

Tree-based Models for Regression

- Regression trees
- Regression forests
 - `randomForest` based on bagging
 - `gbm` based on boosting

Tree-based Models for Regression

- Input vector $X = (X_1, X_2, \dots, X_p) \in \mathcal{X}$
- Response variable $Y \in \mathbb{R}$
- Trees are constructed by recursively splitting regions of \mathcal{X} into two sub-regions, beginning with the whole space \mathcal{X} .

For simplicity, focus on recursive binary partitions.

- R page: check the fitted regression tree on BostonHousingData based on two features lon and lat.

- Notation: node (t), child node (t_L, t_R), split (var j , value s), leaf/terminal node.
- Every leaf node (i.e. a rectangle region R_m in \mathcal{X}) is assigned with a constant for regression tree

$$\hat{f}(X) = \sum_m c_m I\{X \in R_m\}.$$

Advantages of Trees

- Easy to interpret
- Variable selection and interactions between variables are handled automatically
- Invariant under any monotone transformation of predictors

How to Build a Tree?

Three elements:

1. Where to split?
2. When to stop?
3. How to predict at each leaf node?

Prediction at Leaf Nodes

Each leaf node (corresponds to region R_m) contains some samples.

Assign the prediction for a leaf node to be the average (of the response variable Y).

$$\hat{f}(X) = \sum_m c_m I\{X \in R_m\}.$$

$$\min_{c_m} \sum_{i=1, x_i \in R_m}^n (y_i - c_m)^2,$$

$$\implies c_m = \text{average of } y_i\text{'s whose } x_i \in R_m$$

Where to Split?

- A split is denoted by (j, s) : split the data into two parts based on whether “**var** j < **value** s ”.
- For each split, define a **split criterion** $\Phi(j, s)$
 - deduction of RSS for regression
- Trees are built in a top-down greedy fashion. Start with the root: try all possible variables $j = 1 : p$ and all possible split values^a, and pick the best split, i.e., the split having the best Φ value. Now, data are divided into the left node and right node. Repeat this procedure in each node.

^aFor each variable j , sort the n values (from n samples), and choose s to be a middle point of two adjacent values. So at most $(n - 1)$ possible values for s .

Goodness of Split $\Phi(j, s)$

For **Regression tree**, we look at the deduction of RSS if we split samples at node t into t_R and t_L :

$$\Phi(j, s) = \text{RSS}(t) - \left[\text{RSS}(t_R) + \text{RSS}(t_L) \right],$$

where

$$\begin{aligned} \text{RSS}(t) &= \sum_{x_i \in t} (y_i - c_t)^2, \\ c_t &= \text{AVE}\{y_i : x_i \in t\}. \end{aligned}$$

Note that $\Phi(j, s)$ is always positive if we split the data into two groups (even randomly), unless the mean of the left node and the one of right node are the same.

Issues: Split Categorical Predictors

- For a categorical predictor with m levels, there are $2^{m-1} - 1$ possible partitions of the m labels into two groups.
- However, for regression with square error, the computation simplifies: order the m levels by their mean values of Y , and then split the categorical variable as if it were an ordered predictor — there are only $(m - 1)$ potential splits.

Issues: Missing Predictor Values

- Discard any observation with missing values \longrightarrow serious depletion of the training set.
- Splitting criteria are evaluated on non-missing observations.
- Once a split (j, s) is determined, what to do with observations missing X_j ?

- Find **surrogate variables** that can predict the binary outcome “ $X_j < s$ ” and “ $X_j \geq s$ ” using a one-split tree.
- Rank those surrogate variables along with the **blind rule** “go with majority”.
- Any observation that is missing X_j is then classified with the first surrogate variable, or if missing that, the second surrogate variable (or the blind rule) is used, and etc.

When to Stop?

- A simple one : stop splitting at a node if the gain from any split is less than some pre-specified threshold.
- BUT, this is short-sighted.
- Another strategy: grow a large tree and then prune it (i.e., cut some branches).

Preliminaries for Pruning

First, grow a vary large tree T_{\max}

1. until all terminal nodes are nearly pure;
2. or when the number of data in each terminal node is less than certain threshold;
3. or when the tree reaches certain size.

As long as the tree is sufficiently large, the size of the initial tree is not critical.

Notation : *subtree* $T' \prec T$, *branch* T_t .

Minimum Complexity-cost Pruning

For any subtree $T \prec T_{\max}$, define the Complexity-cost

$$R_{\alpha}(T) = R(T) + \alpha|T|, \quad (1)$$

- $R(T)$: RSS for regression tree T
- $|T|$: tree size, i.e., the number of leaf nodes
- $\alpha > 0$: cost (penalty) of adding a split

Questions: *i)* How to minimize (1) for a given α ? *ii)* How to choose α ?

Pick the best subtree that minimizes the cost

$$T(\alpha) = \operatorname{argmin}_{T \preceq T_{\max}} R_{\alpha}(T) = \operatorname{argmin}_{T \preceq T_{\max}} \left[R(T) + \alpha |T| \right]$$

$T(\alpha)$ may not be unique.

Define the optimal subtree $T^*(\alpha)$ to be the smallest one among $T(\alpha)$'s

$$(1) R_{\alpha}(T^*(\alpha)) = \min_{T \preceq T_{\max}} R_{\alpha}(T).$$

$$(2) T^*(\alpha) \preceq \text{any } T(\alpha).$$

$T^*(\alpha)$ is unique.

$$R_\alpha(T) = R(T) + \alpha|T|$$

Some Facts

- For a pair of leaf nodes (t_L, t_R) , there exists α^* , such that
 1. for any $\alpha \geq \alpha^*$, we would like to collapse them to just node t ;
 2. for any $\alpha < \alpha^*$, keep the two leaf nodes.

That is, α^* is the maximal price we would like to pay to keep that split.

Next we extend this calculation to compute the maximal price we would like to pay to keep a branch T_t .

- For any non-leaf node t , do the following calculation to find out the maximal price we'd like to pay for keeping the whole branch T_t .

Focus only on samples at node t .

- Cost for keeping branch T_t : $R_\alpha(T_t) = R(T_t) + \alpha|T_t|$
- Cost for cutting branch T_t : $R_\alpha(\{t\}) = R(\{t\}) + \alpha$
- Calculate

$$\alpha^* = \frac{R(\{t\}) - R(T_t)}{|T_t| - 1}.$$

That is, if the given $\alpha > \alpha^*$, then it is too expensive to keep this branch and we would like to cut the whole branch and make t a leaf node.

Weakest-Link Pruning

The weakest-link pruning algorithm.

- Start with $T_0 = T_{\max}$ and $\alpha_0 = 0$.
- For any non-leaf node t , denote the maximal price we'd like to pay to keep T_t by $\alpha(t)$.
- $\alpha_1 = \min_t \alpha(t)$. The corresponding (non-terminal node) t_1 is called the **weakest link**. Cut the branch at t_1 .
- Next update the maximal price for each non-leaf node (we only need to recompute the maximal price for nodes that are parents/grandparents of t_1). Find α_2 and cut the branch at the 2nd weakest link. Keep doing this until we get to the root.

The steps above generate a **Solution Path**:

$$T_{\max} = T_0 \succ T^*(\alpha_1) \succ T^*(\alpha_2) \succ \cdots \succ \{\text{root node}\}$$

$$0 = \alpha_0 < \alpha_1 < \alpha_2 < \cdots$$

All possible values of α are grouped into $(m + 1)$ intervals:

$$I_0 = [0, \alpha_1)$$

$$I_1 = [\alpha_1, \alpha_2)$$

$$\vdots$$

$$I_m = [\alpha_m, \infty)$$

where all $\alpha \in I_i$ share the same optimal subtree $T^*(\alpha_i)$.

Cross-validation

How to Choose α ? K -fold Cross-validation (rpart):

1. Fit a big tree T_{\max} and compute I_0, I_1, \dots, I_m

$$\text{Set } \beta_0 = 0$$

$$\beta_1 = \sqrt{\alpha_1 \alpha_2}$$

$$\vdots$$

$$\beta_{m-1} = \sqrt{\alpha_{m-1} \alpha_m}$$

$$\beta_m = \infty$$

where each β_j is a ‘typical value’ for its interval I_j .

2. Divide data into K groups and repeat $k = 1, \dots, K$:
 - Fit a full model on the data set except the k -th group and determine the optimal subtrees:

$$T_0 \succ T^*(\beta_1) \succ \dots \succ T^*(\beta_m) \succ \{\text{root node}\}$$

- Compute the prediction error on the k -th group for each tree models.
3. Produce the CV plot over different α values and pick the optimal α_{min} or α_{1se} .

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Bagging (Bootstrap Aggregation)

- Training data: $\mathbf{Z} = \{(x_i, y_i)_{i=1}^n\}$
- Bootstrap samples^a: $\mathbf{Z}^{*b} = \{(x_i^{*b}, y_i^{*b})_{i=1}^n\}$, where $b = 1 : B$

$$\mathbf{Z}^{*1} : (x_1^{*1}, y_1^{*1}), (x_2^{*1}, y_2^{*1}), \dots, (x_n^{*1}, y_n^{*1})$$

$$\mathbf{Z}^{*2} : (x_1^{*2}, y_1^{*2}), (x_2^{*2}, y_2^{*2}), \dots, (x_n^{*2}, y_n^{*2})$$

$$\vdots$$

$$\mathbf{Z}^{*B} : (x_1^{*B}, y_1^{*B}), (x_2^{*B}, y_2^{*B}), \dots, (x_n^{*B}, y_n^{*B})$$

^asample with replacement from \mathbf{Z} .

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- Bootstrap samples^a: $\mathbf{Z}^{*b} = \{(x_i^{*b}, y_i^{*b})_{i=1}^n\}$, where $b = 1 : B$
- \hat{f}^{*b} : classification/regression function trained by \mathbf{Z}^{*b}
- The bagging estimate is defined to be

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

- **Advantage: reduce variance.** So works well for high-variance, low-bias procedures, such as trees.

^asample with replacement from \mathbf{Z} .

Random Forest

1. For $b = 1 : B$:
 - (a) Draw a bs sample \mathbf{Z}^{*b} from the training data.
 - (b) Grow a **BIG** tree T_b (with some restriction).
2. Output the forest $\{T_b\}_{b=1}^B$.

To make a prediction at a new point x

Regression: $\frac{1}{B} \sum T_b(x)$.

Restriction when growing a tree in the forest:

- At each split, randomly select m variables from the p variables, and then pick the best split among them.
- The recommended value for m is \sqrt{p} for classification and $p/3$ for regression.
- Purpose: reduce the correlation between trees in the forest.

Out-of-Bag (OOB) Samples

- OOB samples: sample points which are not included in \mathbf{Z}^{*b} , i.e., they are not used in building the tree T_b
- The OOB samples can be used to get a test error for T_b .
- The prediction and error rate returned by randomForest are calculated based on OOB. The error is usually close to a CV error.

Variable Importance

- Measure the importance of a variable by the improvement of RSS contributed by this variable.
- At each split, attribute the improvement of RSS to the corresponding splitting variable.
- For each variable, accumulate its improvement of RSS across the tree and then averaged over all the trees in the forest.

- Another measure is computed from **permuting** OOB samples: For each tree T_b in the forest, calculate the prediction error (MSE for regression) based on OOB samples. Then the same is done after permuting the j th predictor in the OOB samples. The difference between the two (**before and after** permutation) is then averaged over all trees, and further normalized by the corresponding standard deviation^a.

^aIf the standard deviation of the differences is equal to 0 for a variable, then the division is not applied.

Boosting Trees

- **Boost** the performance of a set of weak regression trees by cleverly combining them.
- **Forward stagewise additive modeling**: consider an additive model,

$$F(x) = f_1(x) + f_2(x) + \cdots + f_{T-1}(x) + f_T(x).$$

It is difficult to solve for all f_t 's. Instead we solve it using a forward stagewise greedy algorithm.

Forward Stagewise Optimization

1. $F(x) = 0$ and record the current residual $r_i^{(0)} = y_i$
2. For $t = 1$ to T
 - Fit a regression tree f_t to the current residual $r_i^{(t-1)}$
 - Add f_t to F : $F = F + f_t$
 - Update the current residual $r_i^{(t)} = r_i^{(t-1)} - f_t(x_i)$

Tuning parameters for GBM: learning rate η , number of trees T , complexity of f_t 's (depth of trees), and subsampling rate.

- Advantages of ensemble methods based on trees
 - Less-processing is needed, e.g., NA can be handled automatically, and no scaling/normalization is required
 - Can handle large number of predictors
- GBM vs randomForest
 - randomForest has less number of tuning parameters, while GBM has more, but with proper tuning, GBM can perform better than randomForest.
- Categorical Predictors
 - Each package treats categorical predictors differently: maximal 32 levels for randomForest and 1024 levels for GBM; XGBoost and some python packages only take numerical input.

Overview

Regression Tree

1. How to build a tree
2. How to use tree to form prediction
3. Pros and cons of tree models

Regression Forest

1. **randomForest** based on bagging
2. **gbm** based on boosting

Case Study: Ames Housing Data

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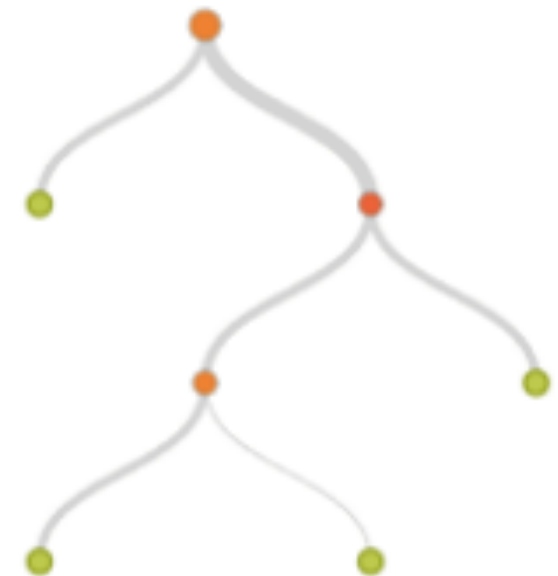
Case Study: Ames Housing Data

Tree Models

<http://www.r2d3.us/visual-intro-to-machine-learning-part-1/>

Build a Tree

- **Top-down greedy** fashion: **recursively** divide data into small subgroups, and then fit a simple model (**constant**) for each subgroup.
- **Internal node**: variable/split_point
- **Leaf node**: a constant prediction



Make Predictions

Tree Models

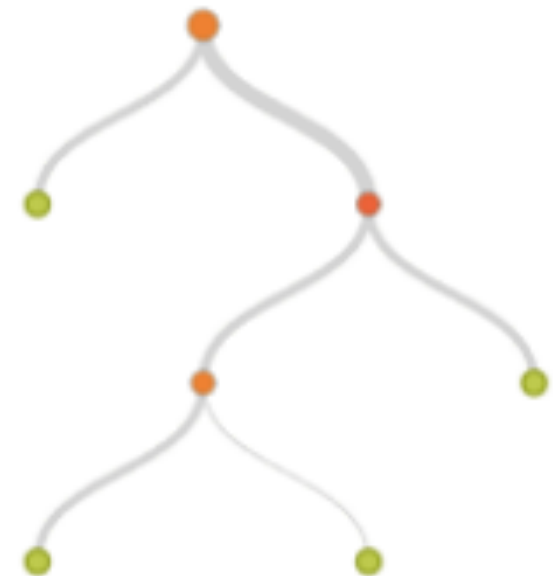
<http://www.r2d3.us/visual-intro-to-machine-learning-part-1/>

Pros

- Easy to interpret
- Automatic variable selection and interaction
- Invariant under any monotone transformations on predictors

Cons

- Unstable
- Weak performance



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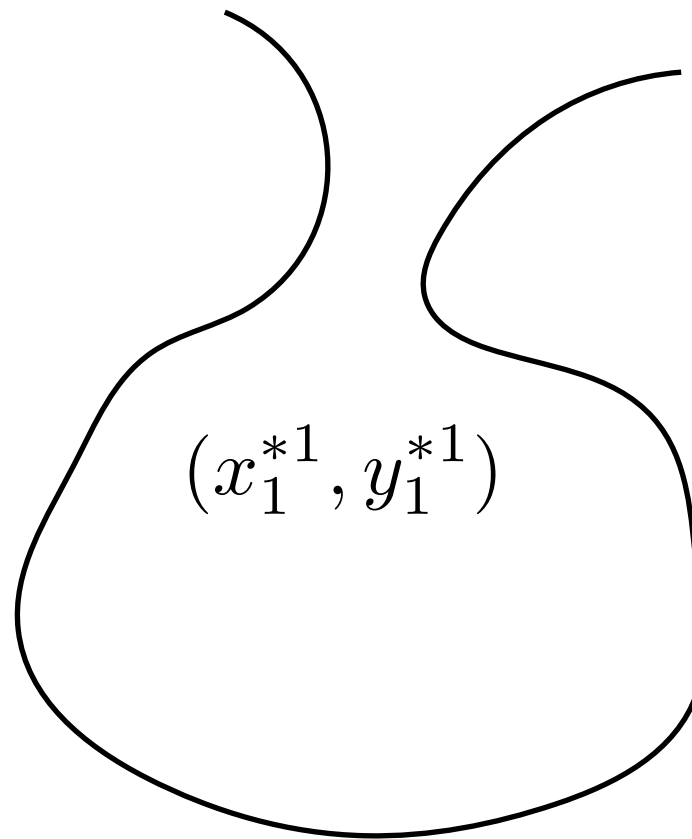
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Bagging (Bootstrap Aggregation)

Training Data

$$\mathbf{Z} = \{(x_1, y_1), (x_2, y_2), \dots, (x_n, y_n)\}$$

Bootstrap Sample 1



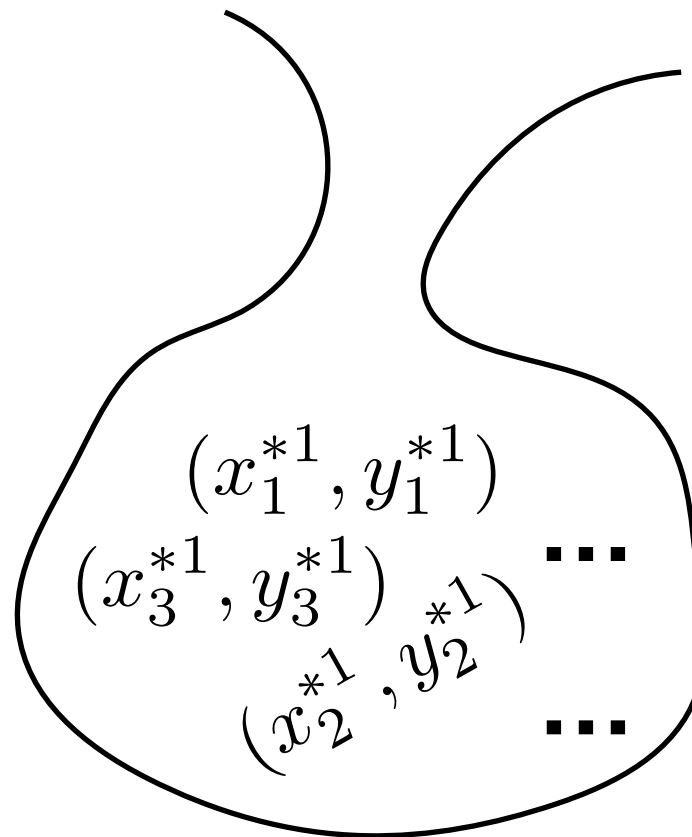
Sample with Replacement

Bagging (Bootstrap Aggregation)

Training Data

$$\mathbf{Z} = \{(x_1, y_1), (x_2, y_2), \dots, (x_n, y_n)\}$$

Bootstrap Sample 1



Sample with Replacement

Bagging (Bootstrap Aggregation)

Training Data

$$\mathbf{Z} = \{(x_1, y_1), (x_2, y_2), \dots, (x_n, y_n)\}$$

Bootstrap Sample 1

$$\mathbf{Z}^{*1} = \{(x_1^{*1}, y_1^{*1}), (x_2^{*1}, y_2^{*1}), \dots, (x_n^{*1}, y_n^{*1})\}$$

Bootstrap Sample 2

$$\mathbf{Z}^{*2} = \{(x_1^{*2}, y_1^{*2}), (x_2^{*2}, y_2^{*2}), \dots, (x_n^{*2}, y_n^{*2})\}$$

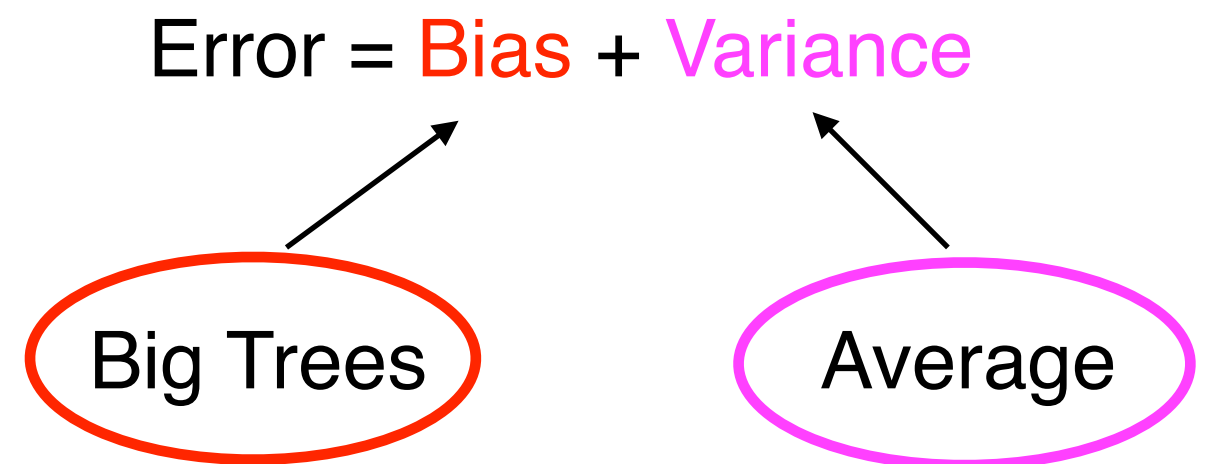
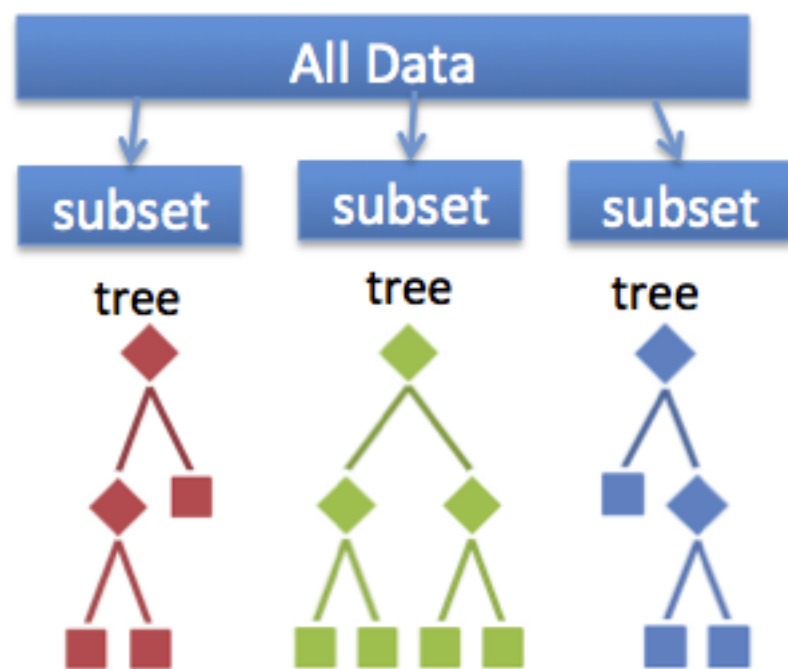
.....

Bootstrap Sample B

$$\mathbf{Z}^{*B} = \{(x_1^{*B}, y_1^{*B}), (x_2^{*B}, y_2^{*B}), \dots, (x_n^{*B}, y_n^{*B})\}$$

Bagging (Bootstrap Aggregation)

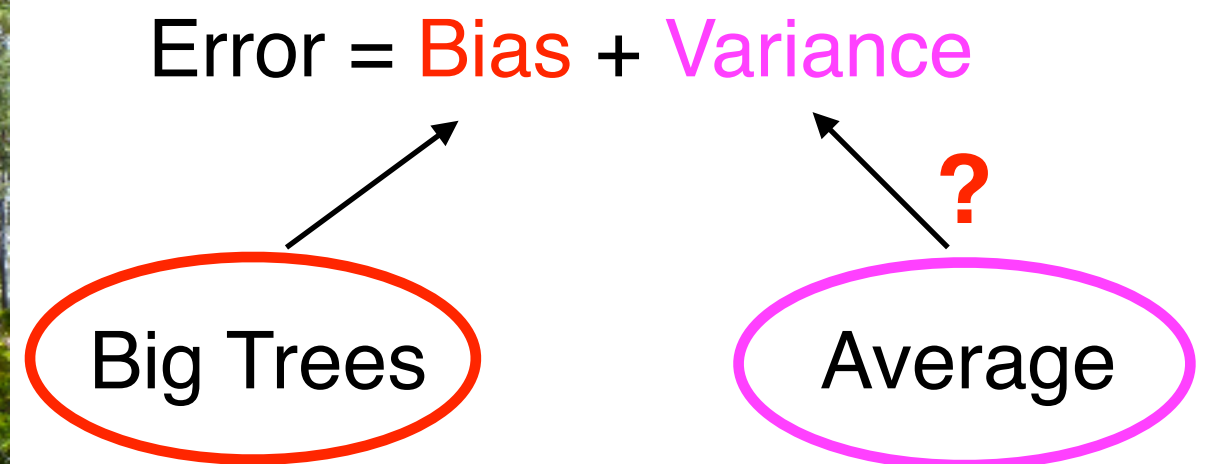
We can fit **B** trees, each based on one bootstrap sample, then when making predictions, we aggregate over the **B** trees.



$$\frac{1}{3} \left(f_1(x) + f_2(x) + f_3(x) \right)$$

Bagging (Bootstrap Aggregation)

We can fit **B** trees, each based on one bootstrap sample, then when making predictions, we aggregate over the **B** trees.



$$\frac{1}{B} \sum_{b=1}^B f_b(x)$$

Averaging won't reduce variance if outcomes are (positively) correlated.

Random Forest

a modification of Bagging; de-correlates trees by randomizing the choice for split-variables; minimal tuning; my favorite out-of-the-box learning algorithm.

```
Input: Training Data, B (# of trees)
for i = 1 to B do
|   Generate a bootstrap sample of the original data
|   Grow a big regression tree to the bootstrapped data
|   for each split do
|       |   Select m variables at random from all p variable
|       |   Pick the best variable/split_point among the m
|       |   Split the node into two
|       |   end
|   end
| end
```

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Boosting Trees

Boosting

Algorithms that can boost the performance of a set of weak regression (or classification) trees via combining them.

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Algorithms that can boost the performance of a set of weak regression (or classification) trees via combining them.

Forward stage-wise additive model

$$F(x) = f_1(x) + f_2(x) + \cdots + f_{T-1}(x) + f_T(x)$$

It is difficult to solve for all f_t 's. Instead we solve them sequentially using a forward stage-wise greedy algorithm.

Forward Stage-wise Optimization

$$F(x) = f_1(x) + f_2(x) + \cdots + f_{T-1}(x) + f_T(x)$$

Input: Training Data, T (# of iterations)

Initialization: $F(x) = 0$ and current residuals $r_i = y$

for $t = 1$ to T do

| Fit a regression tree f_t to the current residuals r_i

| Add f_t to F :

$$F = F + f_t$$

| Update the current residual $r_i \leftarrow r_i - f_t(x_i)$

| end

Forward Stage-wise Optimization

$$F(x) = f_1(x) + f_2(x) + \cdots + f_{T-1}(x) + f_T(x)$$

Input: Training Data, T (# of iterations)

Initialization: $F(x) = 0$ and current residuals $r_i = y$

for $t = 1$ to T do

| Fit a regression tree f_t to the current residuals r_i

| Add f_t to F :

| $F = F + f_t$

$f_t \leftarrow \eta f_t$

| Update the current residual $r_i \leftarrow r_i - f_t(x_i)$

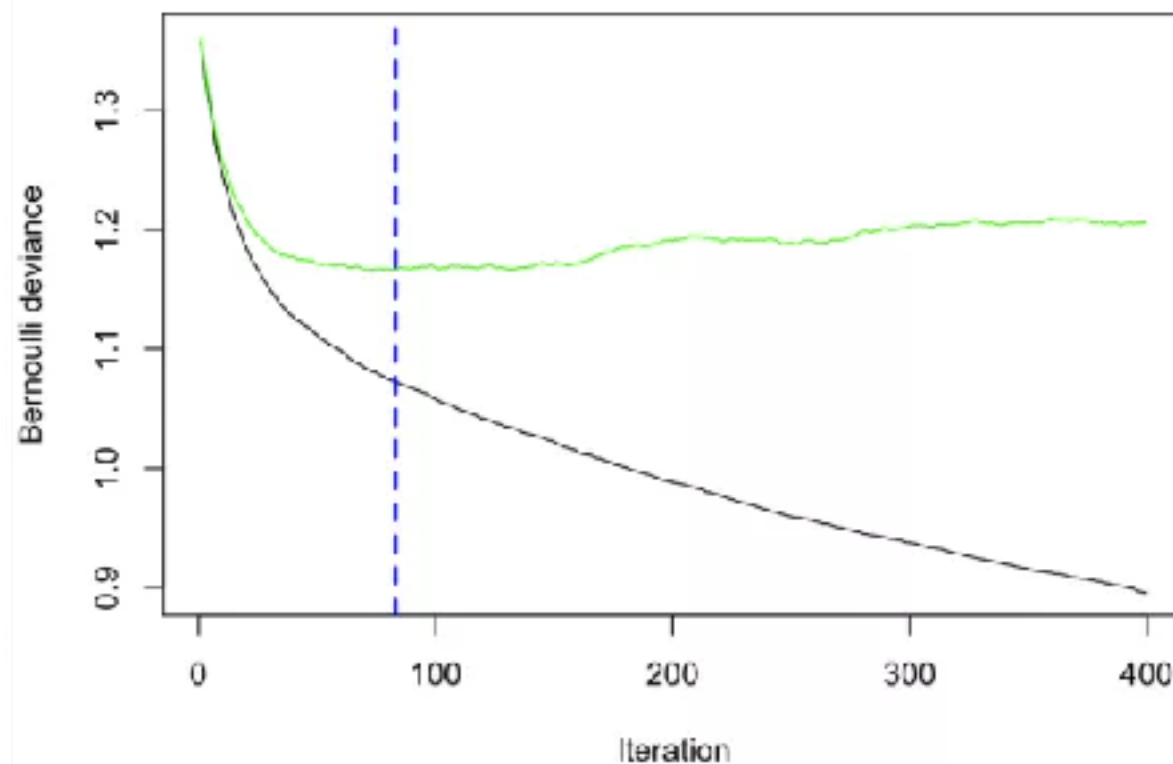
| end

Tuning parameters: learning rate η , number of trees T , complexity of f_t 's (depth of trees), and subsampling rate.

Forward Stage-wise Optimization

$$F(x) = f_1(x) + f_2(x) + \dots + f_T(x)$$

```
Input: Training data
Initialize
for t = 1 to T
  Fit a regression model
  Add f_t to F
  Update residuals
end
```



```
r_i = y_i - f_t(x_i)
residuals r_i
```

Tuning parameters: learning rate η , **number of trees** T , complexity of f_t 's (depth of trees), and subsampling rate.

Forward Stage-wise Optimization

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Tuning parameters: learning rate η , number of trees T , complexity of f_t 's (**depth of trees**), and subsampling rate.

Relatively small trees (weak regression trees)

Forward Stage-wise Optimization

$$F(x) = f_1(x) + f_2(x) + \cdots + f_{T-1}(x) + f_T(x)$$

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 Add f_t to

 Update the

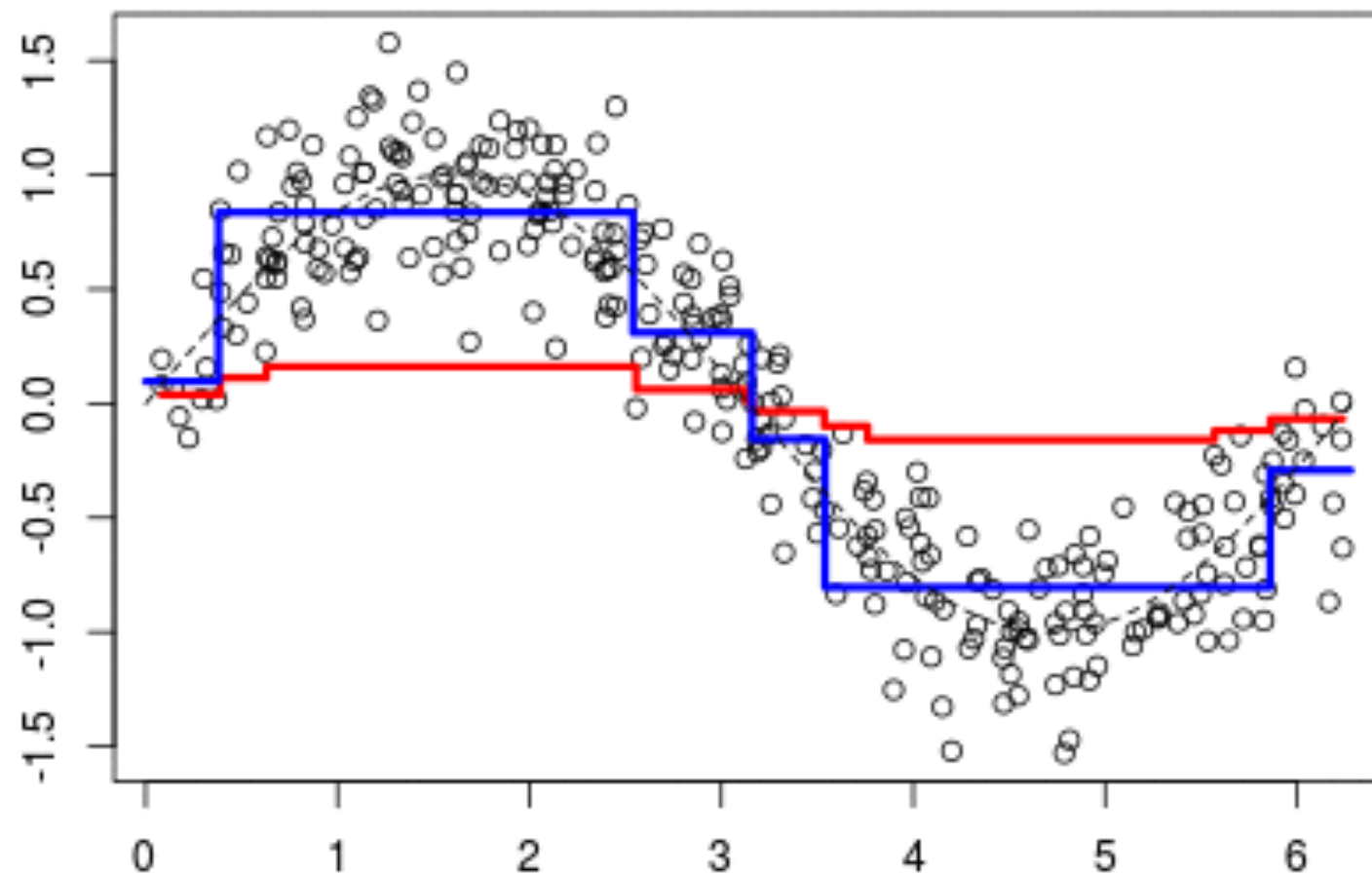
end

Sampling without replacement, i.e., less # of samples will be used when fitting a single tree (computation advantage).

Tuning parameters: learning rate η , number of trees T , complexity of f_t 's (depth of trees), and **subsampling rate**.

Demo: Boosting Tree for Curve Fitting

http://uc-r.github.io/public/images/analytics/gbm/boosted_stumps.gif



Comparison

	randomForest	BoostingTree	SingleTree
Accuracy	★★	★★★	★
Interpretation	★	★	★★★
Easy-to-Use	★★★	★	★★★
Computation	★	★★	★
Tree Size	Large	Small	
Parallel	Yes	No	

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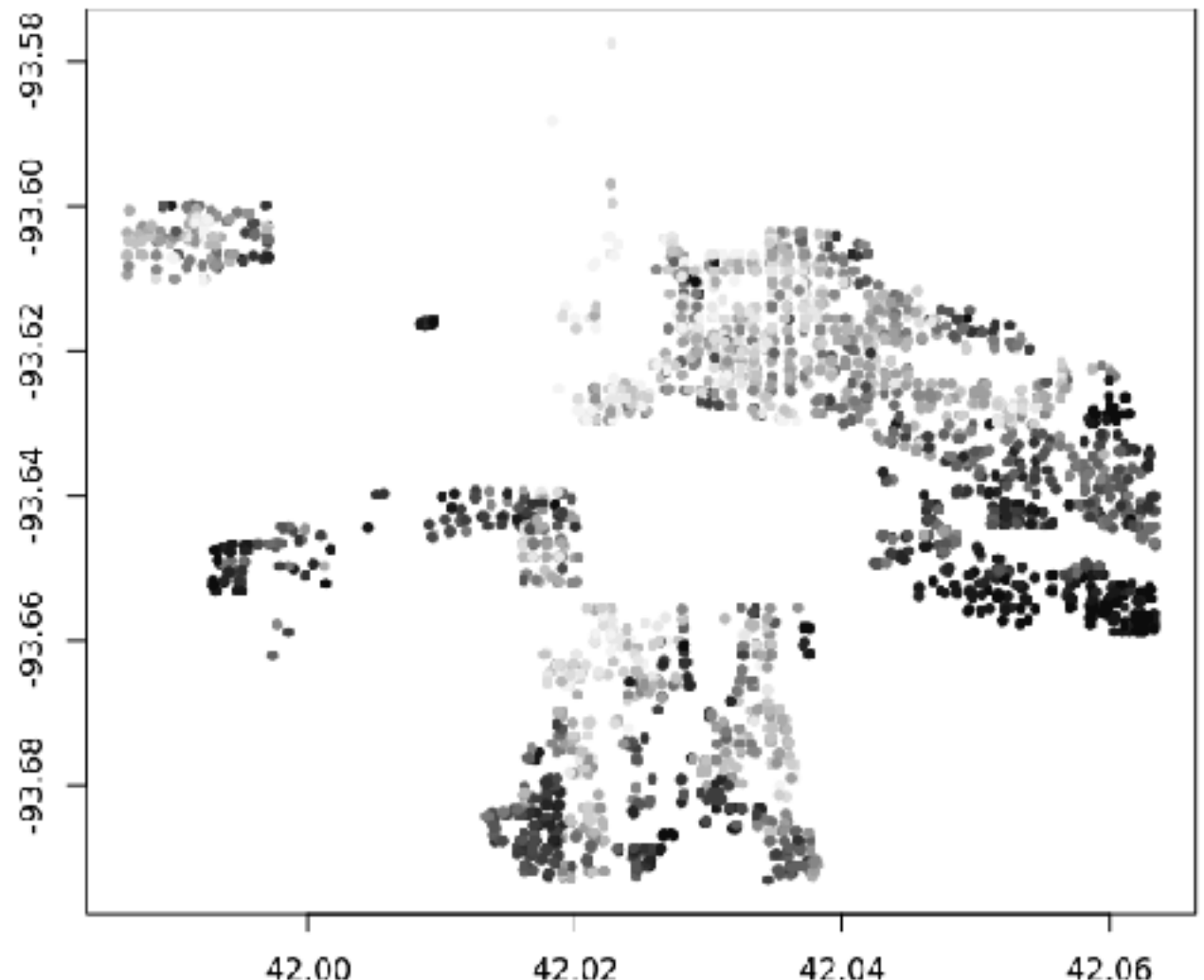
Ames Housing Data

<https://www.kaggle.com/c/house-prices-advanced-regression-techniques>

Full data from R package [AmesHousing]

- $n = 2930$ (houses)
- $p = 83$ (features, including **PID** and **Sale_Price**)

[1] "PID"	"MS_SubClass"	"MS_Zoning"
[4] "Lot_Frontage"	"Lot_Area"	"Street"
[7] "Alley"	"Lot_Shape"	"Land_Contour"
[10] "Utilities"	"Lot_Config"	"Land_Slope"
[13] "Neighborhood"	"Condition_1"	"Condition_2"
[16] "Bldg_Type"	"House_Style"	"Overall_Qual"
[19] "Overall_Cond"	"Year_Built"	"Year_Remod_Add"
[22] "Roof_Style"	"Roof_Matl"	"Exterior_1st"
[25] "Exterior_2nd"	"Mas_Vnr_Type"	"Mas_Vnr_Area"
[28] "Exter_Qual"	"Exter_Cond"	"Foundation"
[31] "Bsmt_Qual"	"Bsmt_Cond"	"Bsmt_Exposure"
[34] "BsmtFin_Type_1"	"BsmtFin_SF_1"	"BsmtFin_Type_2"
[37] "BsmtFin_SF_2"	"Bsmt_Unf_SF"	"Total_Bsmt_SF"
[40] "Heating"	"Heating_QC"	"Central_Air"
[43] "Electrical"	"First_Flr_SF"	"Second_Flr_SF"
[46] "Low_Qual_Fin_SF"	"Gr_Liv_Area"	"Bsmt_Full_Bath"
[49] "Bsmt_Half_Bath"	"Full_Bath"	"Half_Bath"
[52] "Bedroom_AbvGr"	"Kitchen_AbvGr"	"Kitchen_Qual"
[55] "TotRms_AbvGrd"	"Functional"	"Fireplaces"
[58] "Fireplace_Qu"	"Garage_Type"	"Garage_Yr_Blt"
[61] "Garage_Finish"	"Garage_Cars"	"Garage_Area"
[64] "Garage_Qual"	"Garage_Cond"	"Paved_Drive"
[67] "Wood_Deck_SF"	"Open_Porch_SF"	"Enclosed_Porch"
[70] "Three_season_porch"	"Screen_Porch"	"Pool_Area"
[73] "Pool_QC"	"Fence"	"Misc_Feature"
[76] "Misc_Val"	"Mo_Sold"	"Year_Sold"
[79] "Sale_Type"	"Sale_Condition"	"Longitude"
[82] "Latitude"	"Sale_Price"	



```
> sort(abs(y.pred - y.test), decreasing = TRUE)[1:10]
```

randomForest

```
> library("randomForest")  
> set.seed(123)  
> m1 = randomForest(Sale_Price ~ ., importance=TRUE,  
                    tmpdata[-test.id, ], ntree=500)  
> y.pred = predict(m1, newdata = tmpdata[test.id, ])
```

```
> y.test = tmpdata$Sale_Price[test.id]  
> sqrt(mean((y.pred - y.test)^2))
```

Minimal pre-processing:

- no transformation;
- fill in some missing values;
- no one-hot coding for cat.

GBM

```
> library("gbm")  
> gbm.fit <- gbm(  
  formula = Sale_Price ~ .,  
  distribution = "gaussian",  
  data = tmpdata[-test.id, ],  
  n.trees = 5000,  
  interaction.depth = 2,  
  shrinkage = 0.01,  
  cv.folds = 5,  
  bag.fraction = 0.75,  
  verbose = FALSE  
)
```

```
> y.pred = predict(gbm.fit, n.trees = 4971, testdata)  
> sqrt(mean((y.test - y.pred)^2))
```



```
> sort(abs(y.pred - y.test), decreasing = TRUE)[1:10]
```

randomForest

```
> library("randomForest")  
> set.seed(123)  
> m1 = randomForest(Sale_Price ~ ., importance=TRUE,  
                    tmpdata[-test.id, ], ntree=500)  
> y.pred = predict(m1, newdata = tmpdata[test.id, ])
```

```
> y.test = tmpdata$Sale_Price[test.id]  
> sqrt(mean((y.pred - y.test)^2))
```

Project 1 for F18 Stat 542

10 Splits of Training/Test
Target perf < 0.132

Very difficult for some
splits, e.g., Split 3. Why?

GBM

```
> library("gbm")  
> gbm.fit <- gbm(  
  formula = Sale_Price ~ .,  
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  n.trees = 5000,  
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  cv.folds = 5,  
  bag.fraction = 0.75,  
  verbose = FALSE  
)
```

```
> y.pred = predict(gbm.fit, n.trees = 4971, testdata)  
> sqrt(mean((y.test - y.pred)^2))
```

[illegible]