PGE 383 Lecture 26
Machine Learning - PCA

- Decision Tree
- Ensemble Methods

Michael Pyrcz, The University of Texas at Austin

Machine Learning

Introduction

Prerequisites

Data Preparation

Univariate Analysis

Multivariate Analysis

Spatial Characterization

Spatial Estimation

Spatial Simulation

Uncertainty Analysis

Model Checking

Decision Making

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Decision Making

Training and Testing

Training Phase

- The training subset of the data is applied to select the model parameters (fit the model) usually optimized to minimize the mean square error.

$$MSE = \frac{1}{n}\sum_{i=1}^{n}\left[\left(y_i - \hat{f}(x_1^i, \dots, x_m^i)\right)^2\right], \; for \; i = 1, \dots, n_{train}$$

Testing Phase

- Apply the model to the testing data (data withheld from training)
- Optimize the model hyperparameters (e.g. complexity) to minimize mean square error with the testing data

$$MSE = \frac{1}{n}\sum_{i=1}^{n}\left[\left(y_i - \hat{f}(x_1^j, \dots, x_m^j)\right)^2\right], for \; i = 1, \dots, n_{test}$$

Do not use all data to train or you will likely overfit to the data and not predict well with new data. Various methods, **k-fold cross validation** is common.

Decision Trees

- Decision trees are used for supervised learning.

$$Y = f(X_1, \dots, X_m) + \epsilon$$

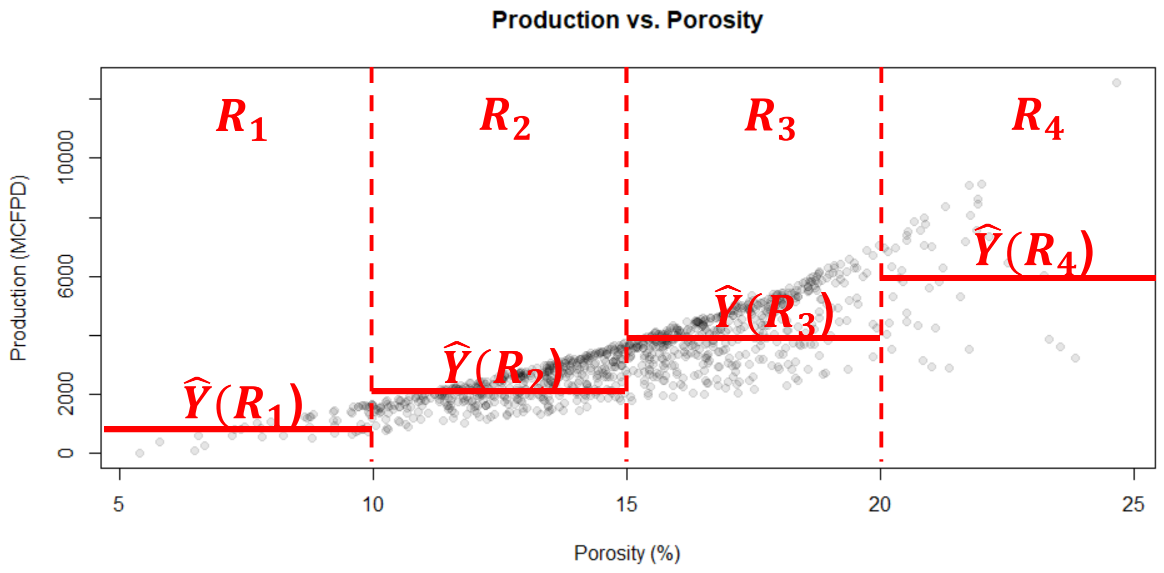
  we are predicting a response, Y, from a set of features, $X_1, \dots, X_m$
- May work with continuous Y for regression tree or categorical Y for classification tree.

- Why cover decision trees?
  - They are not the most powerful, cutting edge method in machine learning
  - But they are likely the most understandable, interpretable
  - Decision trees are expanded with random forests, bagging and boosting to be cutting edge.

"Let's learn first about a single tree and then we can comprehend the forest."

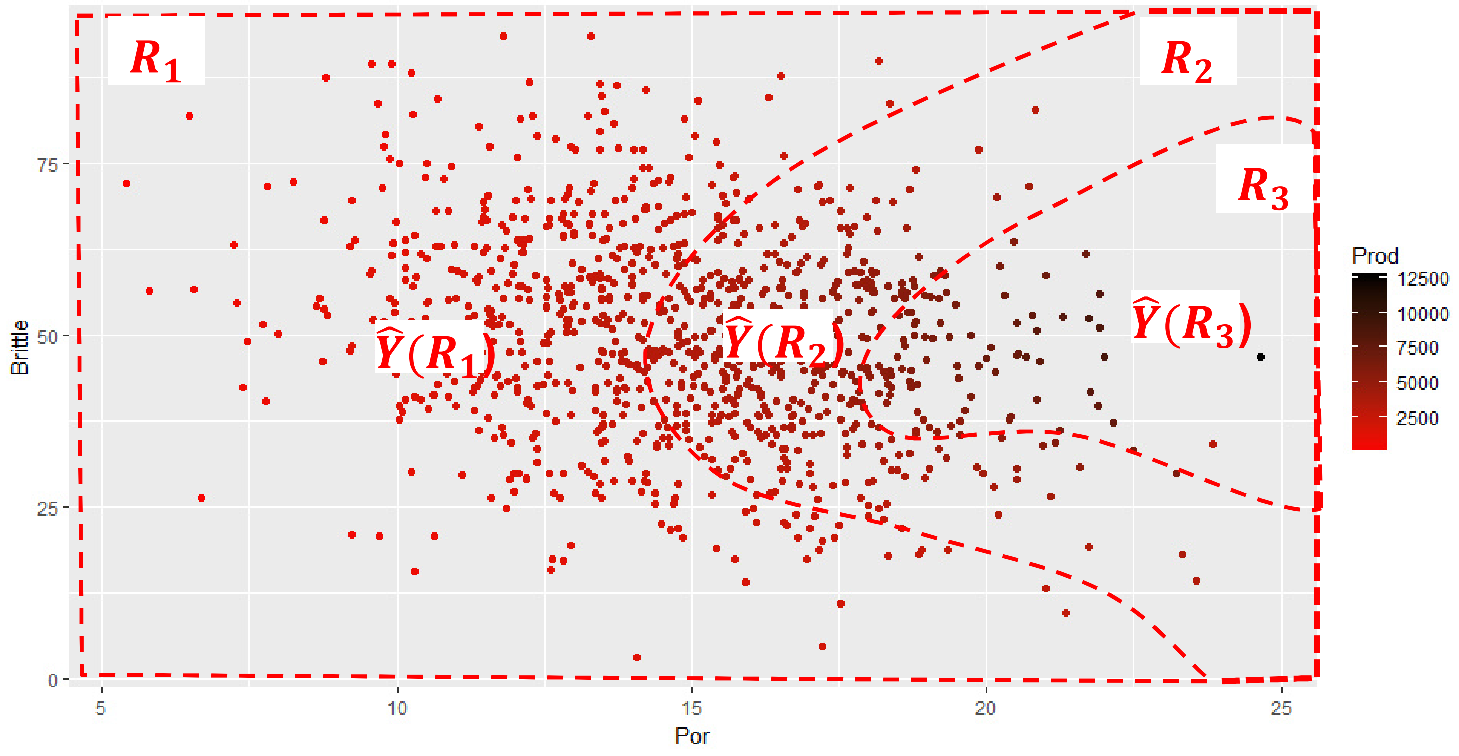
Decision Trees

- The fundamental idea is to divide the predictor space, $X_1, \dots, X_m$, into J mutually exclusive, exhaustive regions
  - mutually exclusive – any combination of predictors only belongs to a single region, R_j
  - exhaustive – all combinations of predictors belong a region, R_j, regions cover entire feature space (range of the variables being considered)
- For every observation in a region, R_j, we use the same prediction, $\hat{Y}(R_j)$
- For example predict production, $\hat{Y}$, from porosity, X_1



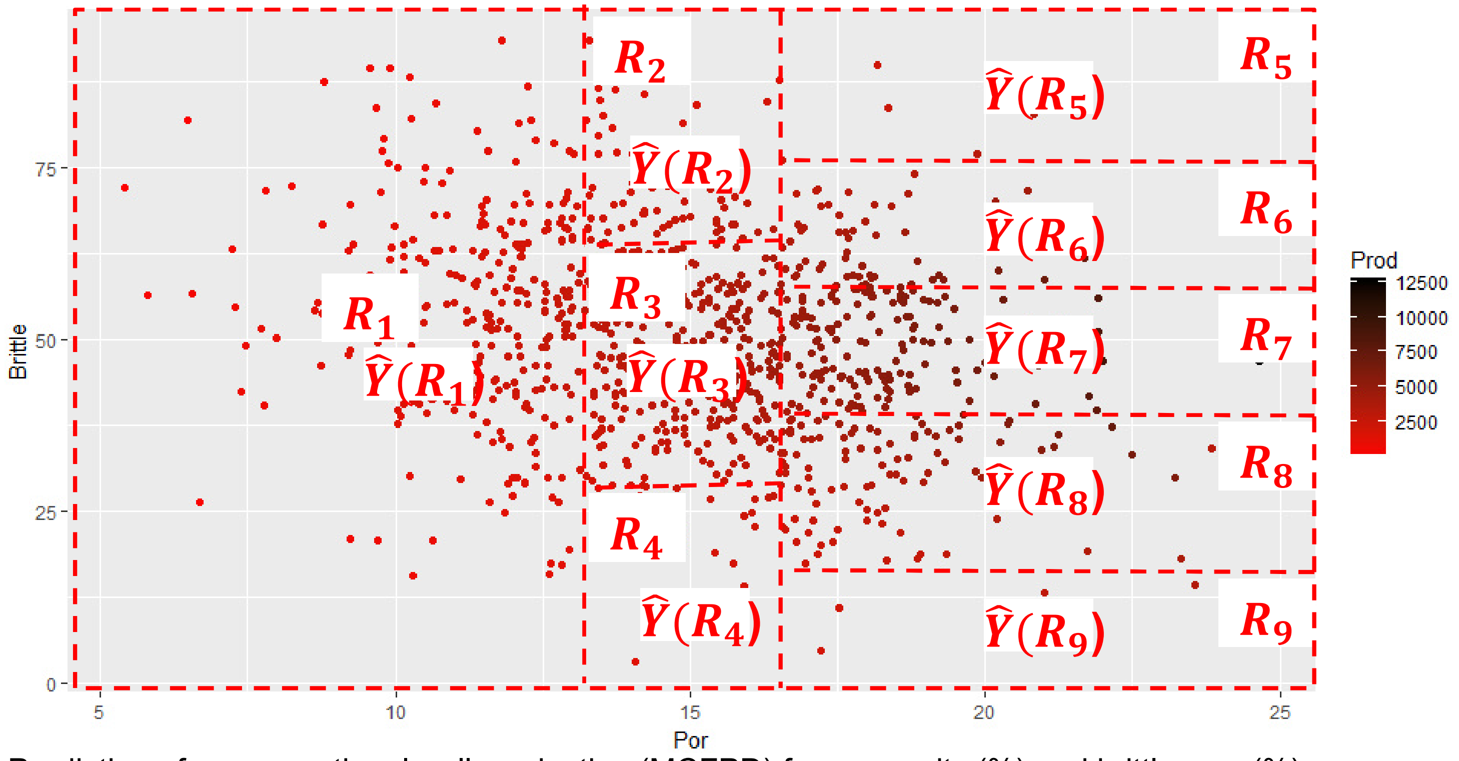
Decision Trees
The Regions

- How do we construct the Regions, $R_{1,} R_2 , \ldots , R_J$?
  - They could be any shape!
  - Consider the 3 variable problem below.
- Prediction of unconventional well production (MCFPD) from porosity (%) and brittleness (%)



Decision Trees
The Regions

- How do we construct the Regions, $R_{1,} R_2 , \dots , R_J$?
  - They could be any shape!
  - Consider the trivariate (3 variable) problem below.
  - We decide to use high-dimensional rectangles or boxes ⇨simple interpretation / rules
    - » Hierarchical segmentation over the features – **very flexible, compact model!**



Prediction of unconventional well production (MCFPD) from porosity (%) and brittleness (%)

Decision Trees
The Regions

How do we construct the Regions, $R_{1,} R_2, \dots, R_J$?

– We want to minimize the Residual Sum of Squares:

$$RSS = \sum_{j=1}^{J} \sum_{i \in R_j} (y_i - \hat{y}_{R_j})^2$$

looping over J regions and data in each region, $i \in R_j$

– This is the sum of squares of all the data vs. the estimate in their region (the mean of the training data in the region)

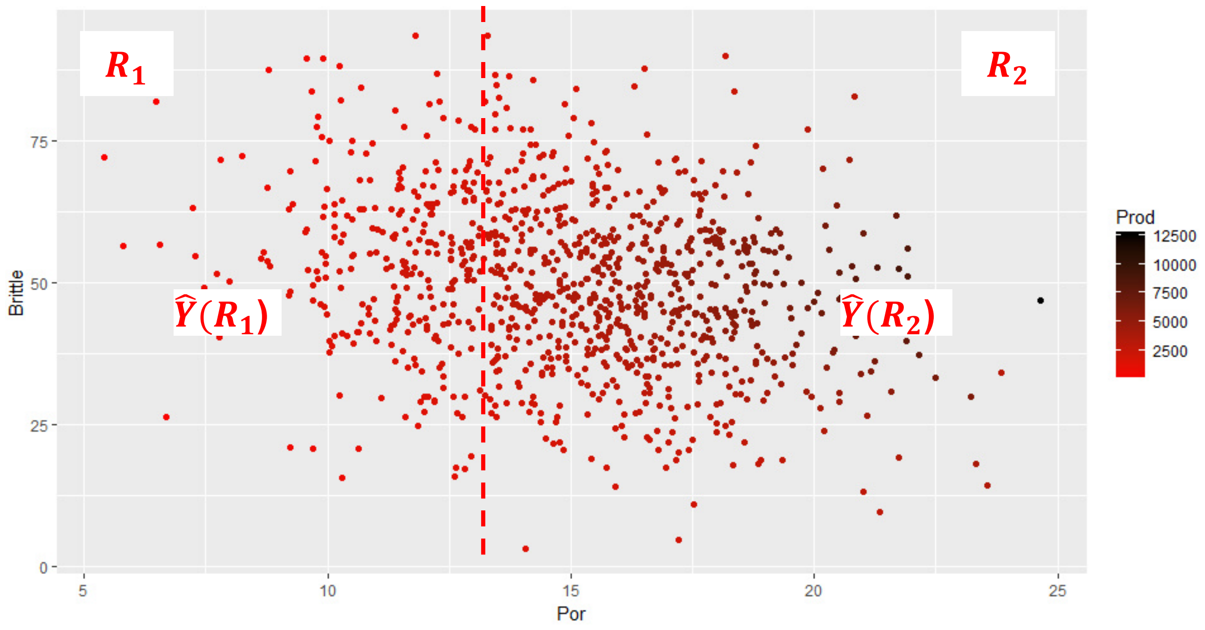
– Hint: somehow we need to account for the cost of complexity

» We do this through cross validation and pruning

Decision Trees
The Regions

How do we construct the Regions, $R_{1,} R_2, \ldots, R_J$?

- Recursive, binary splitting
  - Greedy - at each step the method selects the choice that minimizes RSS. There is no attempt to look ahead, jointly optimize over multiple choices
  - Top-down - at the beginning all data belong to a single region, top of the tree, greedy selection of the single best split over any feature that best reduces the RSS



Prediction of unconventional well production (MCFPD) from porosity (%) and brittleness (%)

Decision Trees
The Regions

How do we construct the Regions, $R_{1,} R_2 , \ldots , R_J$?

- Let's start with one region, $R_{1,}$ with all the training data in it
  - We will place the region boundary based on a threshold, s, inside a this region, j, such that it minimize the RSS.
  - This requires search over all possible thresholds over all features within that region.
  - This is not computationally impossible (not a big space to search)

$$R_{1(m,s)} = \{X|X_m < s\} \text{ and } R_{2(m,s)} = \{X|X_m \geq s\}$$

  - X_m are the features and s is the threshold for the segmentation into R_1 and R_2
  - We segment such that we minimize the Residual Sum of Squares:

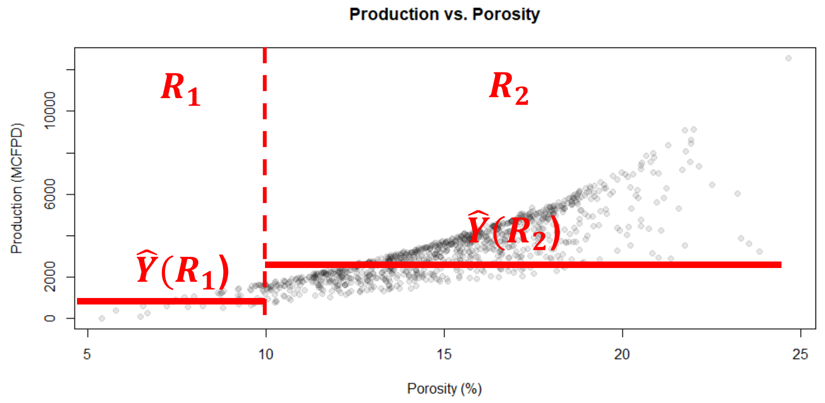
$$RSS = \sum_{i:x_i \in R_1(m,s)} (y_i - \hat{y}_{R_1})^2 + \sum_{i:x_i \in R_2(m,s)} (y_i - \hat{y}_{R_2})^2$$

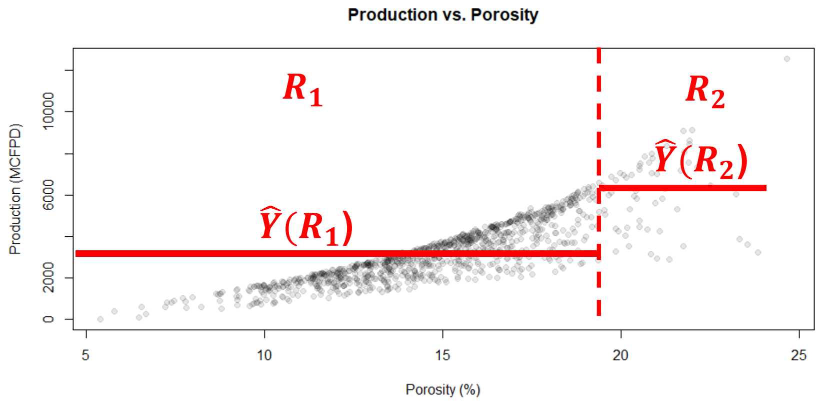
  - Then we just repeat for over the two region to find the next best segmentation.

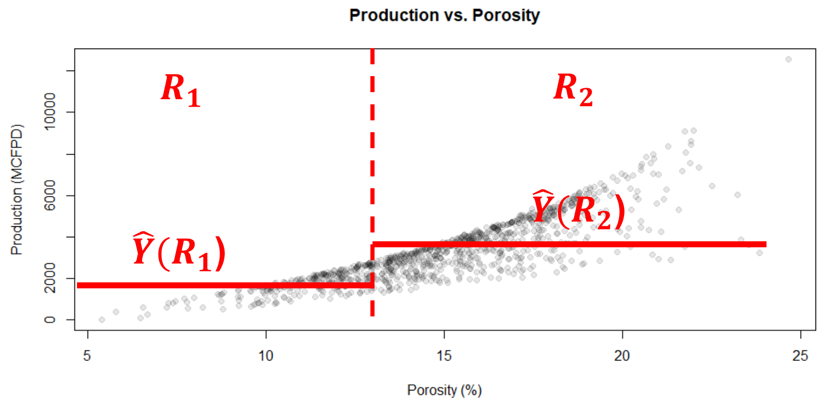
Decision Trees
The Regions

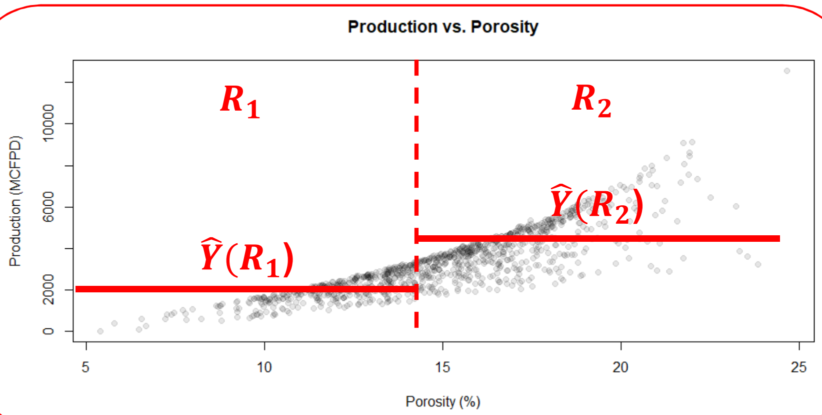
Let's pause and go back to our initial univariate problem and make a tree by hand!

- Where should we split to minimize the error in a tree-based estimate (minimize the residual sum of square)?





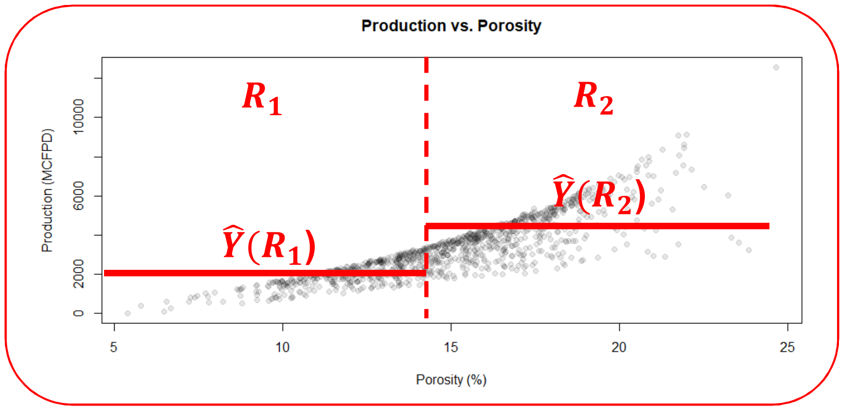


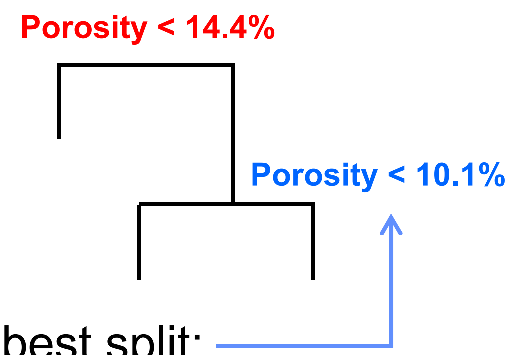


Decision Trees
The Regions

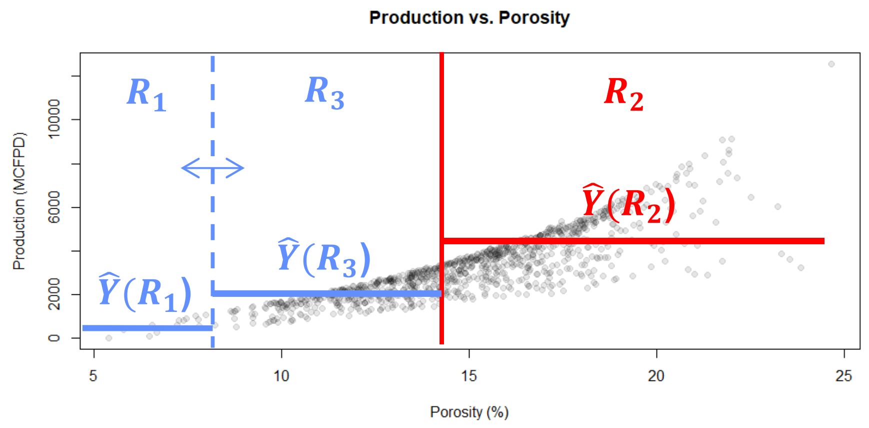
Let's pause and go back to our initial bivariate problem and make a tree by hand!

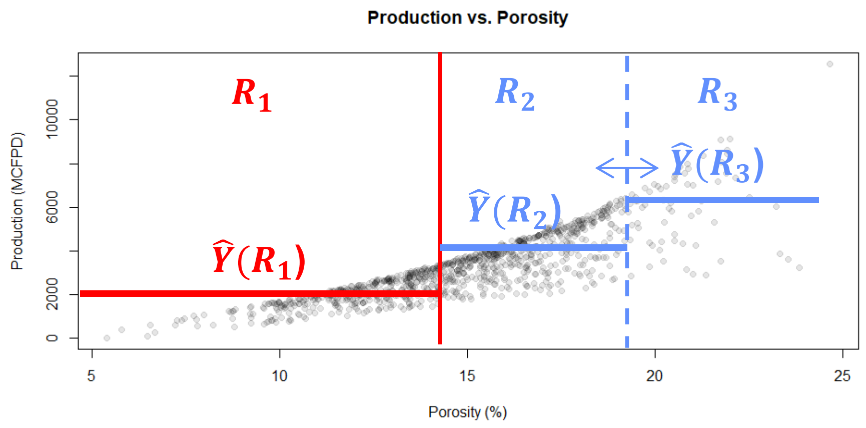
- Found first split, now check for next split the maximizes accuracy





- Search over all regions and variables, to find the next best split:



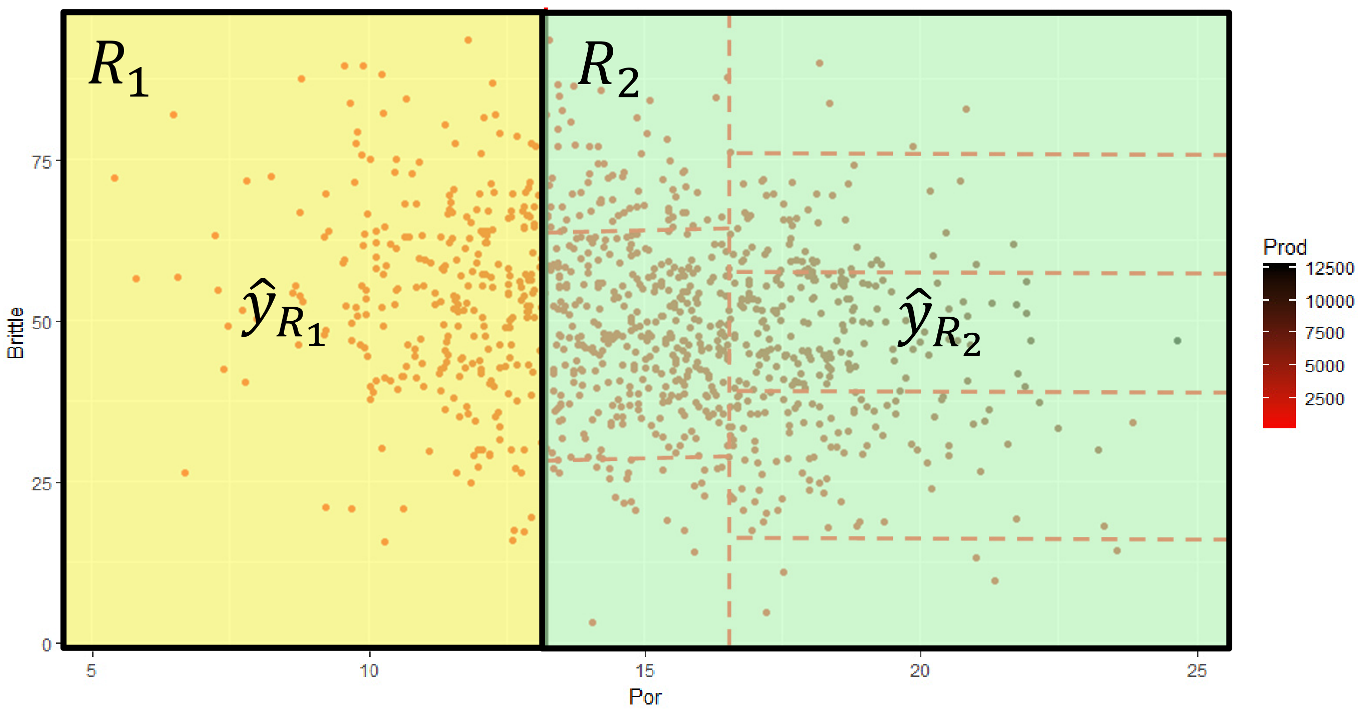


Decision Trees
The Regions

How do we construct the Regions, $R_{1,} R_2 , \dots , R_J$?

- The we continue sequentially segmenting region with threshold.
  - We will place the region boundaries based on a threshold, s, inside a previous

$$RSS = \sum_{i:x_i \in R_1} (y_i - \hat{y}_{R_1})^2 + \sum_{i:x_i \in R_2} (y_i - \hat{y}_{R_2})^2 + \cdots + \sum_{i:x_i \in R_J} (y_i - \hat{y}_{R_J})^2$$



Prediction of unconventional well production (MCFPD) from porosity (%) and brittleness (%)

Decision Trees
The Regions

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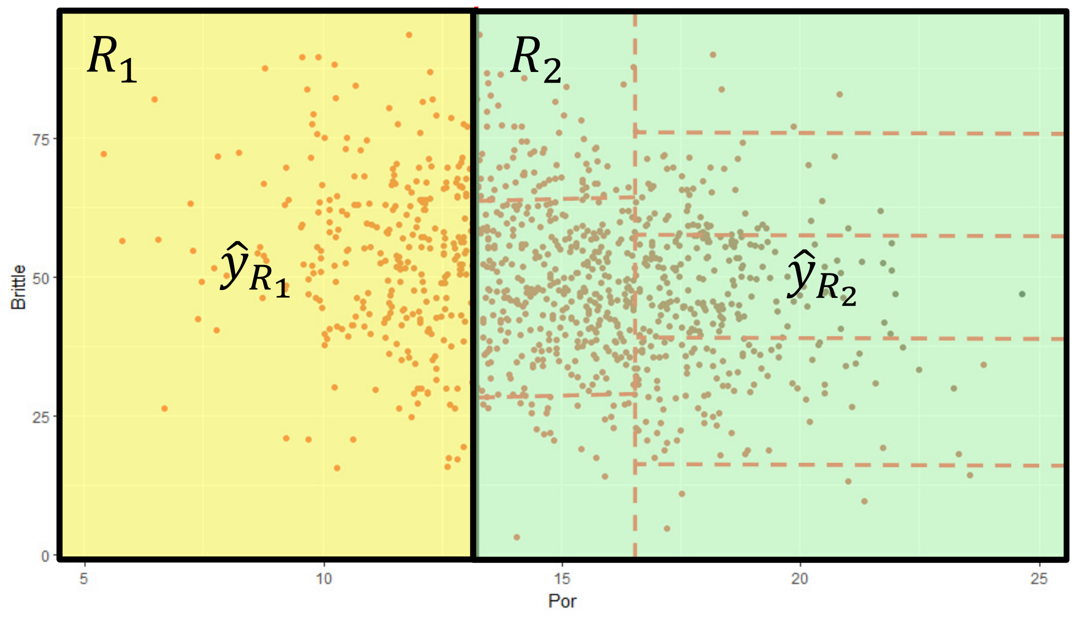

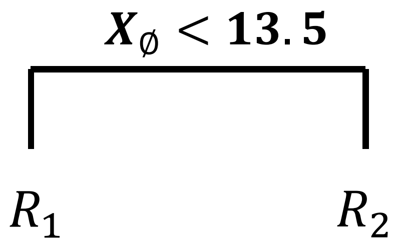

Decision Trees
The Regions

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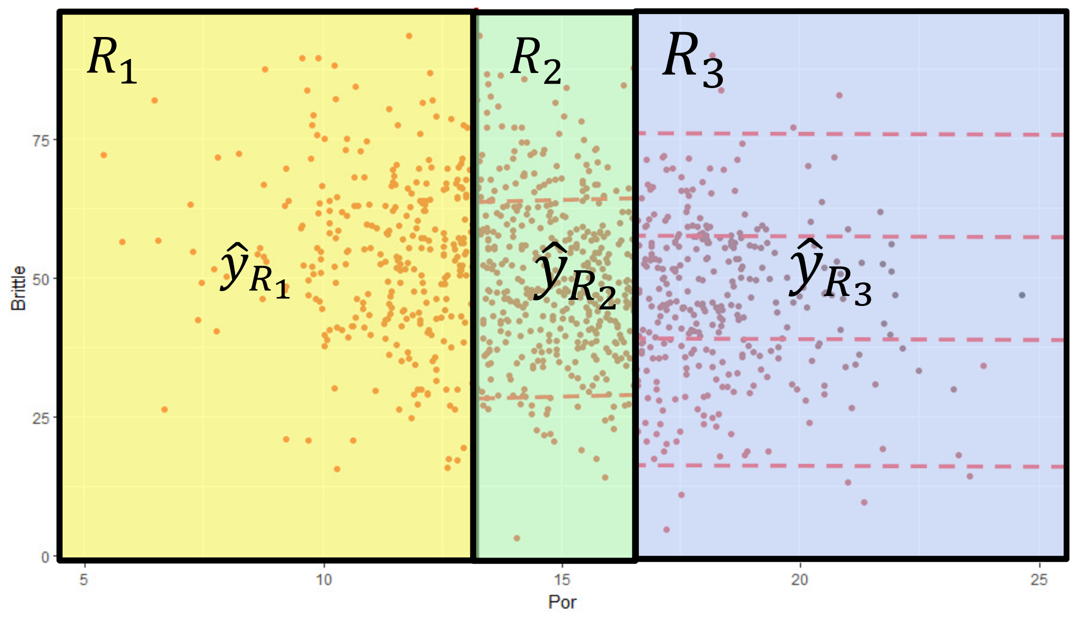

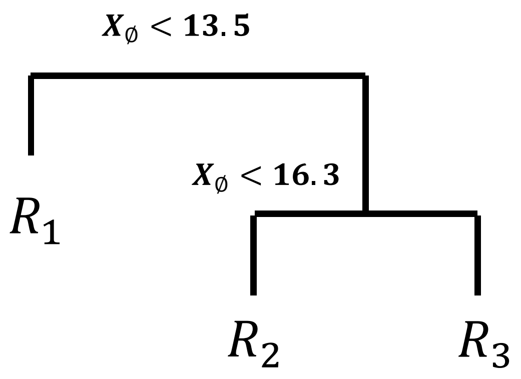

Decision Trees
The Regions

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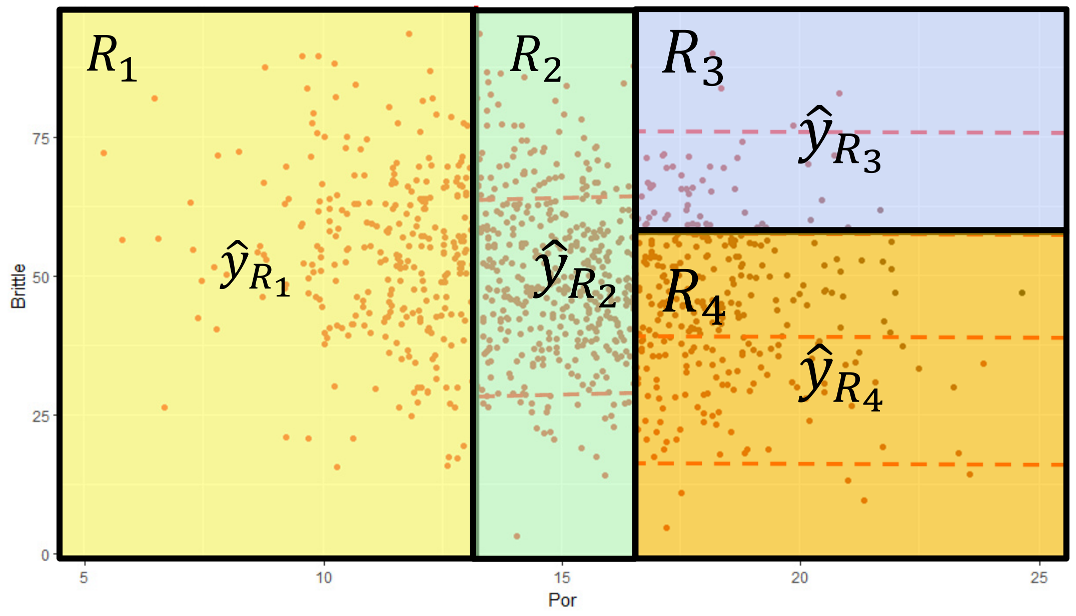
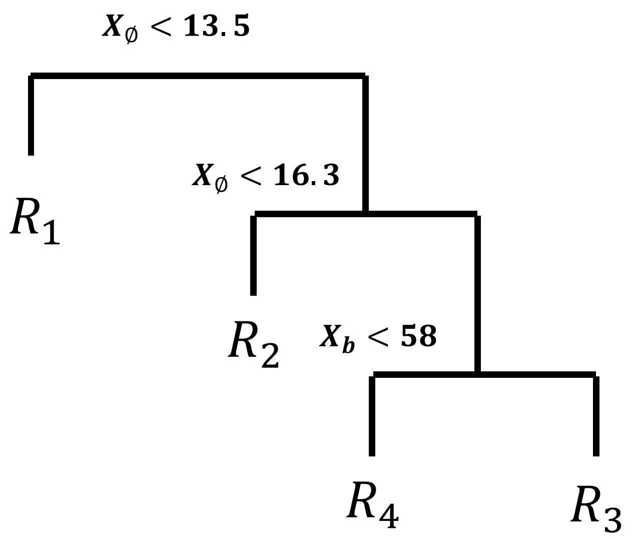


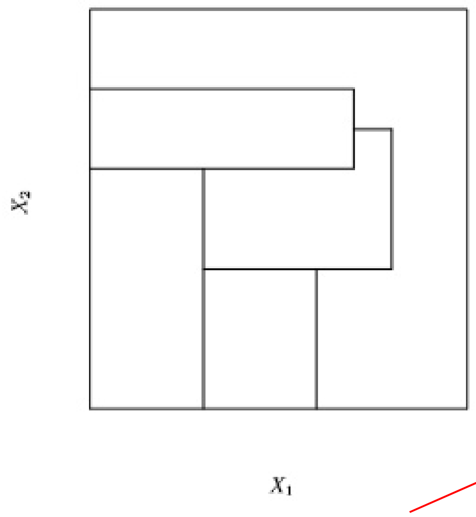


Decision Trees
The Regions

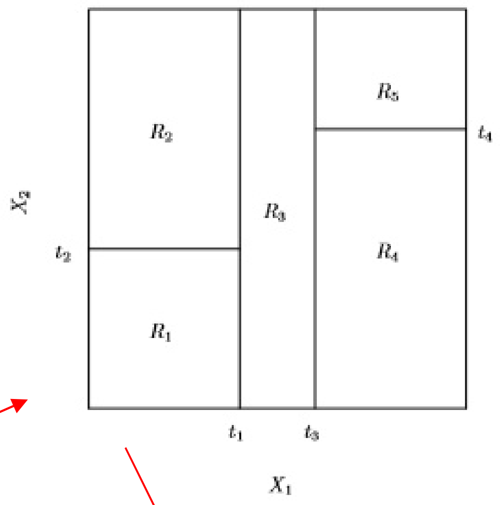
Example from James et al. (2017)

- Top-left 2D feature space partitioning that could not result from recursive binary splitting
- Top-right feature space partitioning, decision tree and estimation surface for feature space.

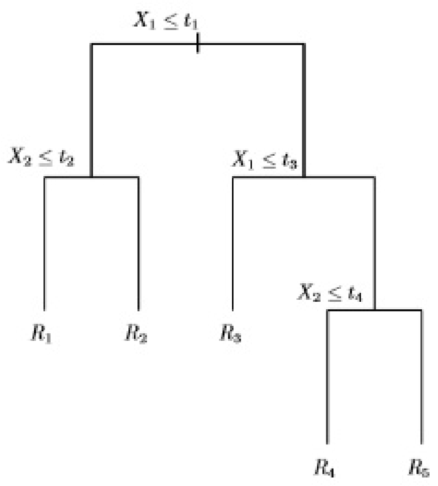
Not from recursive binary splitting



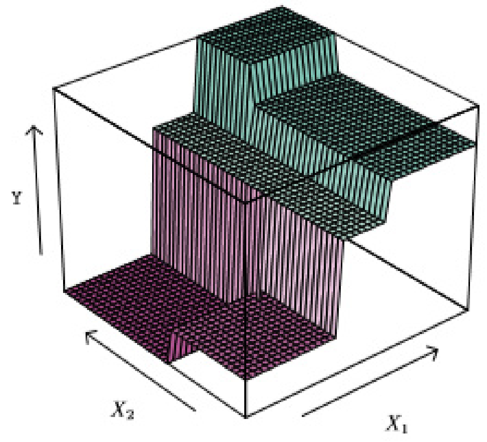
Segmented Feature Space



Decision Tree



Prediction Surface



Decision Trees Termination

When do we stop recursive binary splitting?

- We could continue until every training data value is in it’s own region!
  - This would be overfit!

- The typical approach is to apply a minimum training data in each region criteria
  - The algorithm stops when all boxes have reached the minimum

- We could continue until we cannot not significantly reduce RSS
  - But the current split could lead to an even better split $\Rightarrow$ short sighted

Decision Trees Pruning

Why do we want a less complicated tree?

- Decision trees, if allowed to grow very complicated are generally overfit.
- It is better to simplify the tree to a smaller tree with fewer splits
  - » lower model variance
  - » better interpretation
  - » with little added model bias
- Limiting tree growth with a high decrease in RSS hurdle is short sighted
- Best strategy is to build a large, complicated tree and then to prune the tree.
  - » We then select the sub tree to provides the lowest test error rate
  - » We cannot consider all possible sub trees (too vast of a solution space)

Decision Trees – Steps

Building a Regression Tree

1. Apply recursive binary splitting to train / grow a large tree with training data, stop when each terminal node has fewer than a minimum number of data or insufficient RSS decrease.
2. Obtain the sequence of best subtrees as a function of complexity (number of terminal nodes) and RSS with training.
3. Use k-fold cross validation to chose the best complexity value. Divide the training observations into K folds. For each fold, $k = 1, \ldots K$:
   a) Repeats steps from 1-2 on all training excluding those in k fold.
   b) Evaluate the RSS on the left out data in the k fold.
4. Average the error for each α (K results over each fold) and select complexity (number of terminal nodes) that provides low enough RSS.

K-fold Cross Validation

Cross Validation

- Withhold subset of the data during model training
- Then testing the trained model with withheld subset dataset
- Must make sure cross validation is fair
- Training data set (used for training), Testing data set (withheld for testing)

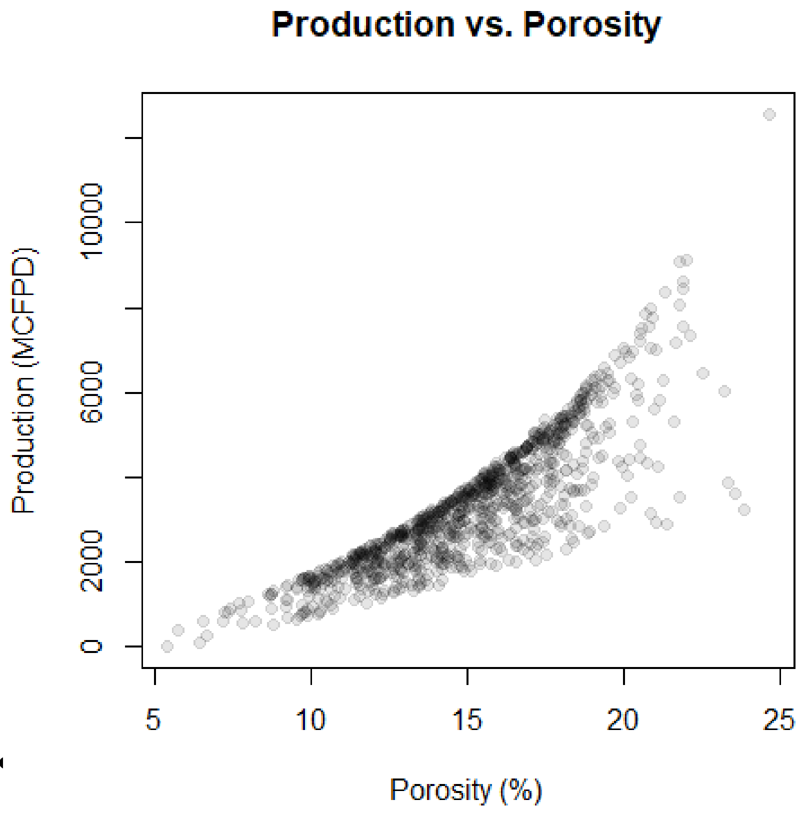
K-fold Approach

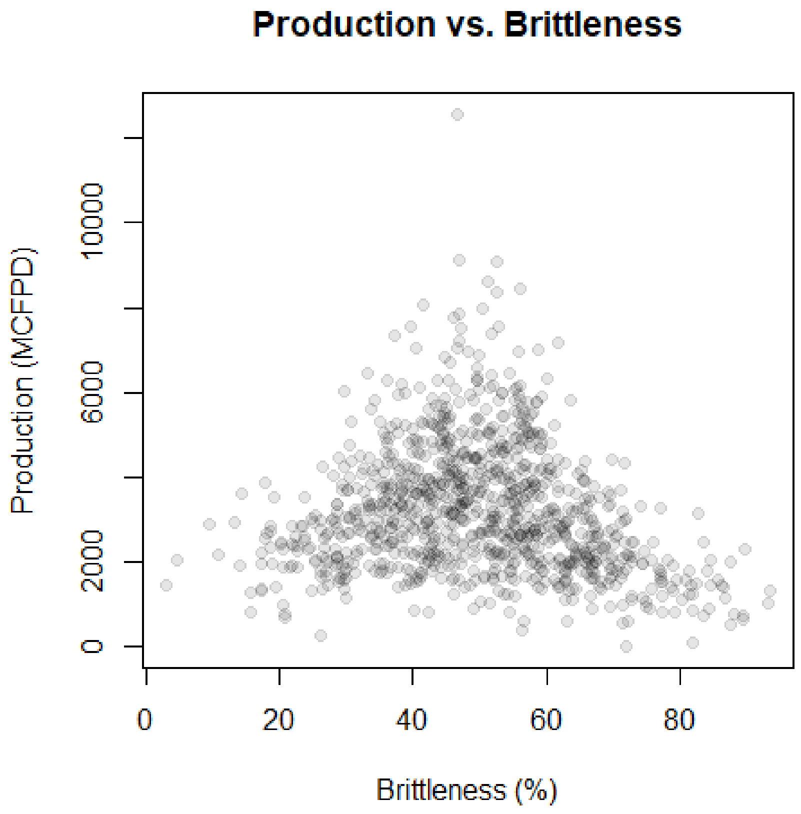
- Select K, for example
- Break data set into K subsets
- Loop over K subsets:
  - use data outside the K part to predict inside the K subset
- Average to summarize the result

Decision Trees Example

Let's use our Unconventional Multivariate Data

- We added in a production variable for prediction
- Both porosity and brittleness have interesting relationships with production

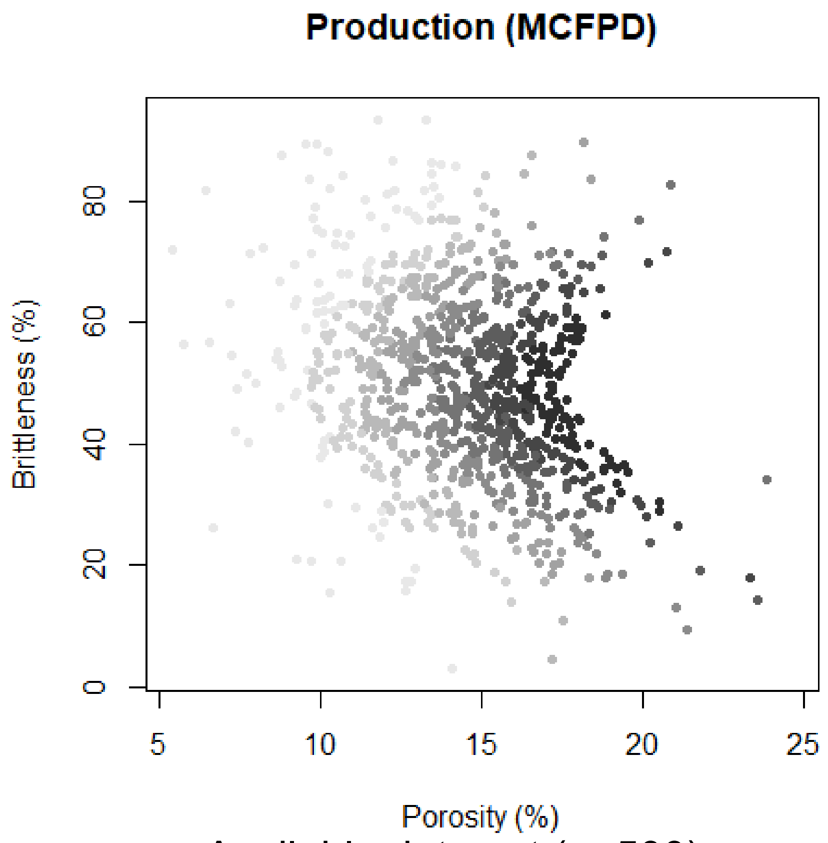




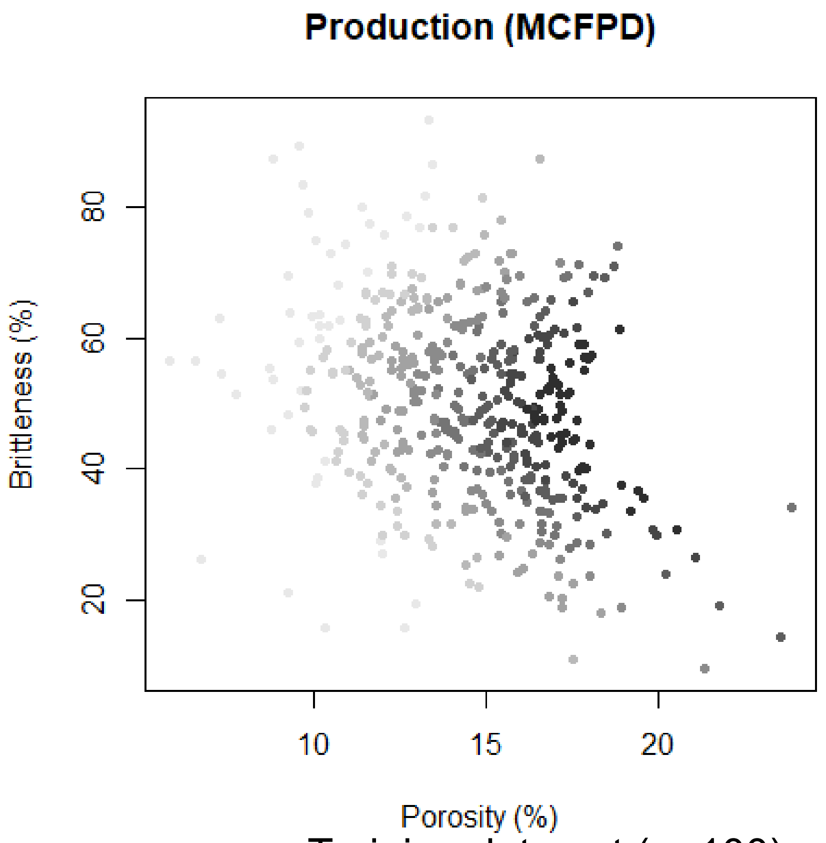
Decision Trees Example

Let's use our Unconventional Multivariate Data

- There is a complicated relationships between porosity, brittleness and production.



Available data set (n=500)

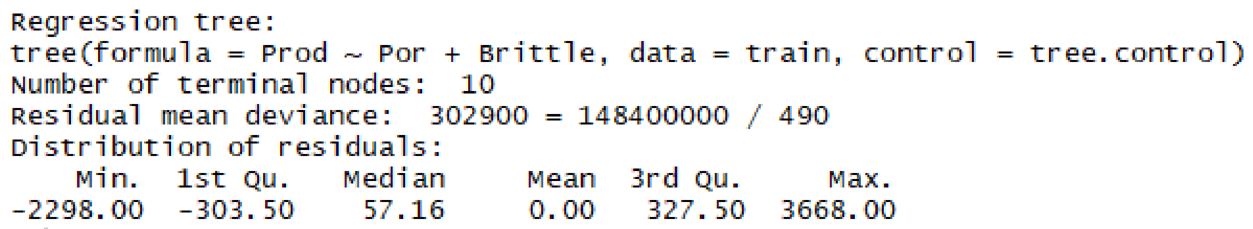


Training data set (n=100)

Decision Trees Example

Build the initial reasonably complicated tree

- By using the default tree controls we get an 10 terminal node tree.
- We can use the summary command to:



```
Regression tree:
tree(formula = Prod ~ Por + Brittle, data = train, control = tree.control)
Number of terminal nodes:  10
Residual mean deviance:  302900 = 148400000 / 490
Distribution of residuals:
    Min.  1st Qu.   Median     Mean  3rd Qu.     Max.
-2298.00  -303.50    57.16     0.00   327.50  3668.00
```

  - check the complexity of the resulting tree (number of terminal nodes)
  - check the summary statistics of the residuals and ensure that the model is not biased (mean = 0.0)
  - residual mean deviance is the total residual deviance divided by (the number of observations – number of terminal nodes)
  - for a regression trees the total residual deviance is the RSS, reminder:

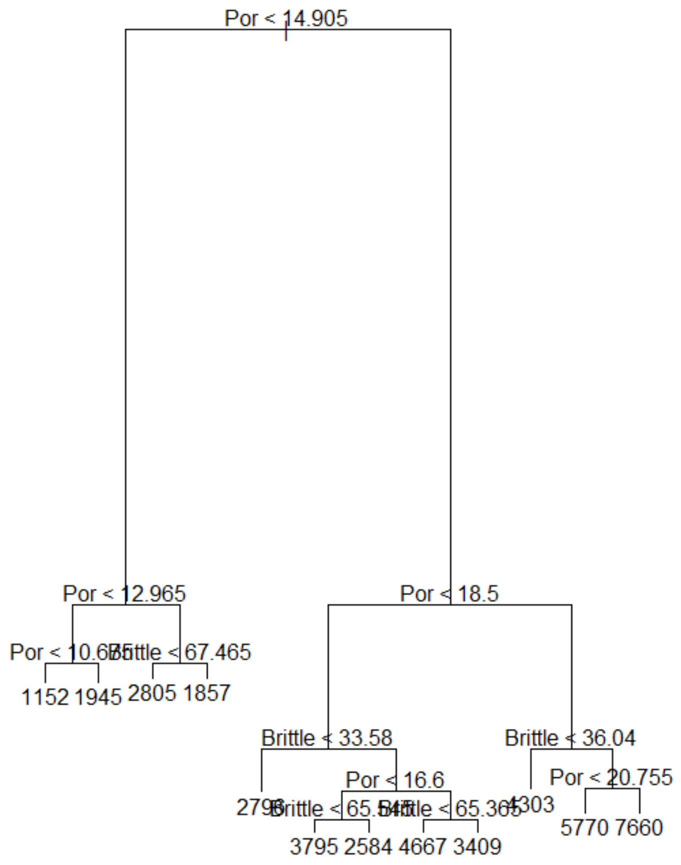
$$\text{RSS} = \sum_{j=1}^{J} \sum_{i \in R_j} (y_i - \hat{y}_{R_j})^2$$

Decision Trees Example

Build the initial reasonably complicated tree

Here's the tree:

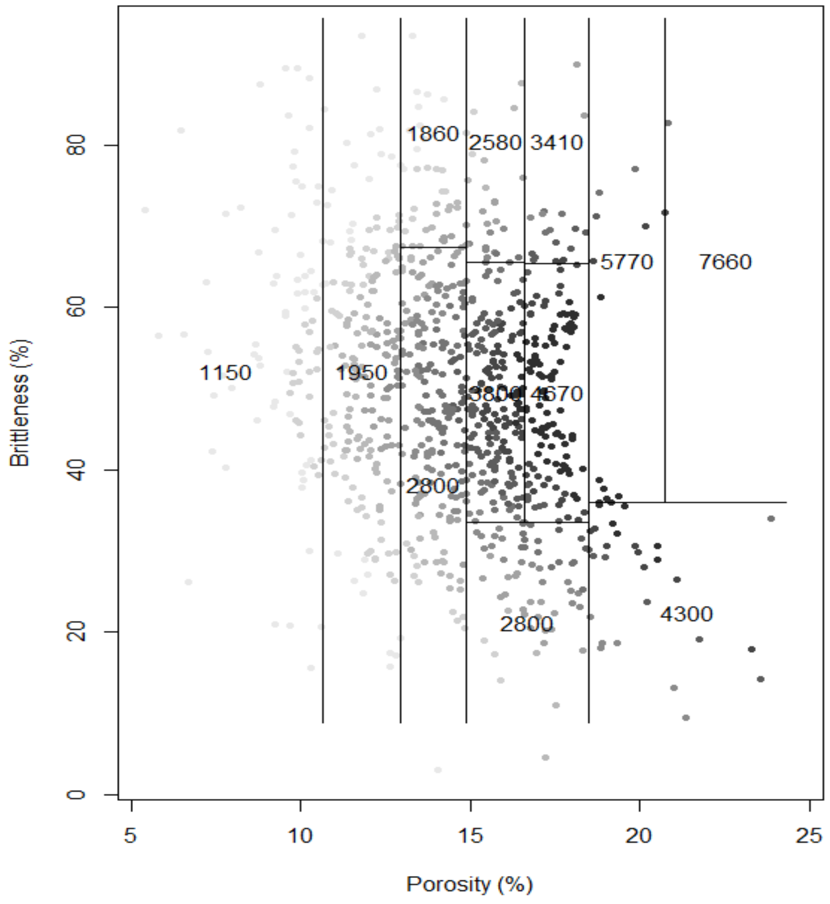
- first choice is porosity < or > 14.9%
- we get to the 3rd decision before brittleness is considered
- length of the branches is proportional to decrease in impurity
    - decress in RSS of the model for regression tree
    - a measure of node heterogeneity for classification trees



Decision Trees Example

Build the initial reasonably complicated tree

- We can plot the original data and the binary recursive boundaries outlining the various regions and the mean values in each region used as the estimate.

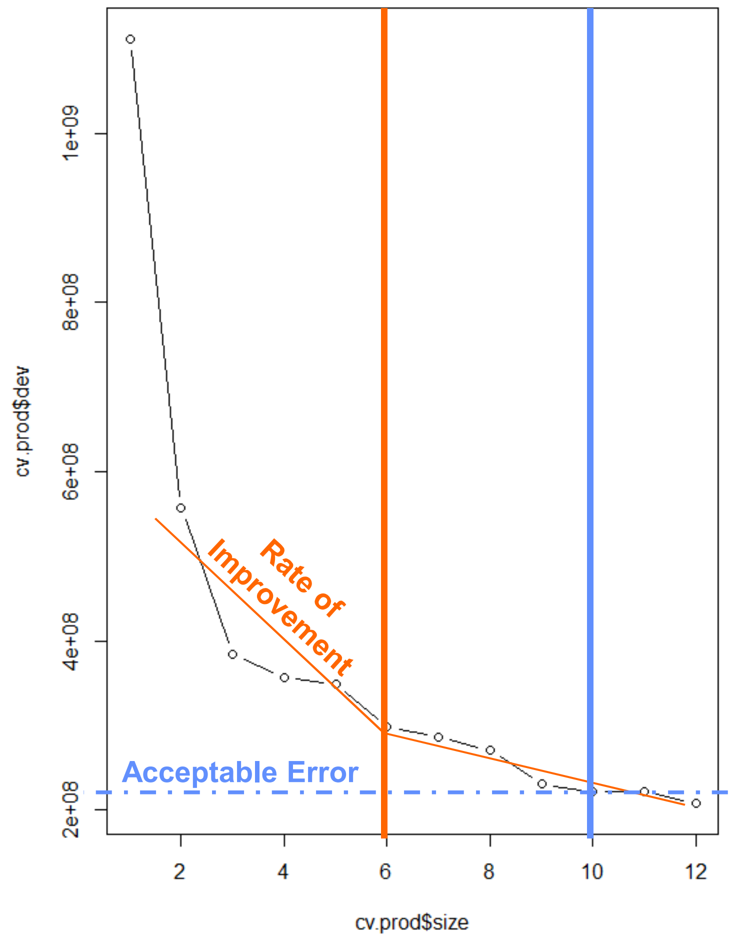


Decision Trees Example

Build the initial reasonably complicated tree

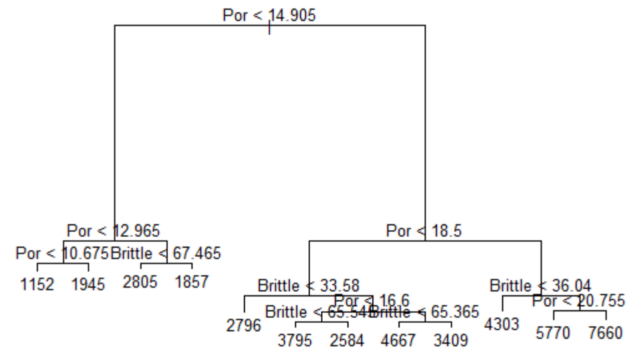
Then we perform k fold cross validation.

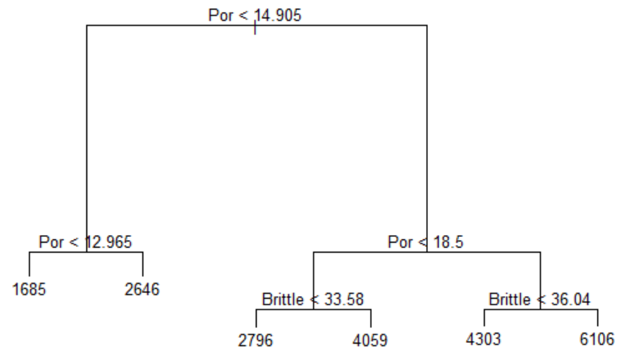
- Decrease tree complexity from 12 nodes (current model) to 1 node (uniform model)
- Calculate the RSS by averaging over k folds of the training data
- We can observed that each additional node improves the model
- Prune complexity based on:
  - Diminishing returns
  - Acceptable level of error

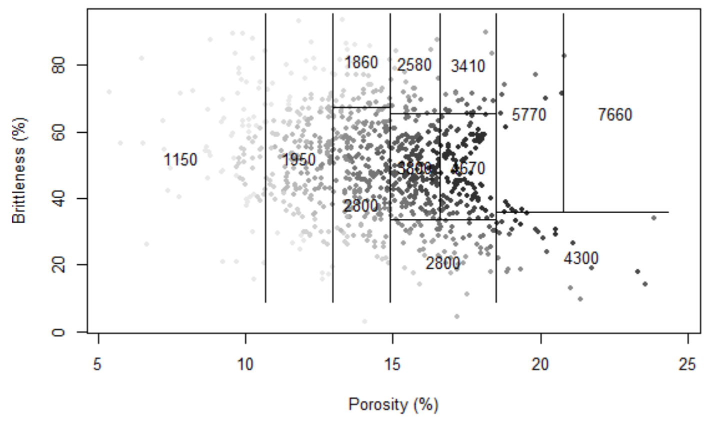


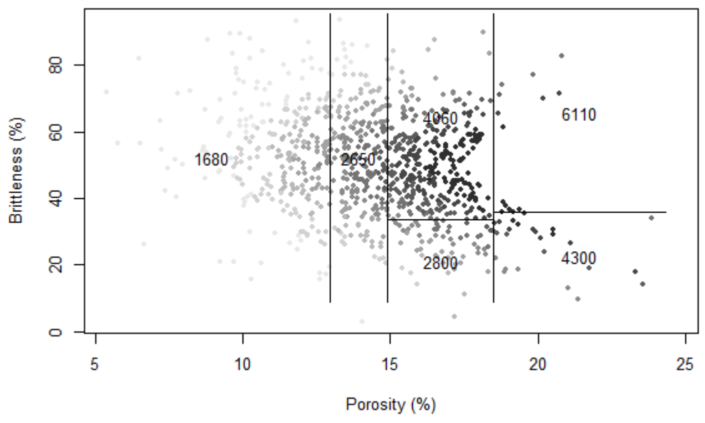
Decision Trees Example

Original and pruned tree:



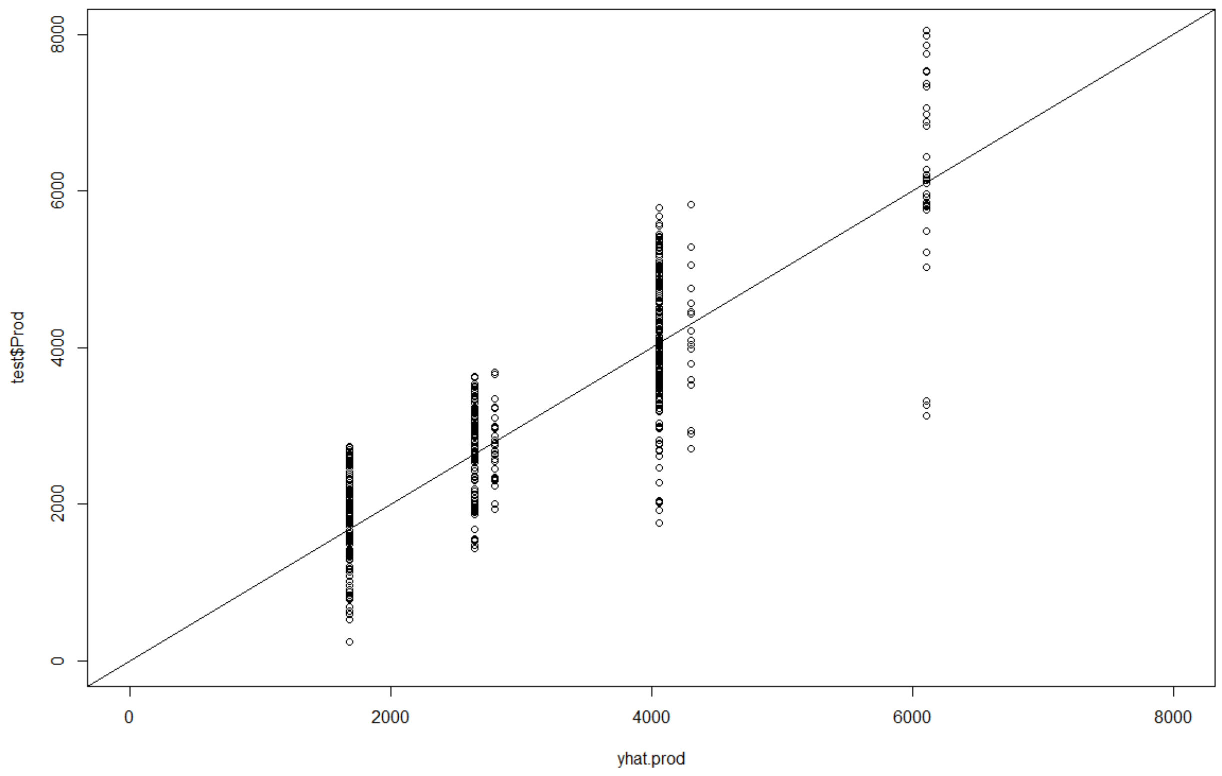






Decision Trees Example

Cross validation with the testing data set



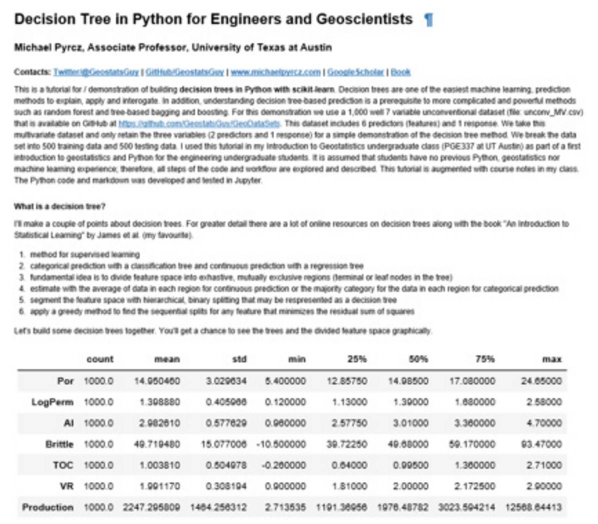
- Note: the binning due to estimation with the mean of only 6 regions
- We can calculate MSE to assess model accuracy

Decision Trees Demonstration in Python

Decision Tree Tutorial with Subsurface Demonstration in **Python** for Geoscientists and Geo-engineers

Michael Pyrcz, University of Texas at Austin (@GeostatsGuy)

Decision Tree is one of the most simple, explainable and interpretable predictive models in machine learning; therefore, it is a great introduction to regression and classification with machine learning. In addition, the recursive binary segmentation is analogous to human decision making. Finally, understanding a decision tree is a prerequisite for more powerful bagging, random forest and boosting. This tutorial is in Jupyter with Markdown and a realistic unconventional dataset. There is enough documentation that any geoscientists or engineer should be able to try out machine learning.



Decision Tree in Python for Engineers and Geoscientists ¶

Michael Pyrcz, Associate Professor, University of Texas at Austin

Contacts: Twitter/@GeostatsGuy | GitHub/GeostatsGuy | www.michaelpyrcz.com | GoogleScholar | Book

This is a tutorial for / demonstration of building **decision trees in Python with scikit-learn**. Decision trees are one of the easiest machine learning, prediction methods to explain, apply and interogate. In addition, understanding decision tree-based prediction is a prerequisite to more complicated and powerful methods such as random forest and tree-based bagging and boosting. For this demonstration we use a 1,000 well 7 variable unconventional dataset (file: unconv_MV.csv) that is available on GitHub at https://github.com/GeostatsGuy/GeoDataSets. This dataset includes 6 predictors (features) and 1 response. We take this multivariate dataset and only retain the three variables (2 predictors and 1 response) for a simple demonstration of the decision tree method. We break the data set into 500 training data and 500 testing data. I used this tutorial in my Introduction to Geostatistics undergraduate class (PGE337 at UT Austin) as part of a first introduction to geostatistics and Python for the engineering undergraduate students. It is assumed that students have no previous Python, geostatistics nor machine learning experience; therefore, all steps of the code and workflow are explored and described. This tutorial is augmented with course notes in my class. The Python code and markdown was developed and tested in Jupyter.

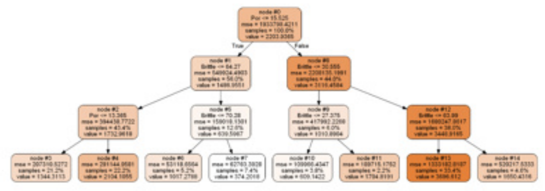
What is a decision tree?

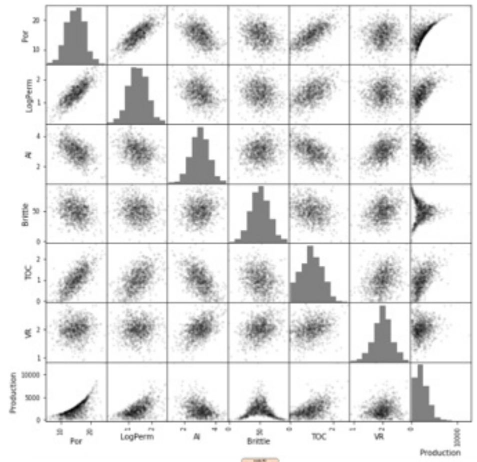
I'll make a couple of points about decision trees. For greater detail there are a lot of online resources on decision trees along with the book "An Introduction to Statistical Learning" by James et al. (my favourite).

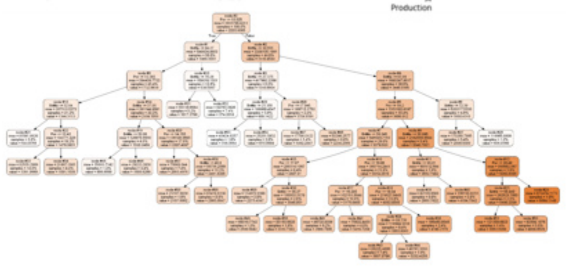
1. method for supervised learning
2. categorical prediction with a classification tree and continuous prediction with a regression tree
3. fundamental idea is to divide feature space into exhastive, mutually exclusive regions (terminal or leaf nodes in the tree)
4. estimate with the average of data in each region for continuous prediction or the majority category for the data in each region for categorical prediction
5. segment the feature space with hierarchical, binary splitting that may be respresented as a decision tree
6. apply a greedy method to find the sequential splits for any feature that minimizes the residual sum of squares

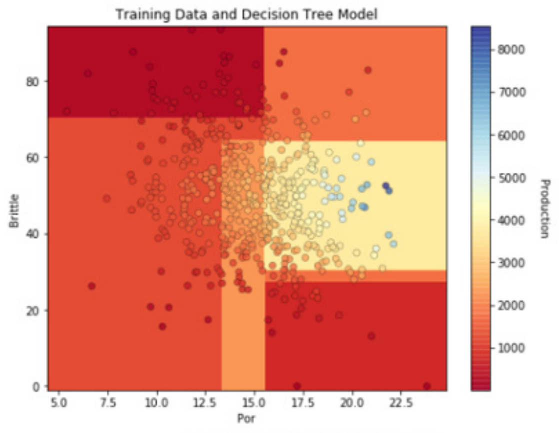
Let's build some decision trees together. You'll get a chance to see the trees and the divided feature space graphically.

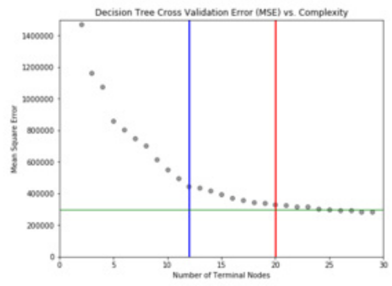
	count	mean	std	min	25%	50%	75%	max
Por	1000.0	14.950460	3.029634	5.400000	12.85750	14.98500	17.080000	24.65000
LogPerm	1000.0	1.398880	0.405966	0.120000	1.13000	1.39000	1.680000	2.58000
AI	1000.0	2.982610	0.577629	0.960000	2.57750	3.01000	3.360000	4.70000
Brittle	1000.0	49.719480	15.077006	-10.500000	39.72250	49.68000	59.170000	93.47000
TOC	1000.0	1.003810	0.504978	-0.260000	0.64000	0.99500	1.360000	2.71000
VR	1000.0	1.991170	0.308194	0.900000	1.81000	2.00000	2.172500	2.90000
Production	1000.0	2247.295809	1464.256312	2.713535	1191.36956	1976.48782	3023.594214	12568.64413











Decision Trees Comments

General Comments on Decision Trees

- Easy to explain
- Analog to human decision making
- Graphically displayed
- Continuous or categorical variables

- Lower predictive accuracy than other machine learning methods
- Model bias may be high

PGE 383 Lecture 26
Machine Learning - PCA

- Decision Tree
- Ensemble Methods

Michael Pyrcz, The University of Texas at Austin

Machine Learning

Introduction

Prerequisites

Data Preparation

Univariate Analysis

Multivariate Analysis

Spatial Characterization

Spatial Estimation

Spatial Simulation

Uncertainty Analysis

Model Checking

Decision Making

Bagging, Random Forest and Boosting

These are all methods to improve the prediction accuracy of trees

- Bagging (used with many types of models)
  - the use of bootstrap on the training dataset to get B training sets
  - train a tree on each data set
  - then use all models and average the result to get the prediction

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

  - the trees are allowed to grow large
  - 100s to 1,000s of trees (forest of mediocre estimates!)
  - classification by majority vote
  - out-of-bag data (about 1/3 for each tree) are used as a test data set!

Bagging, Random Forest and Boosting

These are all methods to improve the prediction accuracy of trees

- Random Forest
  - same as bagging, but we randomize selection of on about $\sqrt{m}$ of the features!
  - prevents a single strong predictor form dominating the entire set of trees – forces diversity among the trees
  - decorrelating the trees

Bagging, Random Forest and Boosting

These are all methods to improve the prediction accuracy of trees

- Boosting (used with many types of models)
  - sequential modeling of a simple tree
  - build a tree, calculate residual
  - build a tree to model residual from 1st tree
  - build a tree to model the residual from 2nd tree
  - etc.

Summary

Short Summary of:

- Decision Trees