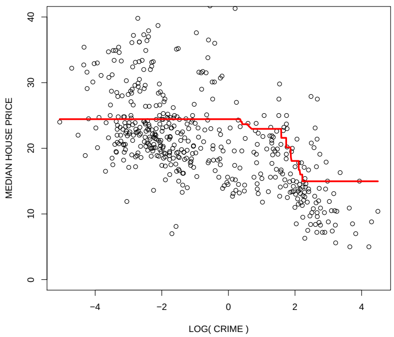
$$(x_{j_1}, y_{j_1}), \ldots, (x_{j_n}, y_{j_n})$$

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.
- In general, bagging reduces the variance of predictions

Variance Reduction Through Aggregation

- Consider an ideal world where we can draw a complete new dataset at will without having to perform bootstrapping, such that we can construct estimators $\hat{f}_m$ each based on different independent datasets of size n from the true joint distribution of X, Y.
- The aggregated estimator would then be

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

  where expectation is with respect to independent datasets of size n.
- Using the standard bias-variance decomposition and the law of large numbers, the squared-loss to the optimal classifier f_* for input x is

$$\begin{aligned}\mathbb{E}_{\mathcal{D}}[(f_*(x) - \hat{f}_{ag}(x))^2] &= (f_*(x) - \bar{f}(x))^2 + \mathbb{E}_{\mathcal{D}}[(\bar{f}(x) - \hat{f}_{ag}(x))^2] \\ &= (f_*(x) - \bar{f}(x))^2 + \frac{1}{B}\mathbb{E}_{\mathcal{D}}[(\bar{f}(x) - \hat{f}(x))^2] \\ &\to (f_*(x) - \bar{f}(x))^2 \quad \text{as } B \to \infty.\end{aligned}$$

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

Variance Reduction Through Bagging

- For bagging, our setup is similar, but our estimators are now based on the bagging estimators $\hat{f}^b$ trained on resampled versions of the dataset.
- We thus have

$$\hat{f}_{bag}(x) = \frac{1}{B}\sum_{m=1}^{B} \hat{f}^b(x) \to \tilde{f}(x,\mathcal{D}) \triangleq \mathbb{E}_{j_1^1,\dots,j_n^1}[\hat{f}^1(x)|\mathcal{D}] \quad \text{as } B \to \infty$$

where the expectation is now over the resampling indices.

- We thus have (not examinable):

$$\begin{aligned}
\mathbb{E}[(f_*(x) - \hat{f}_{bag}(x))^2] = \mathbb{E}_{\mathcal{D}}\left[\mathbb{E}\left[(f_*(x) - \hat{f}_{bag}(x))^2 \middle| \mathcal{D}\right]\right] \\
&= \mathbb{E}_{\mathcal{D}}\left[\mathbb{E}\left[(f_*(x) - \tilde{f}(x,\mathcal{D}))^2 \middle| \mathcal{D}\right]\right] + \mathbb{E}_{\mathcal{D}}\left[\mathbb{E}\left[(\tilde{f}(x,\mathcal{D}) - \hat{f}_{bag}(x))^2 \middle| \mathcal{D}\right]\right] \\
&= \mathbb{E}_{\mathcal{D}}\left[(f_*(x) - \tilde{f}(x,\mathcal{D}))^2\right] + \frac{1}{B}\mathbb{E}\left[(\tilde{f}(x,\mathcal{D}) - \hat{f}^1(x))^2\right] \\
&\to \mathbb{E}_{\mathcal{D}}\left[(f_*(x) - \tilde{f}(x,\mathcal{D}))^2\right] \quad \text{as } B \to \infty.
\end{aligned}$$

Variance Reduction Through Bagging

- In general, the variance of $\tilde{f}(x, \mathcal{D})$ will be less than that of $\hat{f}(x)$, i.e. the base model trained on the full dataset
  - It is still non-zero as $\tilde{f}(x, \mathcal{D})$ still varies with the dataset.
- Similarly the variance of the bagging estimator $\hat{f}_{bag}(x)$ is generally less than that of $\hat{f}(X)$:

$$\mathbb{E}\left[\left(\hat{f}_{bag}(x) - \mathbb{E}\left[\hat{f}_{bag}(x)\right]\right)^2\right] \lesssim \mathbb{E}\left[\left(\hat{f}(x) - \mathbb{E}\left[\hat{f}(x)\right]\right)^2\right]$$

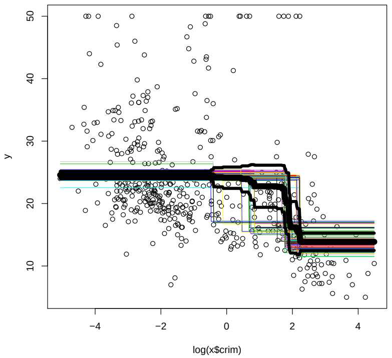
- This variance reduction comes at the cost of a small increase in bias, in general:

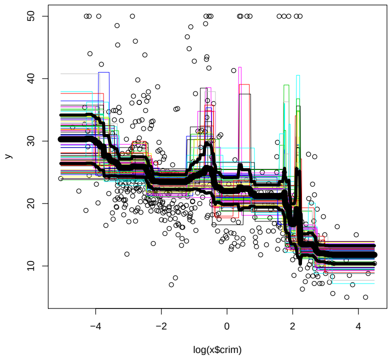
$$\left(\mathbb{E}\left[\hat{f}(x)\right] - f_*(x)\right)^2 \leq \left(\mathbb{E}\left[\hat{f}_{bag}(x)\right] - f_*(x)\right)^2$$

- Bagging is most useful for **flexible estimators with high variance** and **low bias**.

Variance Reduction in Bagging

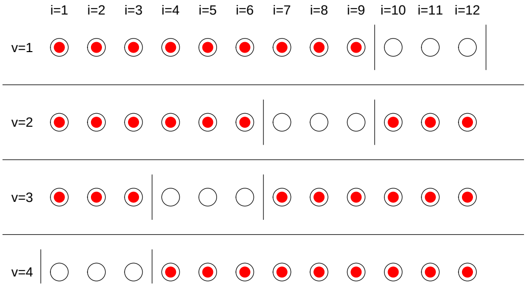
- Deeper trees have higher complexity and variance, but lower bias.
- Compare bagging trees of depth 1 and 3.





Out-of-bag Test Error Estimation

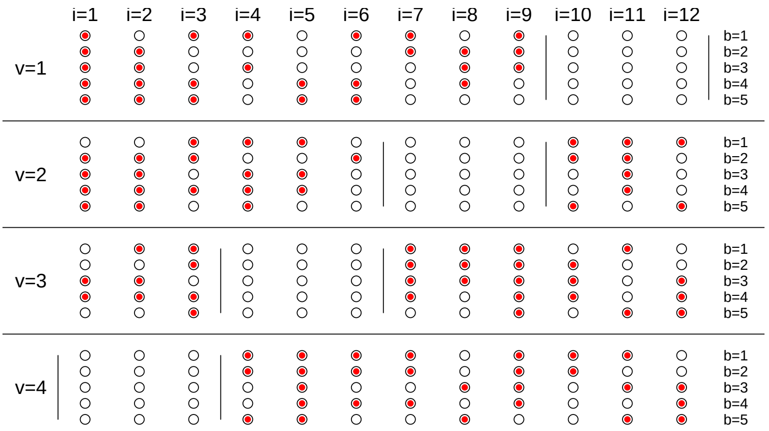
- How well does bagging to? Can we estimate generalization performance, and tune hyperparameters?
- Sledgehammer approach: cross-validation.



- For each $v = 1, \ldots, V$,
  - 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

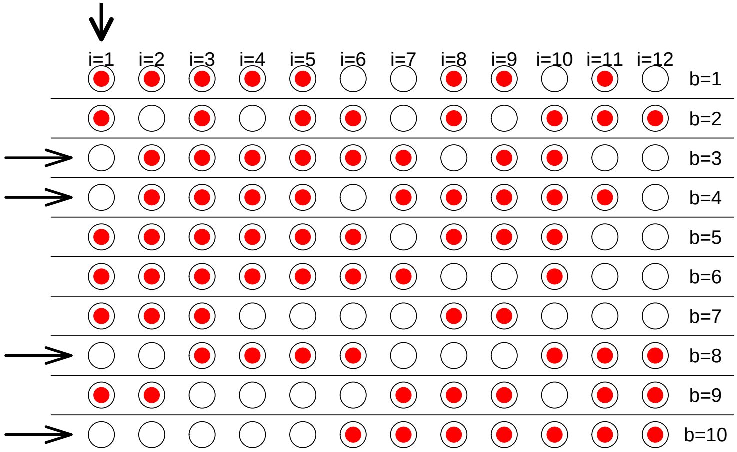
- But to fit $\hat{f}_{Bag}$ on the training set for each $v = 1, \dots, V$, we have to train on B bootstrap samples!



- More elegant approach: **Out-of-bag** test error estimation.

Out-of-bag Test Error Estimation

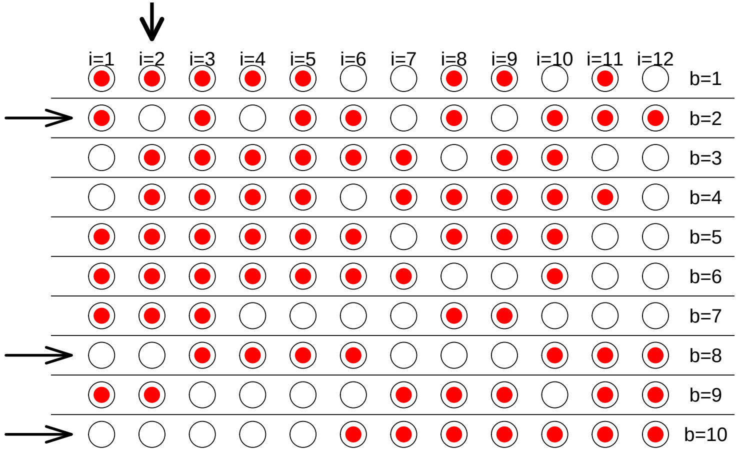
- Idea: test on the “unused” data points in each bootstrap iteration to estimate the test error.



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

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 $i = 1, \ldots, n$, the out-of-bag sample is:

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

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

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

- 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 $i = 1, \ldots, n$.
- The probability π^{oob} of an observation NOT being included in a bootstrap sample $(j_1, \ldots, j_n)$ (and hence being 'out-of-bag') is:

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

- Hence $\mathbb{E}[|\tilde{B}_i|] \approx 0.367B$
- In practice, number of bootstrap samples B is typically between 100 and 1000, meaning that the number $|\tilde{B}_i|$ of out-of-bag samples will be approximately in the range $35 - 400$.
- The obtained test error estimate is asymptotically unbiased for large number B of bootstrap samples and large sample size n.
- For finite B it will generally overestimate the test error as it is effectively using a smaller ensemble

Example: Boston Housing Dataset

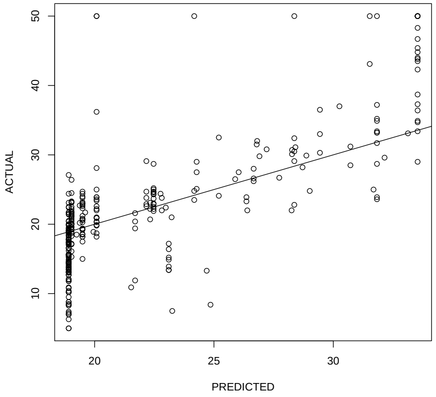
- Apply out of bag test error estimation to select optimal tree depth and assess performance of bagged trees for Boston Housing data.
- Use the entire dataset with $p = 13$ predictor variables.

```
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 pf 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,minsplit=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
```

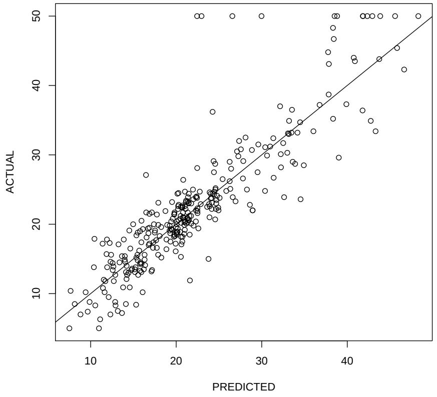
Example: Boston Housing Dataset

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

For depth $d = 1$.



For depth $d = 10$.



Example: Boston Housing Dataset

- Test error / 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 $d = 30$.

Bagging: Summary

- Bagging reduces variance and helps prevent overfitting
  - In general, we do not need to prune when making forests and can often get away without including any early stopping criteria
- Almost always improves performance in practice (for non–trivial data) compared to using a single tree
  - Because they can have more complicated decision boundaries, bagged trees are generally fundamentally more powerful models
- However, bagged trees lose much of the interpretability of single trees
- Bagging is a general strategy: decision trees are the most common base model, but can also be applied to other things like neural networks.

Other Ensembling Approaches

- For some base models, bagging is not best way of creating an ensemble
    - Some models already have natural instabilities that can be exploited without needing to take subsets of the data, e.g. the instability in neural network training with respect to the initialization of the weights and biases
    - In some scenarios, the gains from variance reduction are outweighed by the losses from increased bias due to using subsets of the data
- In other scenarios, bagging does not give enough diversity and we can get further gains by introducing additional randomization into the training process in addition to (or instead of) bagging
- Another common way of introducing diversity is to randomize the way features are accessed by the classifier, such as by manipulating the form of the features (e.g. through using random rotations) or restricting access to certain features during the model training (e.g. using random subspacing)

Random Forests

Random Forests

- In general, bagging trees creates insufficient diversity: it is usually beneficial to further randomize the training process
- **Random Forests** (RFs) are an extension of bagged trees that introduce an additional randomization: random subspacing (we'll cover this next)
    - Implemented in `randomForest` library in R
- This tends to gives a better trade off between diversity and predictive power of individual trees
- RFs and their extensions remain some of the best performing models in machine learning, particularly in the context of "out-of-the-box" use because they typically do not require careful setting of any hyperparameters

Breiman (2001)

Random forests and their extensions give **spectacular out-of-the box performance**: 7 out of the top 20 classifiers from a survey of 180 classifiers on 82 datasets are based on them

Average Rank

Average Error (%)

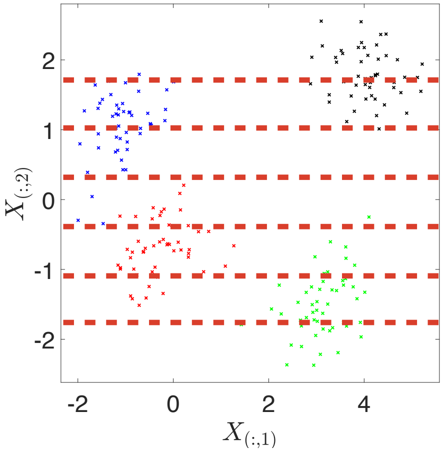
Classifier	R	E
CCF	**28.87**	**14.08**
svmPoly (SVM)	31.53	15.73
svmRadialCost (SVM)	31.84	15.33
svm_C (SVM)	32	15.67
elm_kernel (NNET)	32.19	15.20
parRF (RF)	33.03	15.54
svmRadial (SVM)	33.77	15.68
rf_caret (RF)	34.48	15.56
rforest_R (RF)	40.70	15.82
TreeBagger (RF)	40.91	15.75
Bag_LibSVM (Bag)	42.28	16.65
C50_t (BST)	42.61	16.85
nnet_t (NNET)	42.87	18.74
avNNet_t (NNET)	43.26	18.77
RotationForest	44.62	16.64
pcaNNet_t (NNET)	45.86	19.28
mlp_t (NNET)	46.06	17.38
LibSVM (SVM)	46.50	16.65
MB_LibSVM (BST)	46.90	16.82
RRF_t (RF)	49.56	16.71

[Rainforth, Tom, and Frank Wood. "Canonical correlation forests." *arXiv preprint arXiv:1507.05444* (2015).]

[Fernández-Delgado, Manuel, Eva Cernadas, Senén Barro, and Dinani Amorim. "Do we need hundreds of classifiers to solve real world classification problems?." *The Journal of Machine Learning Research* 15, no. 1 (2014): 3133-3181.]

Random Subspacing

- At **each** node randomly select a random subset of features to use for the split search
- The number of features selected, m_{try} is a hyperparameter
- Typically only select a small number of features (e.g. $m_{try} = \log_2 p$ or $m_{try} = p^{0.5}$)
- This means different trees will split along different dimensions at each node
- Difference at earlier nodes, lead to different data partitions at later nodes and thus further diversity



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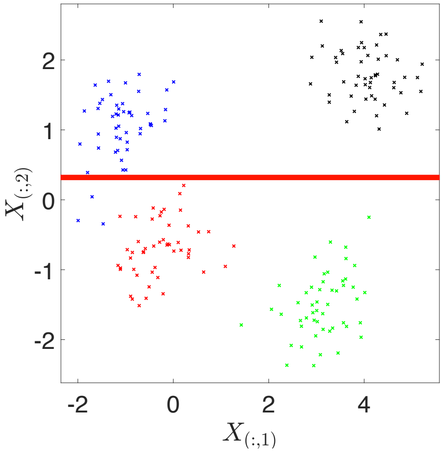

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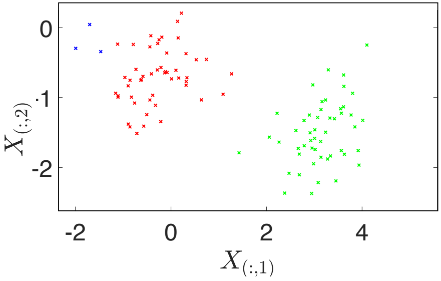

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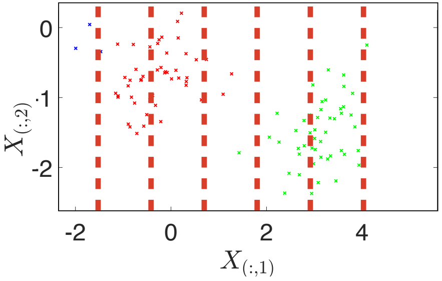

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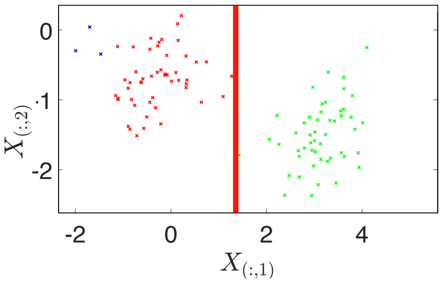
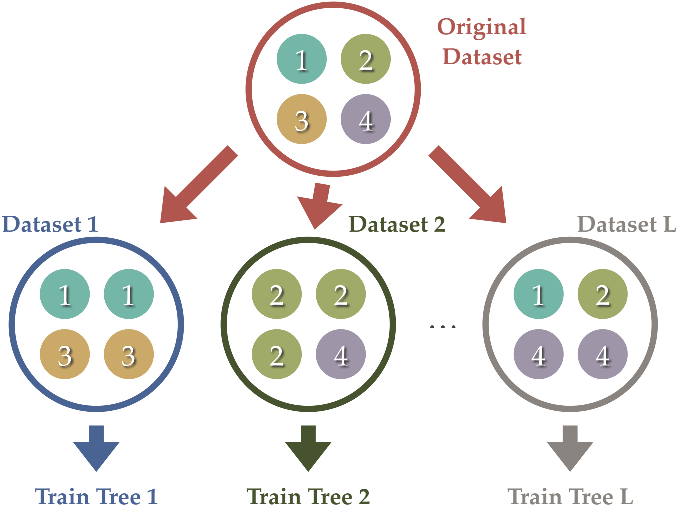
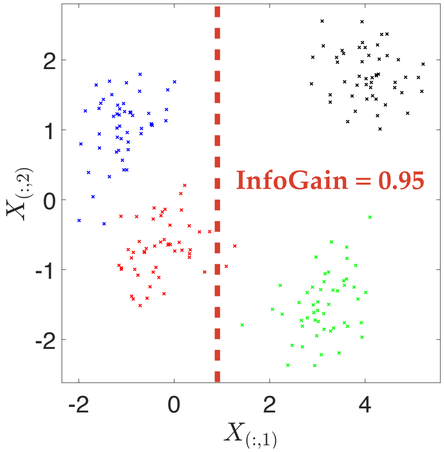


Random Forests = Bagging + Random Subspacing

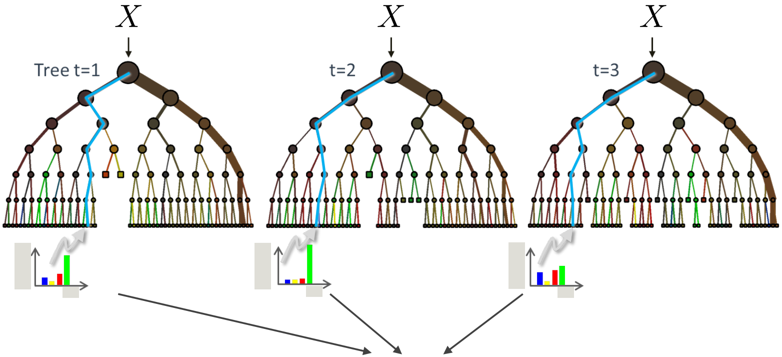
1. Use bagging: generate a separate bootstrap dataset to train each individual tree on



2. Train each tree by recursively greedily choosing the best split (as per the split criterion) from set of randomly selected features until a stopping criterion is reached



3. Make predictions by aggregating the predictions made by individual trees (note bootstrapping is not used for evaluation)



$$p(Y|X) = \frac{1}{L}\sum_{t}^{L} p_t(Y|X)$$

[Adapted from: Criminisi, Antonio, Jamie Shotton, and Ender Konukoglu. "Decision forests: A unified framework for classification, regression, density estimation, manifold learning and semi-supervised learning." *Foundations and Trends® in Computer Graphics and Vision* 7.2–3 (2012): 81-227.]

Looking at the Boston Housing data again

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

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

?randomForest
```

```
> 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

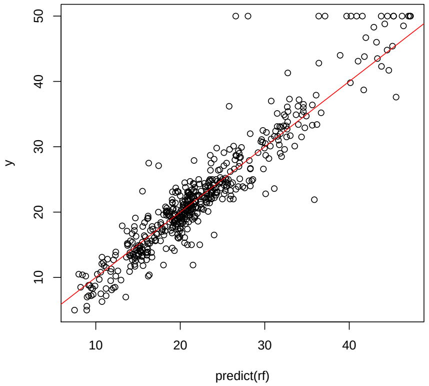
```
> plot( predict(rf), y)
> abline(c(0,1),col=2)
```

Same if treating the training data as new data

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

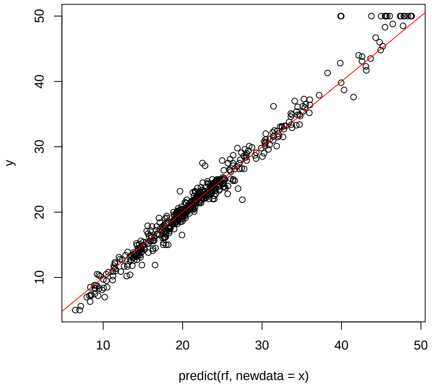
Out-of-bag error.

```
> 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 (i.e. search over two features at each node)

```
> (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
```

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
```

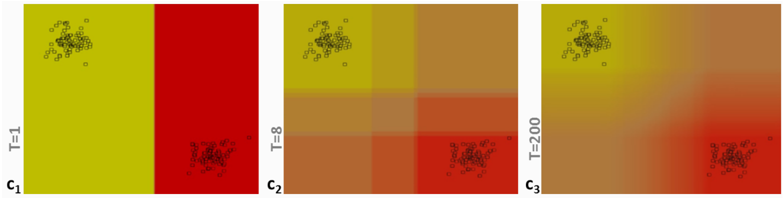
And `mtry` 8 and 10.

```
> (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

> > (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
```

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

Hyperparameters – Number of Trees

- More the merrier — limited by computational budget, having too many does not cause Bagging to overfit
- 500 trees is a typical choice
- More trees gives a smoother surface



[Image taken from: Criminisi, Antonio, Jamie Shotton, and Ender Konukoglu. "Decision forests: A unified framework for classification, regression, density estimation, manifold learning and semi-supervised learning." *Foundations and Trends® in Computer Graphics and Vision* 7.2–3 (2012): 81-227.]

Computational Cost

- Training in $O(n(log(n))^2 Bm_{\text{try}})$ for $n \times p$ data with B trees
- Prediction in $O(\log(n)B)$
- These are not a typos, their costs are actually independent of p!
  - We may wish to increase m_{try} (and potentially also B) as p increases we can indirectly increase cost with larger p
  - Typically though, we set m_{try} to be a sublinear function of p, with $m_{\text{try}} = \lfloor \log_2 p \rfloor$ and $m_{\text{try}} = \lfloor \sqrt{p} \rfloor$ being common choices
- RFs are thus cheaper to train than bagged trees, substantially so for large p
- For large p, training a RF can even be cheaper than training a single decision tree, particularly if we need to use pruning for the latter

Variable “Importance”

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

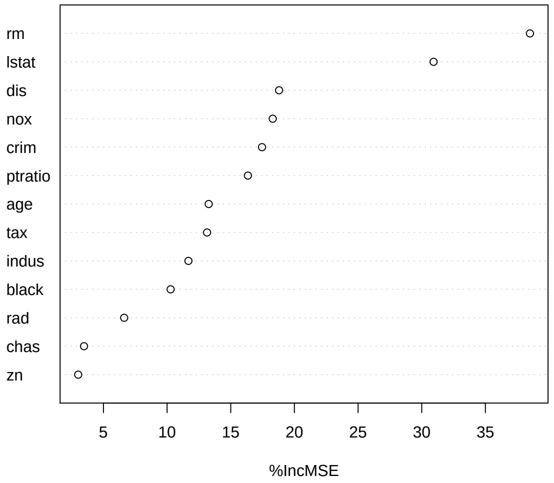
Idea: denote by $\hat{e}$ the out-of bag estimate of the loss when using the original data samples. For each variable $k \in \{1, \ldots, p\}$,

- permute randomly the k-th predictor variable to generate a new set of samples $(\tilde{X}_1, Y_1), \ldots, (\tilde{X}_n, Y_n)$, 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)
```



Random Forests Pros and Cons

+ Very easy to use and applicable to a wide range of problems
+ Fast at train and test time
+ State-of-the-art for many applications
+ Particularly good for small to medium datasets
+ Work very well "out-of-the-box", i.e. without tuning

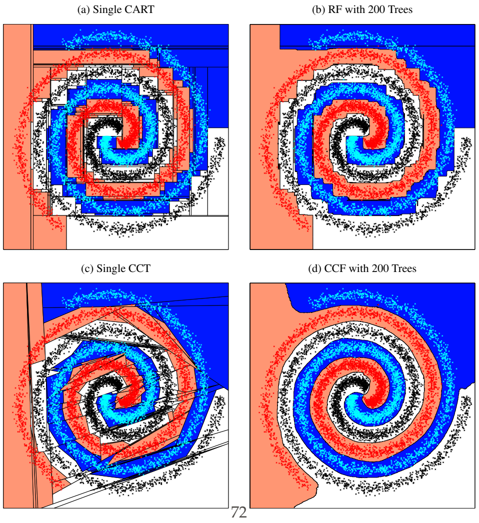
- Typically worse than deep neural nets for huge datasets
- Little flexibility to tune to specific problems
- Good performance can required data preprocessing using some sort of feature extractor

Extensions

- Various further extensions to random forests exist
- Most look to increase diversity even more by adding further randomness to the training process
  - **Extremely Randomized Trees** forms an ensemble where the tree structures are predominantly or even complete random
  - Other methods split along **randomized hyperplanes** rather than using individual features to create further diversity

Breiman (2001), Geurts et al (2006), Rainforth and Wood (2014)

Hyperplane Splits



Rainforth and Wood (2014)

Useful Packages / Further Reading

- Scikit learn (python) - http://scikit-learn.org/stable/ - open source package with lots of machine learning algorithms built in.
- TreeBagger (Matlab) — https://uk.mathworks.com/help/stats/treebagger.html
- C++ — https://github.com/bjoern-andres/random-forest
- R — https://www.tutorialspoint.com/r/r_random_forest.htm
- Weka (stand alone) — http://www.cs.waikato.ac.nz/ml/weka/ - Gui with java back end, operates on csv files and allows lots of algorithms to be used at once
- Complete tutorial paper: Decision Forests for Classification, Regression, Density Estimation, Manifold Learning and Semi-Supervised Learning. Criminisi et al 2014. https://www.microsoft.com/en-us/research/wp-content/uploads/2016/02/decisionForests_MSR_TR_2011_114.pdf
- A good high level introduction with code examples in python: https://www.analyticsvidhya.com/blog/2016/04/complete-tutorial-tree-based-modeling-scratch-in-python/