Introduction to Trees & Random Forests

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Flipped Classroom

Before class:

- Students are assigned reading
  - Chapter 8 in *Introduction to Statistical Learning With Applications in R*
- Students watch online videos.

During class:

- Short lecture
- Lab
  - Guided example
  - Exercises (to be submitted for a grade)

Class Materials

Files at
https://github.com/j3schaue/intro_to_random_forests.git

Prior Knowledge

Regression:

- Linear and regularized models
- Generalized additive models (GAM)

Classification:

- Logistic and regularized models
- Discriminant analyses

Tuning & cross validation

CART & Extensions

- CART = Classification and Regression Trees
- Iterative algorithm that recursively partitions the data
- While trees are not always particularly great on their own, extensions that are based on trees usually are.
  - Random forests
  - Boosted models
- CART extensions are becoming popular
  - Predictive accuracy (He & Hahn, 2020)
  - Causal inference (Hill, 2007; Yeager et al., 2019)

Review: Regression

$$Y = f(\mathbf{X}) + \epsilon$$

- We want to find $\hat{f}$ that gives good predictions of $Y|\mathbf{X}$.
- We usually do this by minimizing an empirical risk function:

$$\sum (Y_i - \hat{f}(\mathbf{X}_i))^2$$

- Example: Linear regression

$$\hat{f} \equiv \arg\min_{\beta} \sum (Y_i - \beta_0 - \beta_1 X_{i1} - ... \beta_p X_{ip})^2$$

Review: Classification

- Classes $1, \ldots, M$ with $P[Y_i \in \text{class } m] = p_{mi}$

$$g(p_{mi}) = f(\mathbf{X})$$

- Optimization problems vary (maximum likelihood, empirical risk minimization,maximum margins, etc.)
- Example: logistic regression with two classes

$$\log \frac{p_i}{1 - p_i} = \beta_0 + \beta_1 X_{i1} + \ldots \beta_p X_{ip}$$

Issues to Remember

- Training vs. test error: Worry if your model is **too good** on the data it's trained on...
- Cross validation: Fold data and use it to tune models and estimate test error.
- Bias-variance trade-off
- Curse of dimensionality

Insight on "good" predictive models

- Take observations with similar $\mathbf{X}$ and assume that they should have similar Y.
- Many techniques (linear/logistic regression) make you specify the structure of $\mathbf{X}$ and $\hat{f}$.
- Why not just try to automatically find observations that have similar $\mathbf{X}$ and Y?

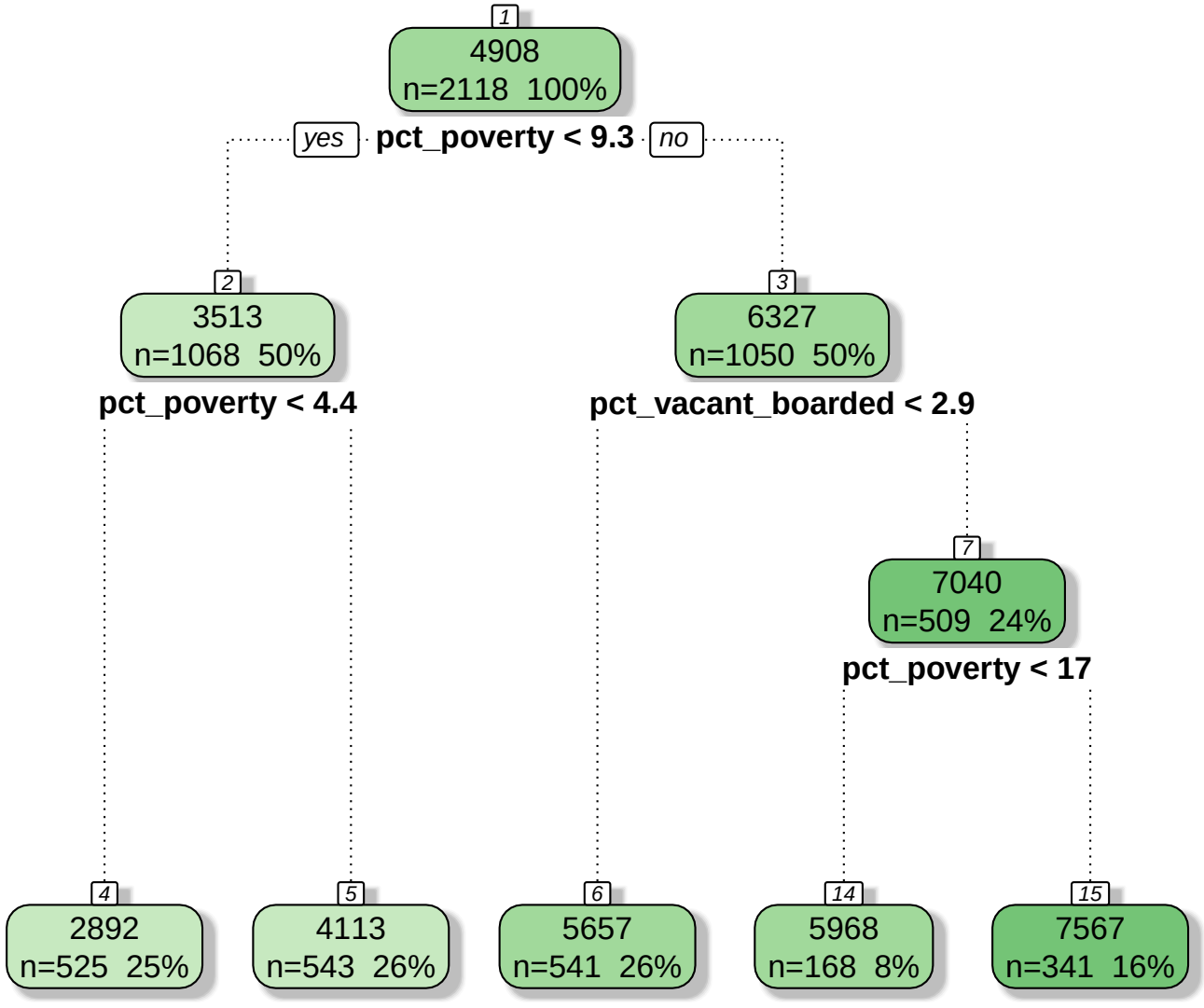
Example: Tree for Nonviolent Crime in Communities

Predict a community's nonviolent crime rate (per 100,000 people) based on the poverty rate and percent of housing that is vacant in that community.

Previously, we've used

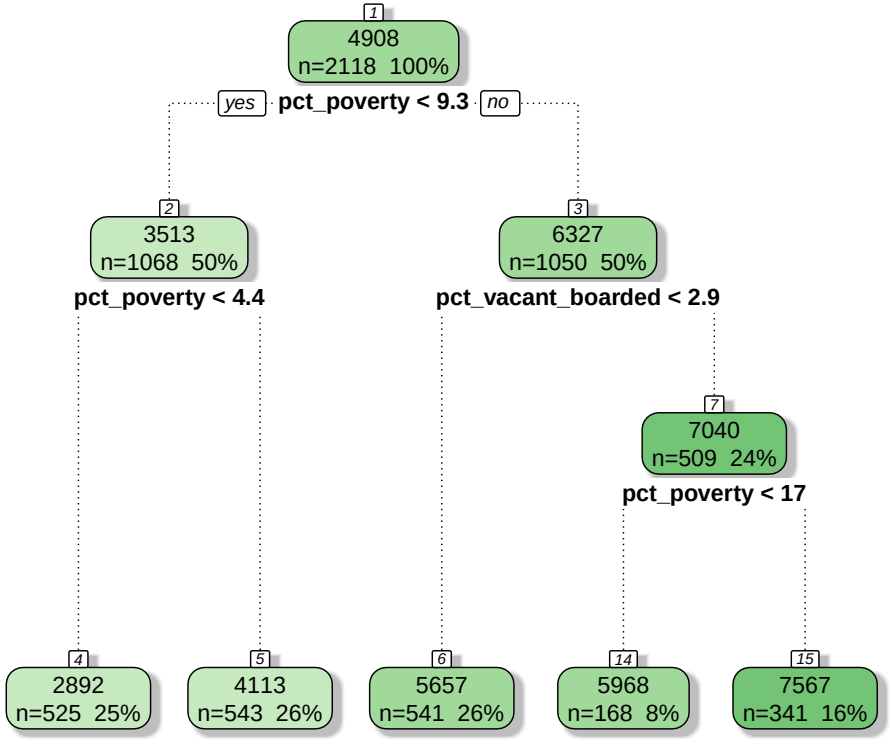
- Linear regression
- Regularized regression
- GAMs

Trees



Tree Predicting Nonviolent Crime in Communities

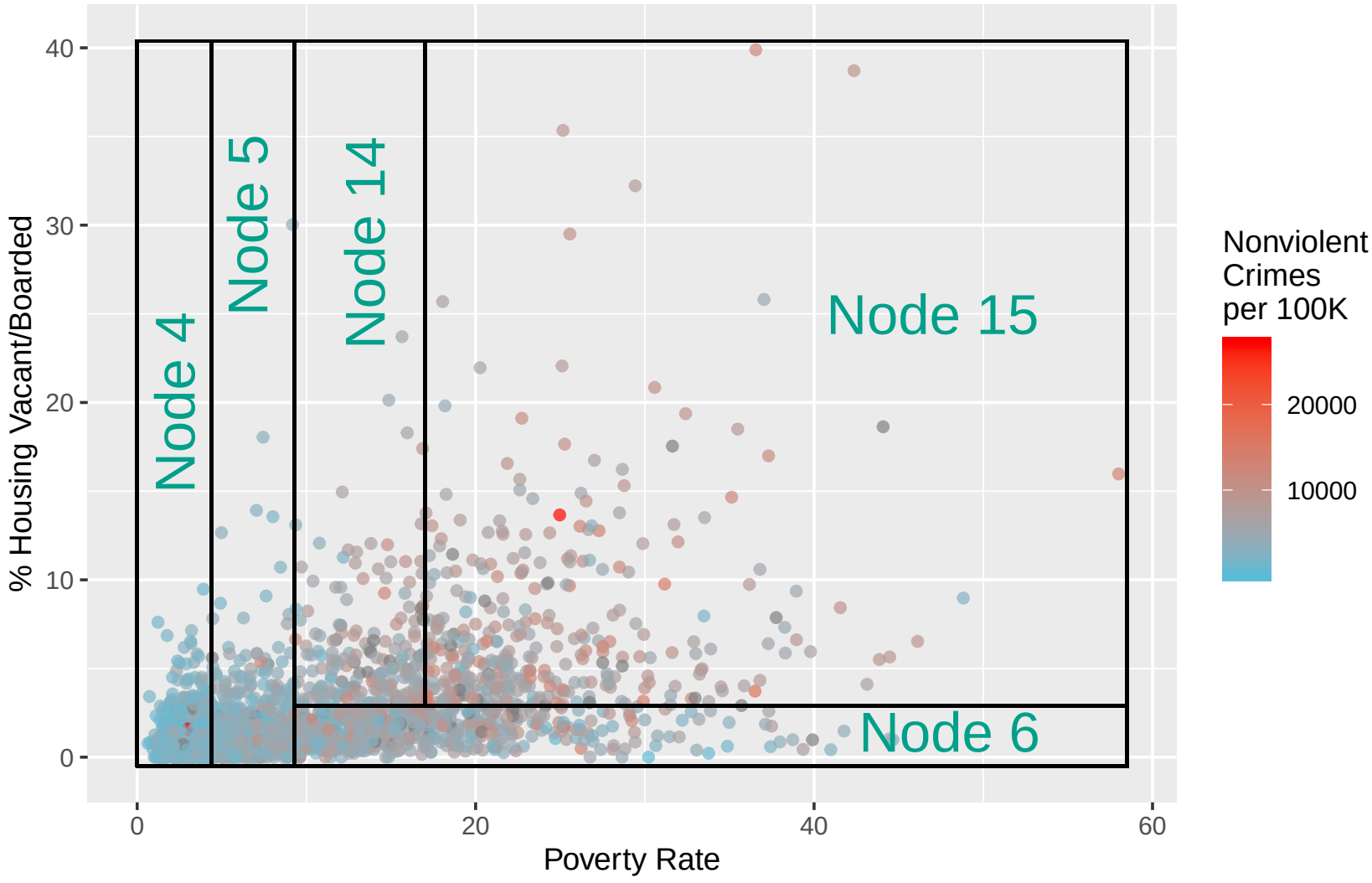
Trees



Tree Predicting Nonviolent Crime in Communities

- Nodes/Splitting rules
- Splitting rules are recursive
- Node/Tree depth
- Terminal nodes (used to make prediction)
- $\hat{f}(X) =$ terminal node mean for X

Trees


Node 4
Node 5
Node 14
Node 15
Node 6
% Housing Vacant/Boarded
Poverty Rate
0
10
20
30
40
0
20
40
60
Nonviolent Crimes per 100K
20000
10000

Regression Trees

Splitting rules are determined by a *greedy algorithm*.

1. Start with a tree with one terminal node (the entire data set).
2. For each value of each predictor:

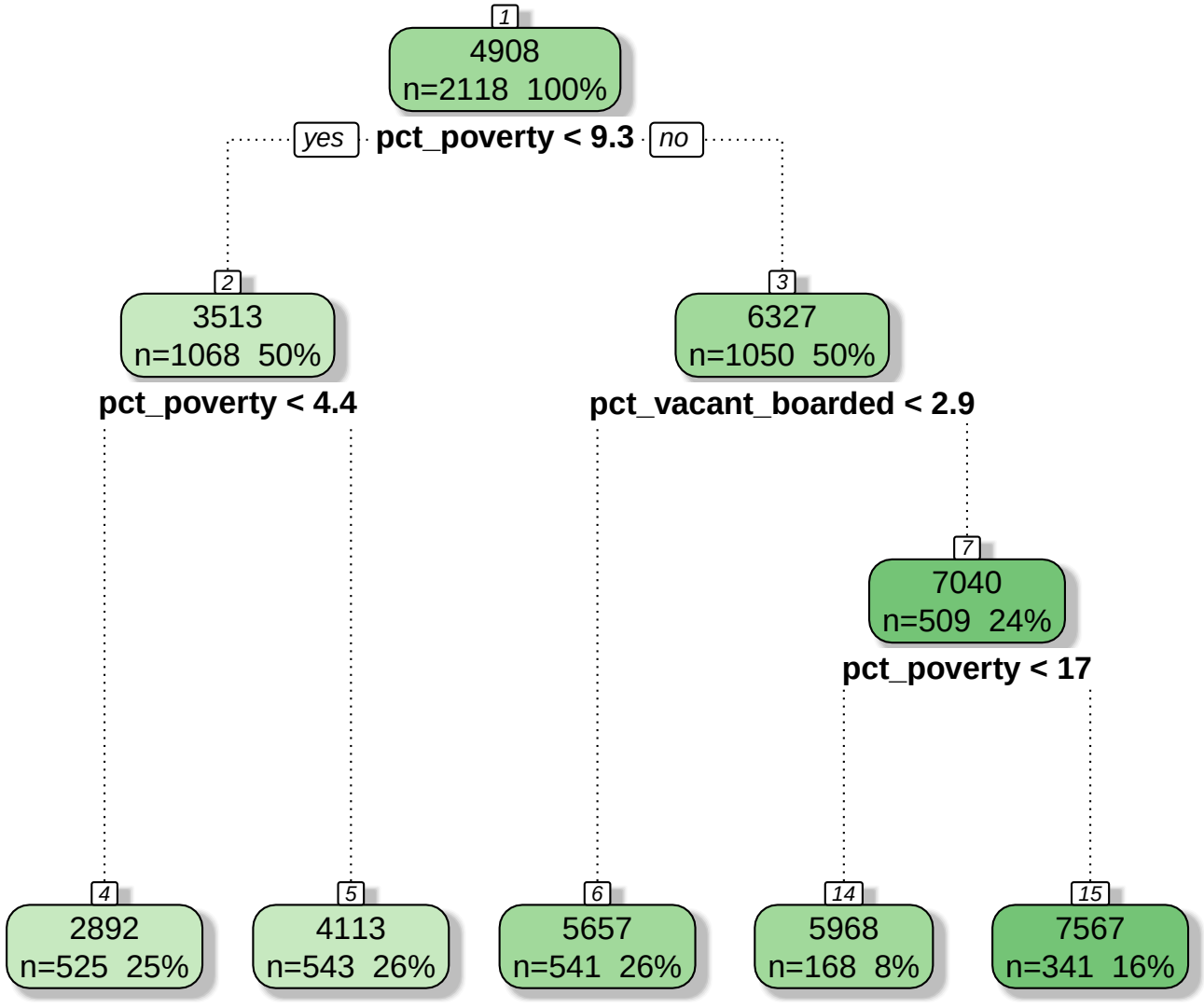
   2a. Split the data on that predictor/value

   2b. Compute sum of squared errors across all resulting terminal nodes SSE $= \sum_{R_j} \sum (Y_i - \hat{Y}_{R_j})^2$

   2c. Choose predictor/value that minimizes SSE
3. Repeat 2 within each resulting terminal node.

Note that at each split, the SSE in terminal nodes decreases.

Recursive Partitioning

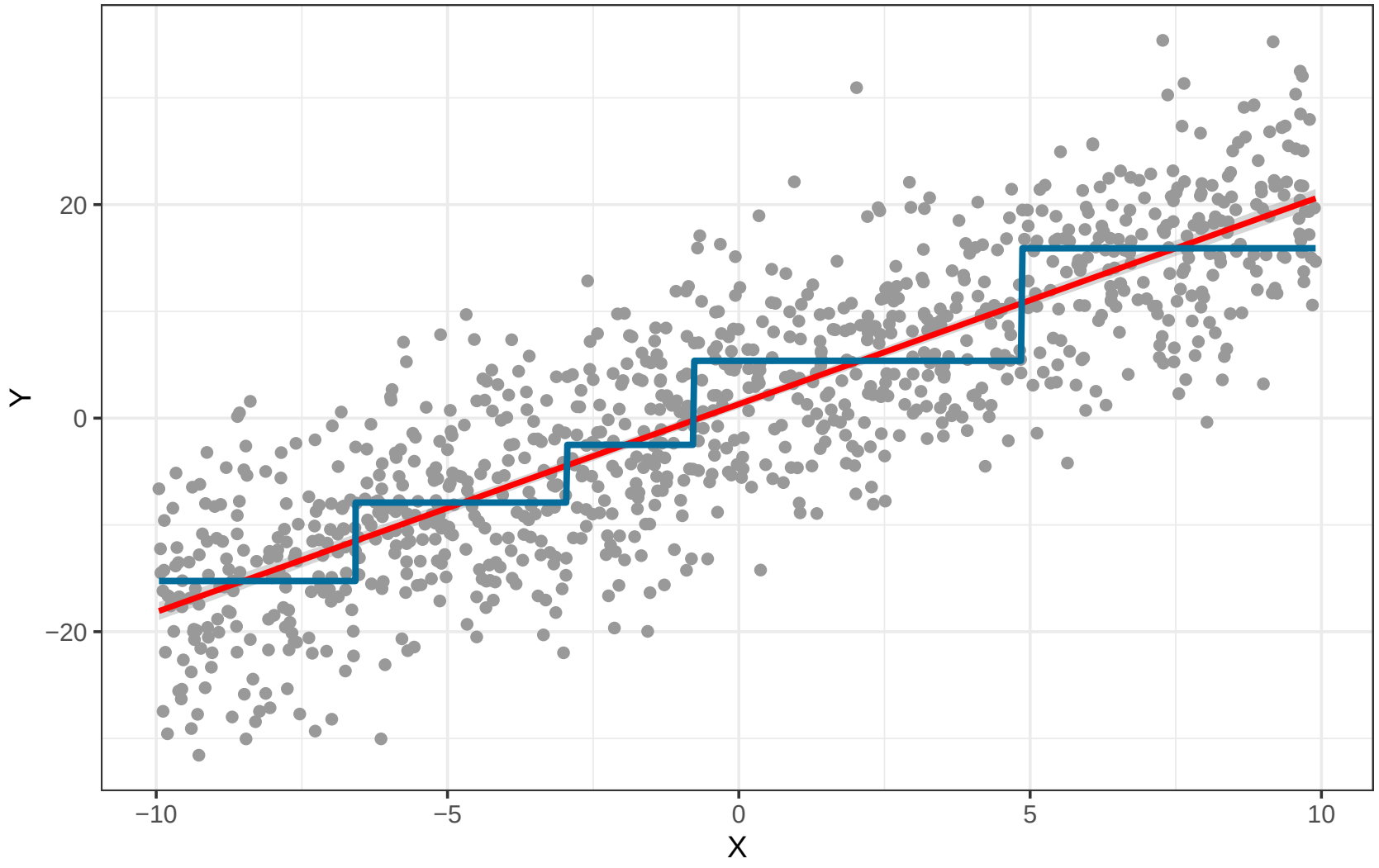


Tree Predicting Nonviolent Crime in Communities

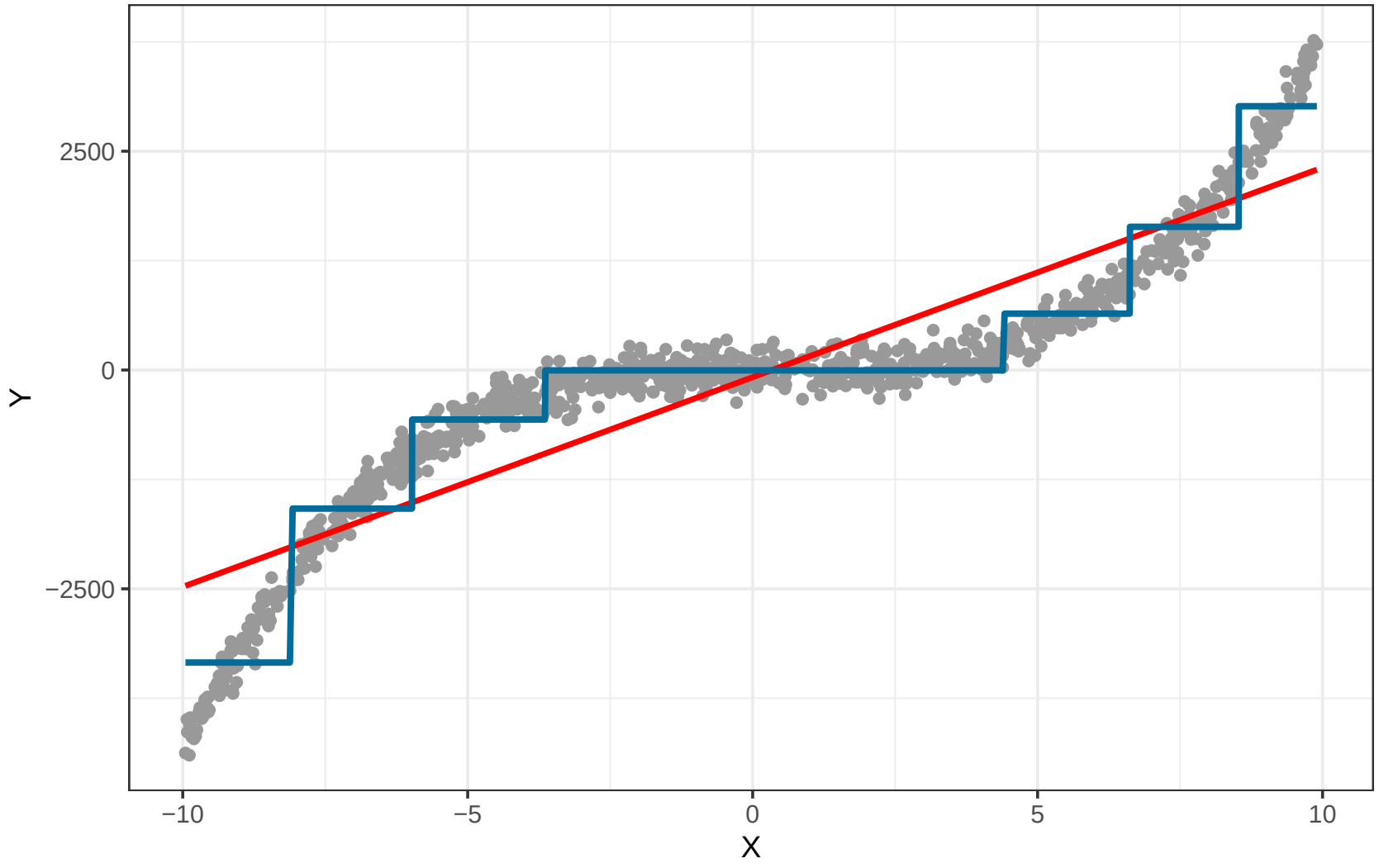
Flexibility

- Nonlinearity does not need to be specified in advance.
  - Split points are similar to step functions with splines.
- Interactions are automatically modeled.
  - Tree splits on predictor X_1 and then later on X_2, then the prediction for a given X_1 will depend on the value of X_2 (an interaction).

Tree vs. Linear Model



Flexibility



Classification Trees

Splitting rules are determined by a *greedy algorithm*.

1. Start with a tree with one terminal node (the entire data set).
2. For each value of each predictor:

   2a. Split the data on that predictor/value

   2b. Compute some metric of impurity (i.e., Gini Index, cross entropy) in the terminal nodes

   2c. Choose predictor/value that minimizes impurity index
3. Repeat 2 within each resulting terminal node.

Note that at each split, the purity of terminal nodes increases

Impurity indices

Suppose our classification problem involves K classes, and our tree has m regions.

- Let $\hat{p}_{mk}$ be the % of observations in region m in class k.
- Gini index: $\sum_{i=1}^{K} \hat{p}_{mk}(1 - \hat{p}_{mk})$
- Cross entropy: $-\sum_{i=1}^{K} \hat{p}_{mk} \log \hat{p}_{mk}$

Trees Notes

- Tree depth can be set *a priori* or could be adaptive (e.g., stop when training MSE is small enough).
- Trees are static given the data set; if you run a tree the same way on the same dataset, you'll always get the same fit.
- Deeper trees tend to have lower bias but more variance; shallower trees tend to have high bias but low variance.
- Deeper trees can be "pruned" to have less variance, but even pruned trees are seldom competitive with more advanced models (even linear models).

Bias-Variance Trade-off for Trees

Fact 1: Trees will have very high variance.

Fact 2: A model that is the average of models can reduce variance.

Proposed solution: Take the average of a bunch of trees.

Averaging Trees

- Since trees are not stochastic, if we fit a bunch of trees on a dataset, they'll all be the same...
- Idea 1: Bootstrapping
  - Bootstrapping = creating B new datasets by sampling rows from your existing dataset **with replacement**.
  - On average, each bootstrap sample will contain about $1/3$ of the rows of the training data (but they will be repeated)
  - Each of these datasets will be a little bit different, which means the trees that are fit on them will be a little bit different.
  - This is gets a handle on how variable the trees are given different datasets you could train them on.

Bootstrap

Bootstrap Samples	1	2	3	...	B
Observation 1	2	0	4		1
Observation 2	1	3	0		0
$\vdots$	$\vdots$	$\vdots$	$\vdots$	$\ddots$	$\vdots$
Observation n	0	1	1		0
	Tree 1	Tree 2	Tree 3		Tree B
	$\hat{f}_1$	$\hat{f}_2$	$\hat{f}_3$		$\hat{f}_B$

Averaging Trees

- Idea 2: Considering only a random subset for splitting.
  - Trees consider **all** p possible predictors for each split.
  - Instead, what if we randomly selected only a few predictors ($m_{try} < p$) to consider at each split?
  - Then, even trees grown this way on the same dataset would be different.

Random Forests

Random forests = Bootstrapping + Randomly selecting predictors

Bootstrap Samples	1	2	3	...	B
Observation 1	2	0	4		1
Observation 2	1	3	0		0
$\vdots$	$\vdots$	$\vdots$	$\vdots$	$\ddots$	$\vdots$
Observation n	0	1	1		0
	Tree 1	Tree 2	Tree 3		Tree B
	$\hat{f}_1$	$\hat{f}_2$	$\hat{f}_3$		$\hat{f}_B$

$$\hat{f}(\mathbf{X}) = \sum_{i=1}^{B} \frac{\hat{f}_i(\mathbf{X})}{B}$$

Conveniences of Random Forests

- Does not matter how many variables you have (though it may get slow).
- Can automatically incorporate nonlinearity (though not all smooth functions).
- Can automatically incorporate interactions (because trees can)
- Potential on-the-fly tuning with out-of-bag (OOB) error
- Open up the "black box"
  - Variable importance
  - Partial dependence

OOB Error

- On average, each tree makes use of about 1/3 of the training data.
- 2/3 of the data are a "test" set for a given tree.
- Predict Y_i of the ith observation with an average of the trees **not** trained on that observation.
- OOB error is a useful approximation to test error and can be used to tune random forests (e.g., if CV is too hard)

Bootstrap Samples	1	2	3	...	B
Observation 1	2	0	4		1
Observation 2	1	3	0		0
$\vdots$	$\vdots$	$\vdots$	$\vdots$	$\ddots$	$\vdots$
Observation n	0	1	1		0
	Tree 1	Tree 2	Tree 3		Tree B
	$\hat{f}_1$	$\hat{f}_2$	$\hat{f}_3$		$\hat{f}_B$

Variable Importance

If a variable is "important" then we will split on it frequently, and those splits will greatly reduce SSE or impurity.

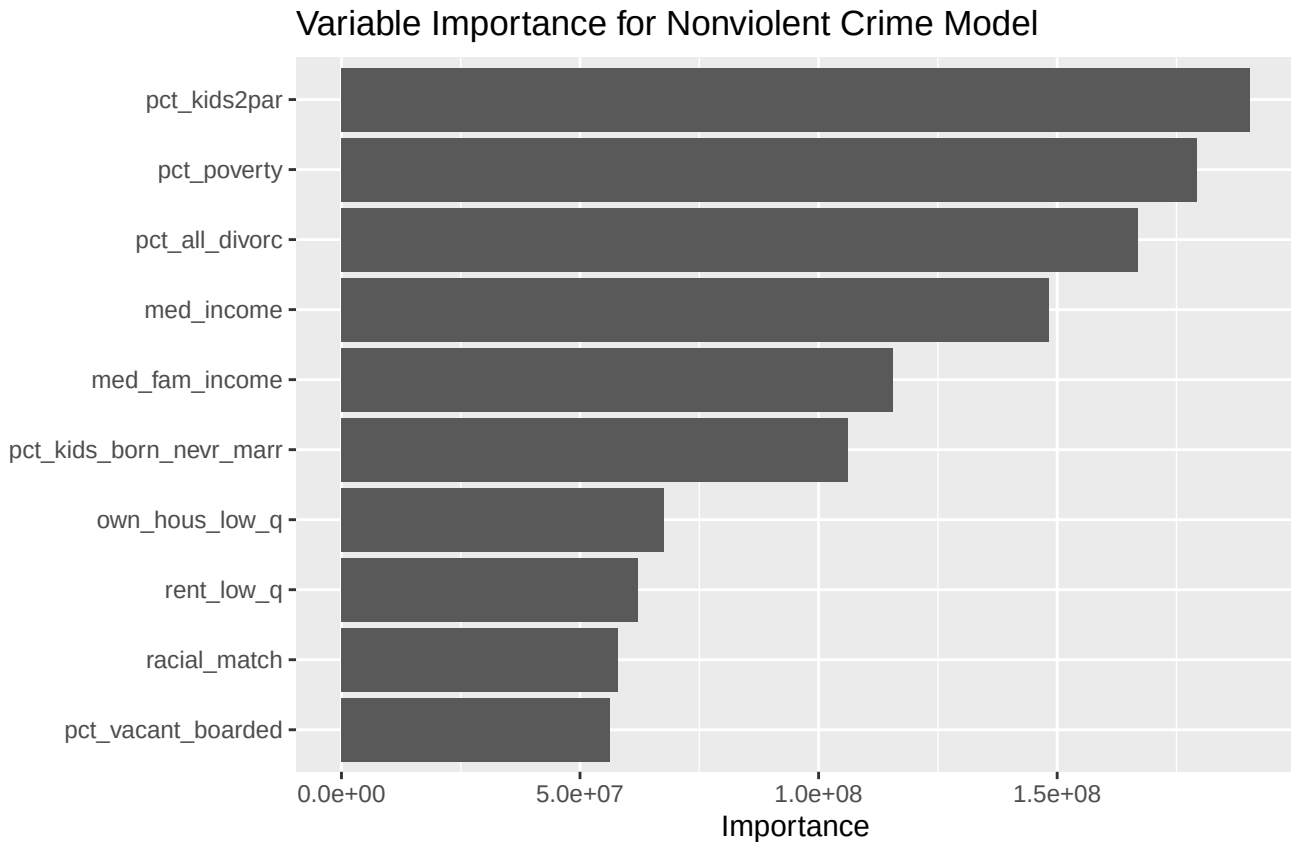
Regression

- Total amount the SSE decreased when a split occurs on variable X_j (summed across all splits on all B trees).

Classification

- Total amount the the impurity metric decreased when a split occurs on variable X_j (summed across all splits on all B trees).

Variable Importance



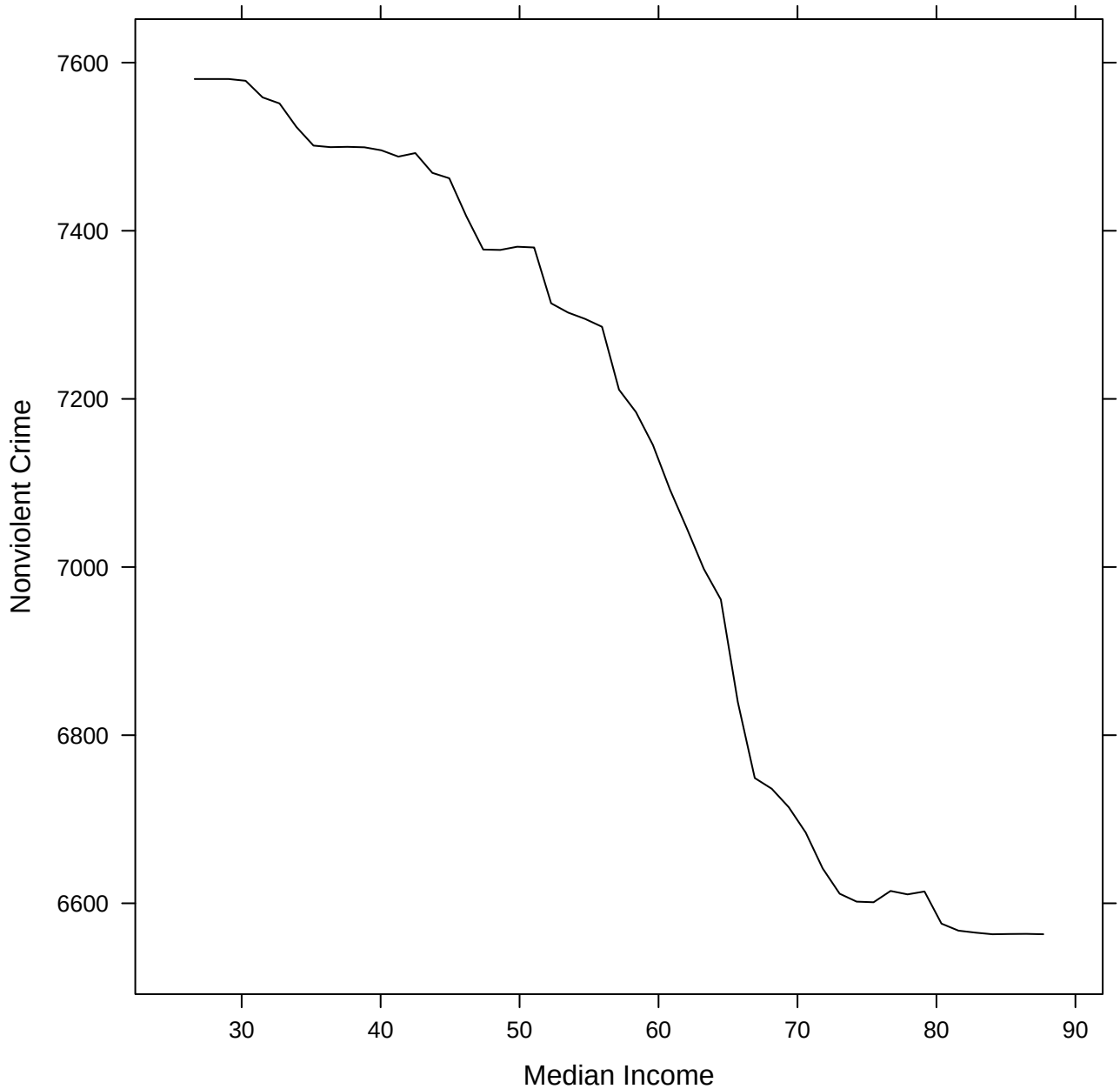
Partial Dependence

We may be interested in the marginal relationship between one predictor X_1 and Y in the random forest: $\hat{f}(X_1)$

We can estimate this from the training data by averaging over the predictions for all other values of $X_2, ..., X_p$ in the data:

$$\hat{f}(x_1) = \sum_{i=1}^{n_{x_1}} \hat{f}(x_1, X_{i2}, ...X_{ip})/n_{x_1}$$

Partial Dependence



Multiple Partial Dependence & Treatment Effect Variation

Suppose $\mathbf{X} = [T, X_1, \ldots X_p]^T$ includes treatment indicator $T \in \{0, 1\}$

Partial dependence can explore the relationship between treatment effect and some variable X_1

$$\hat{f}(T = 1, X_1) = \sum_{i=1}^{n_{T=1,X_1}} \hat{f}(1, X_1, X_{i2}, \ldots X_{ip})/n_{T=1,X_1}$$

$$\hat{f}(T = 0, X_1) = \sum_{i=1}^{n_{T=0,X_1}} \hat{f}(0, X_1, X_{i2}, \ldots X_{ip})/n_{T=0,X_1}$$

$$\hat{f}(T = 1, X_1) - \hat{f}(T = 0, X_1)$$

Tuning Random Forests

1. Number of predictors to consider for each split m_{try}
2. Number of trees
3. Tree depth

How do we find the right tuning parameter values?

Lab Time

Please access the lab on random forests now.