Decision trees

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MSDS program

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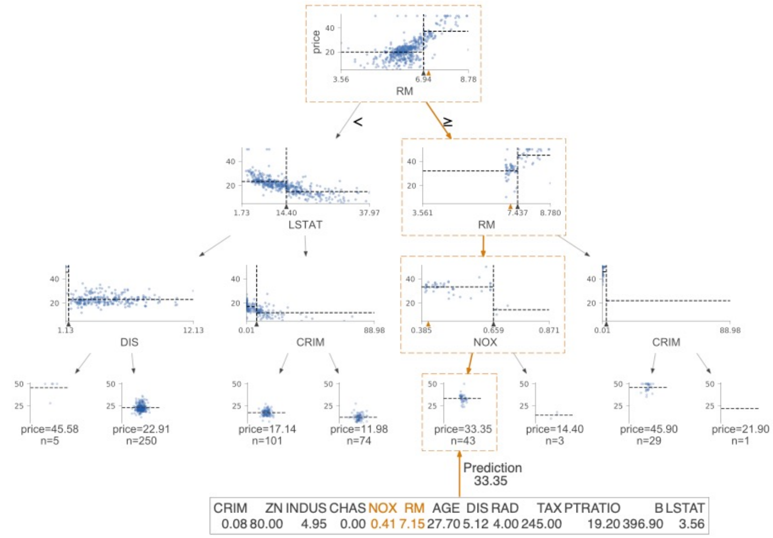
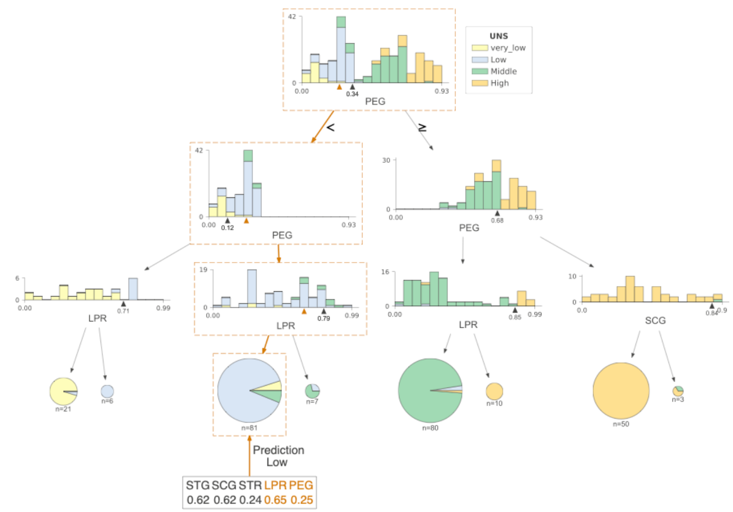
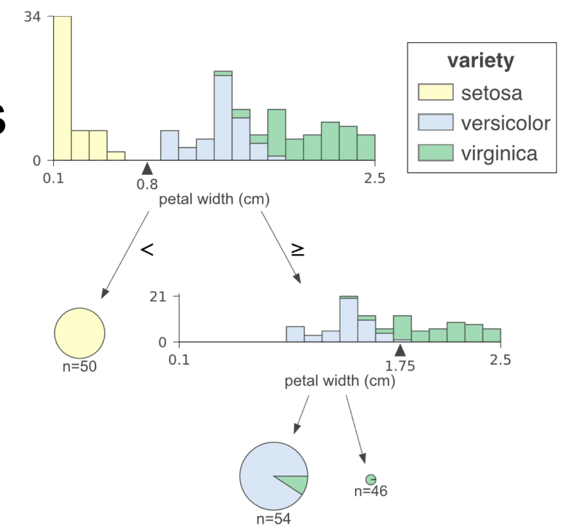




The essence of decision trees

- Decision trees are like *kNN,* but with rectangular not polygonal hypervolumes, dynamic *k* not fixed *k* (based on regions not points)
- Partition feature space into tight rectangular hypervolumes of feature space with constraint that we want y values to be as pure/similar as possible for records in that hypervolume
- Not so tight that the hypervolumes have too few feature vectors (records/samples), which tends to overfit the training data
- Prediction for unknown vector:
  - predict the mean y for training samples in that hypervolume (regression)
  - predict the mode (most common) y in that hypervolume (classification)
- Binary trees just happen to be an efficient implementation

Basic properties of decision tree models



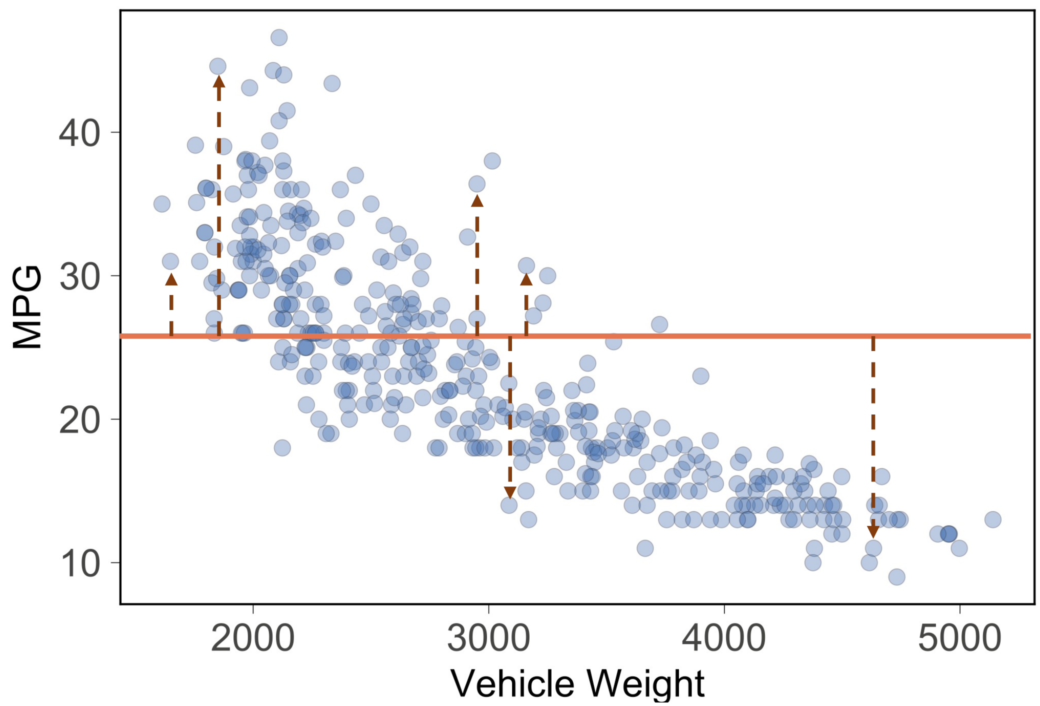
- Decision trees consist of internal decision nodes and leaf nodes that make predictions
- Each input record (feature vector) is contained in exactly one leaf node
- Each leaf has 1 or more records whose y's are as pure as possible (model hyperparameters affect number of records per leaf)
- Prediction proceeds from root to leaf, testing var/value combos
- Regressor: leaf predicts average of y for associated records
- Classifier: leaf predicts mode (most common) class

Most images in these slides from package https://github.com/parrt/dtreeviz

Let’s reinvent decision trees

Let’s create a simple regressor in 1D

Predict MPG from weight



Predict a single constant for entire region (the mean)

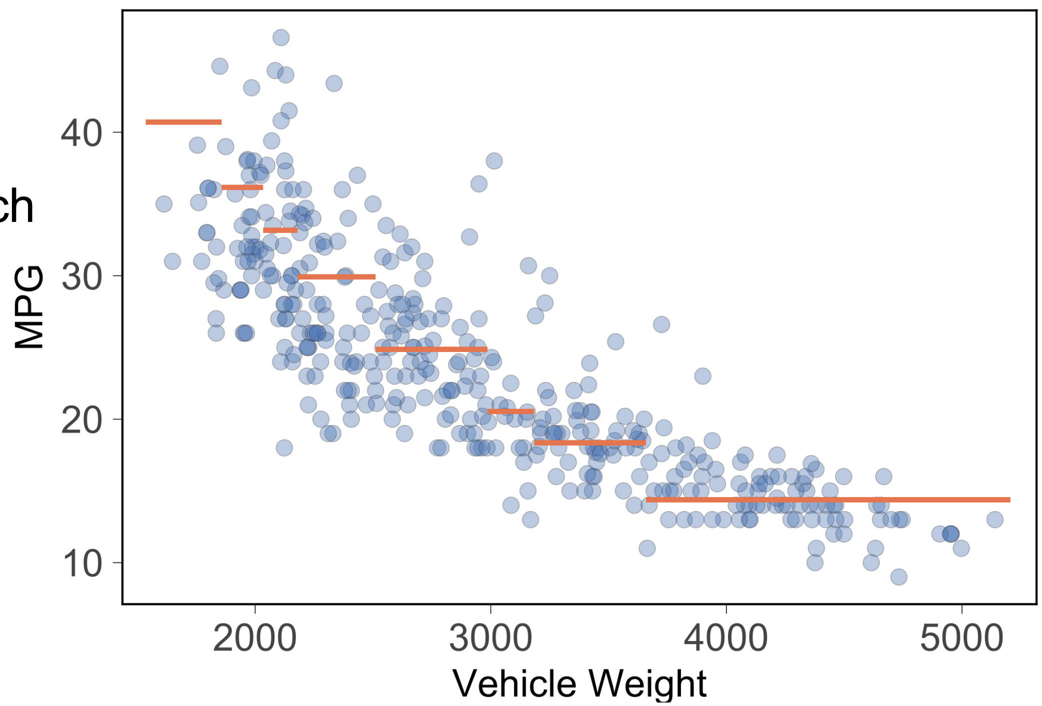
MSE is high, residual variance is high

Residuals from point to region mean

Improve by partitioning, using multiple lines

WHERE DO WE SPLIT??

Find ranges of WGT with similar MPG values, which yields a lower MSE

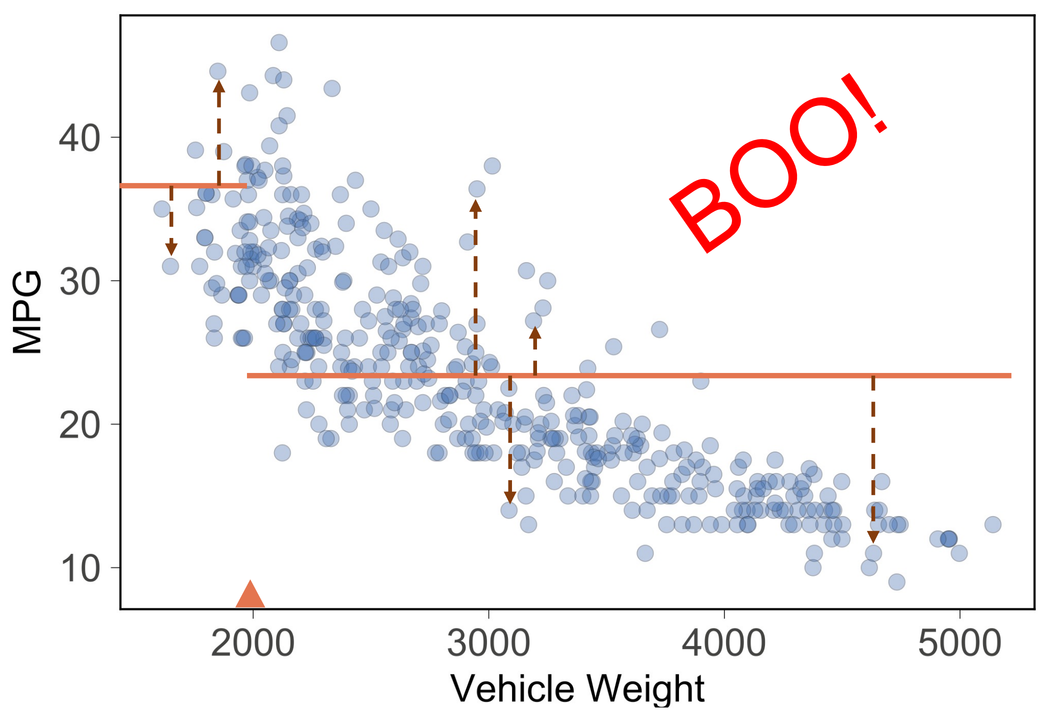


Can only use horizontal lines, but can use lots

Each region predicts mean in piecewise fashion

Strategy: find split point giving least MSE

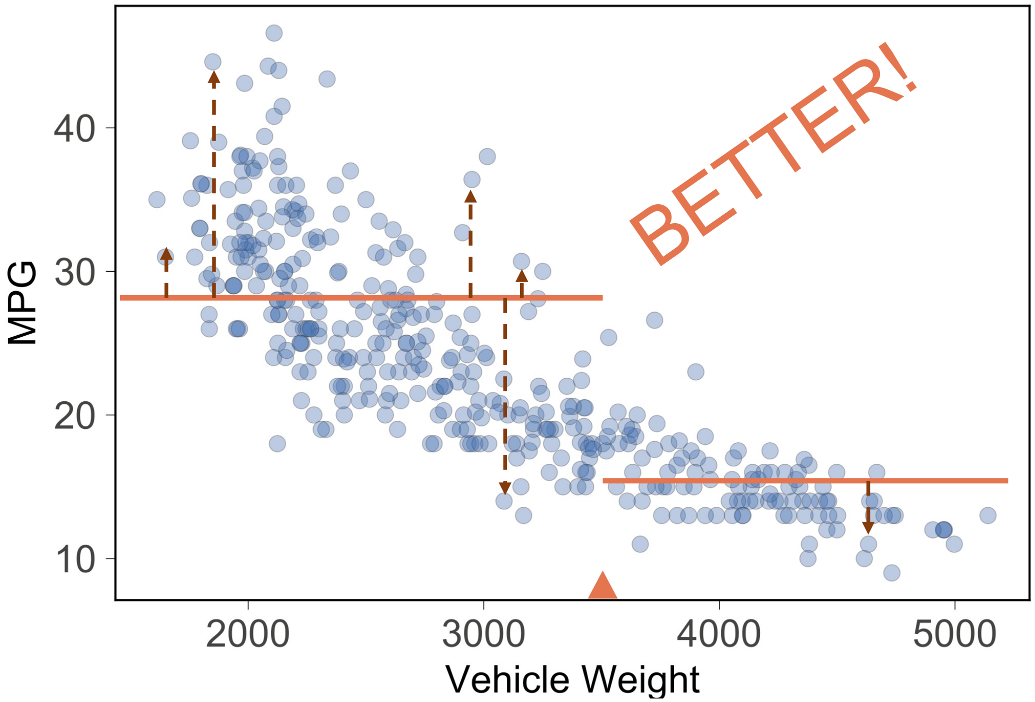
Split WGT into two subregions, each predicting mean



WGT=2000 is BAD CHOICE: MSE very high (subregion y's are still dissimilar)

Strategy: find split point giving least MSE

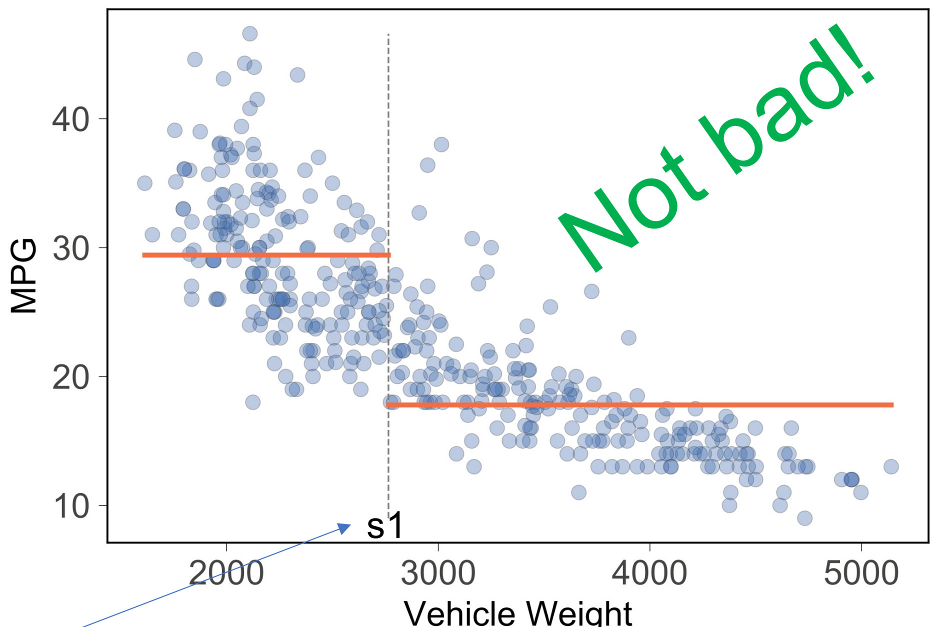
Split WGT into two subregions, each predicting mean



WGT=3500 is ANOTHER BAD CHOICE: MSE very high (still dissimilar)

Note: MSE for mean model is same as variance (average squared difference from mean)

A split exists that gives min MSE for regions



Technique: Exhaustively check all feature values, computing MSE or variance of subregions for each split

Choose split point giving min MSE

Slide s1 from left to right over x_i range, computing subregion MSE
Choose WGT location with min average MSE for subregions

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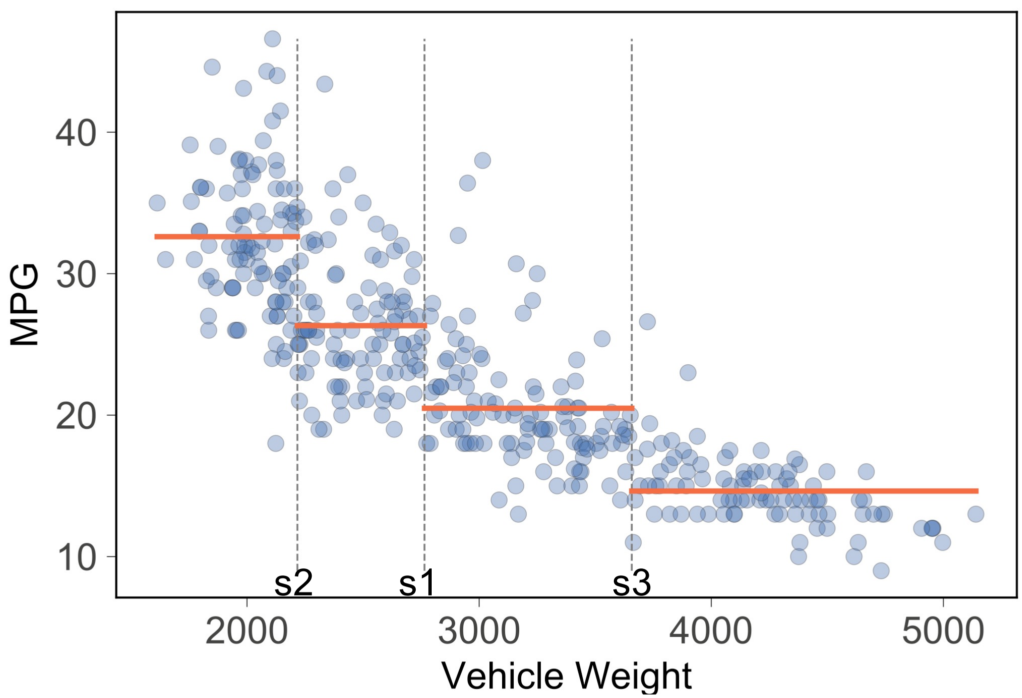
Now split those 2 regions to get 4 regions

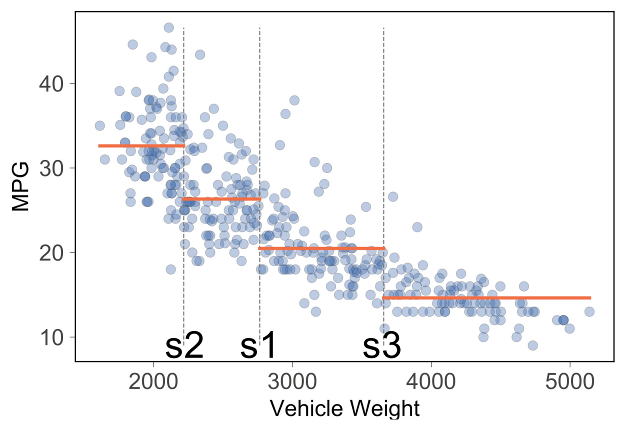


Split s1 stays, *recursively* split left/right regions to get splits s2, s3

Kinda like binary search or other divide-and-conquer strategy

Slide s2 from left to s1, computing MSEs; choose x location with min avg MSE
Slide s3 from s1 to right, computing MSEs; choose x location with min avg MSE

Recursive call-tree from model training gives regions defined by splits s1,s2,s3



s1=split(1000,5000)

s2=split(1000,s1) s3=split(s1,5000)

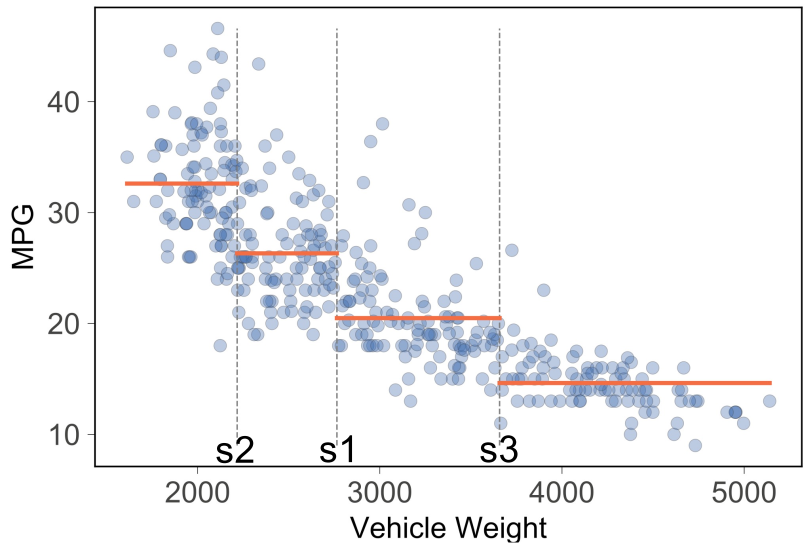
[1000,s2) [s2,s1) [s1,s3) [s3,5000)

Split (recurse) until one of:

- All potential splits do not reduce MSE
- All nodes have min num samples
- Max number of splits reached
- Etc…

Predictions are avg of MPG (target) values in subregions

Hardcoded non-tree model implementation

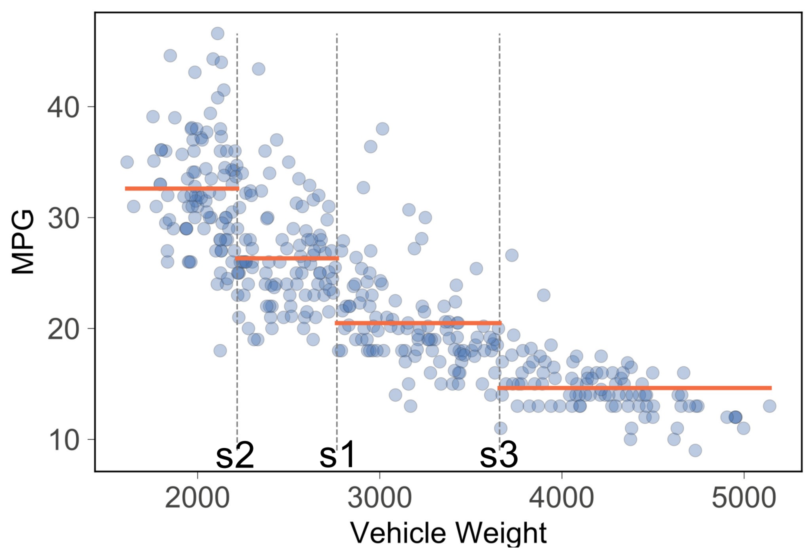


To partition space, test in recursion/split order

```
if x<s1 and x<s2: predict 32.6
if x<s1 and x>=s2: predict 26.3
if x>=s1 and x<s3: predict 20.5
if x>=s1 and x>=s3: predict 14.6
```

Note repeated comparisons!

Factor the split comparisons for efficiency




```
if x<s1:
  if x<s2: predict 32.6
  else: predict 26.3
else:
  if x<s3: predict 20.5
  else: predict 14.6
```

But, don't want to hardcode model!

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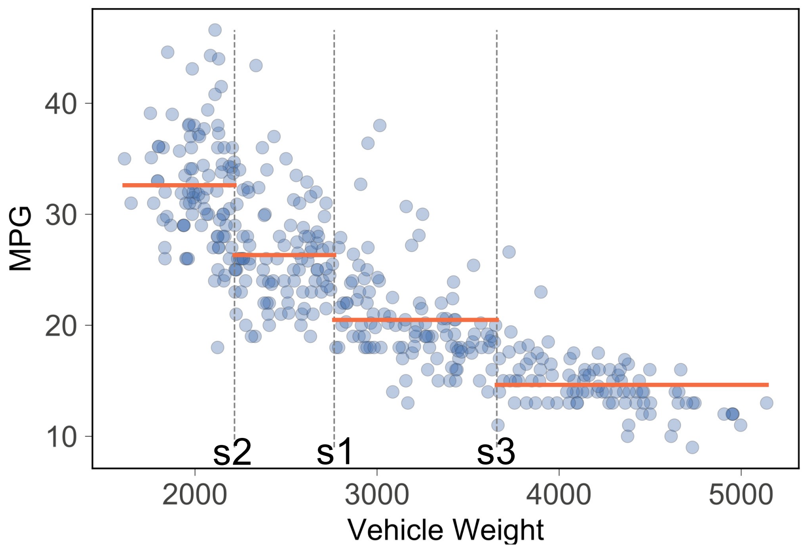
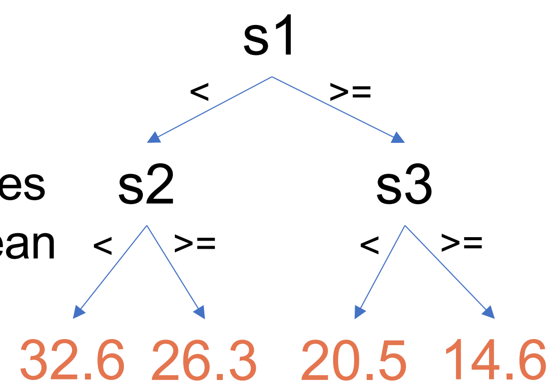
Represent nested conditionals as tree




```
if x<s1:
  if x<s2: predict 32.6
  else: predict 26.3
else:
  if x<s3: predict 20.5
  else: predict 14.6
```

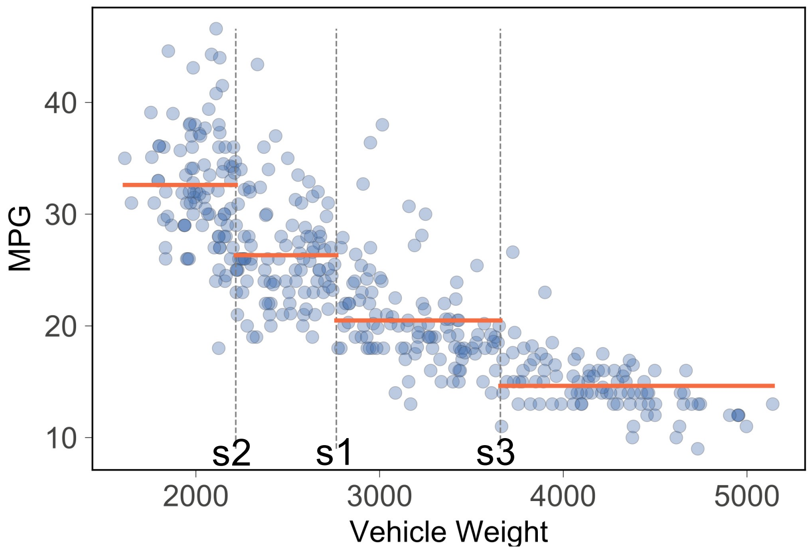
rotate 90°

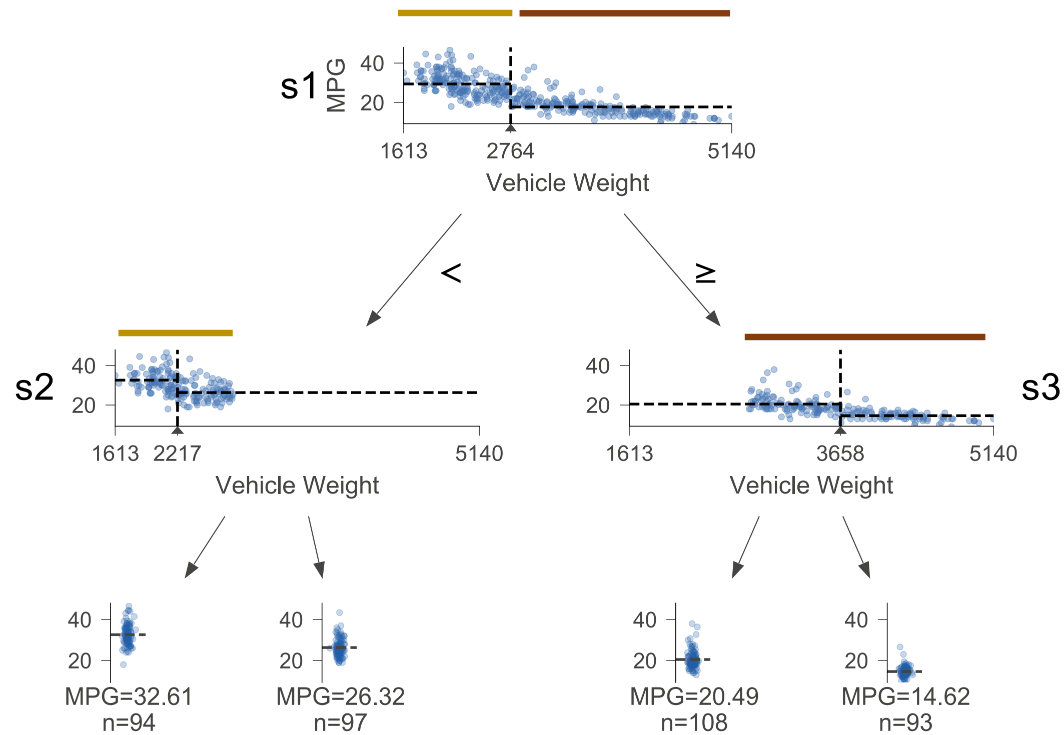
Internal nodes test features
Leaves predict region mean



We morph tree of recursion from training into decision tree!

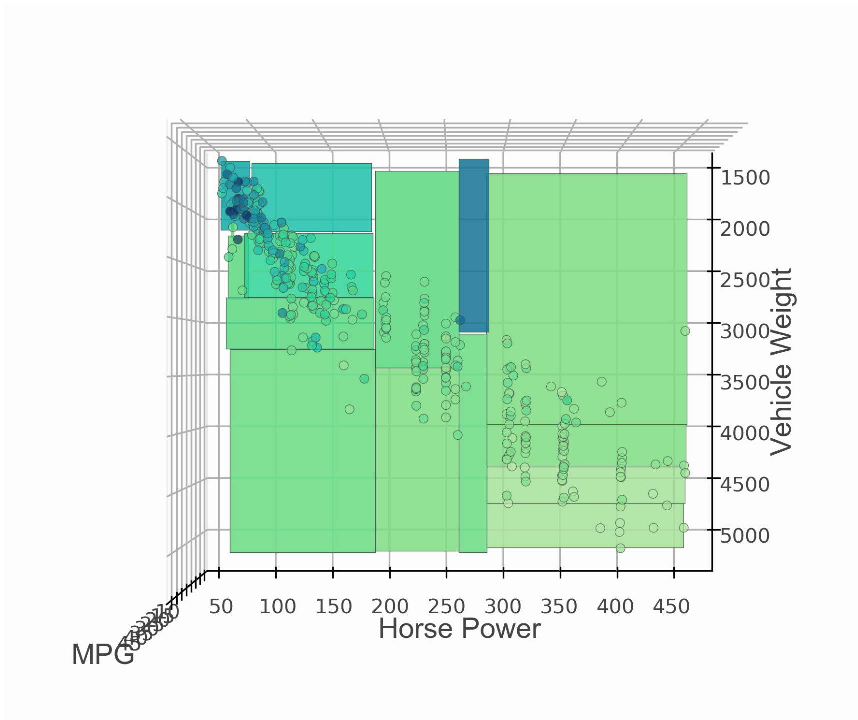
1D feature space vs `dtreeviz` decision tree





https://github.com/parrt/msds621/blob/master/notebooks/trees/partitioning.ipynb

2D regressor feature space (heatmap, 3D)



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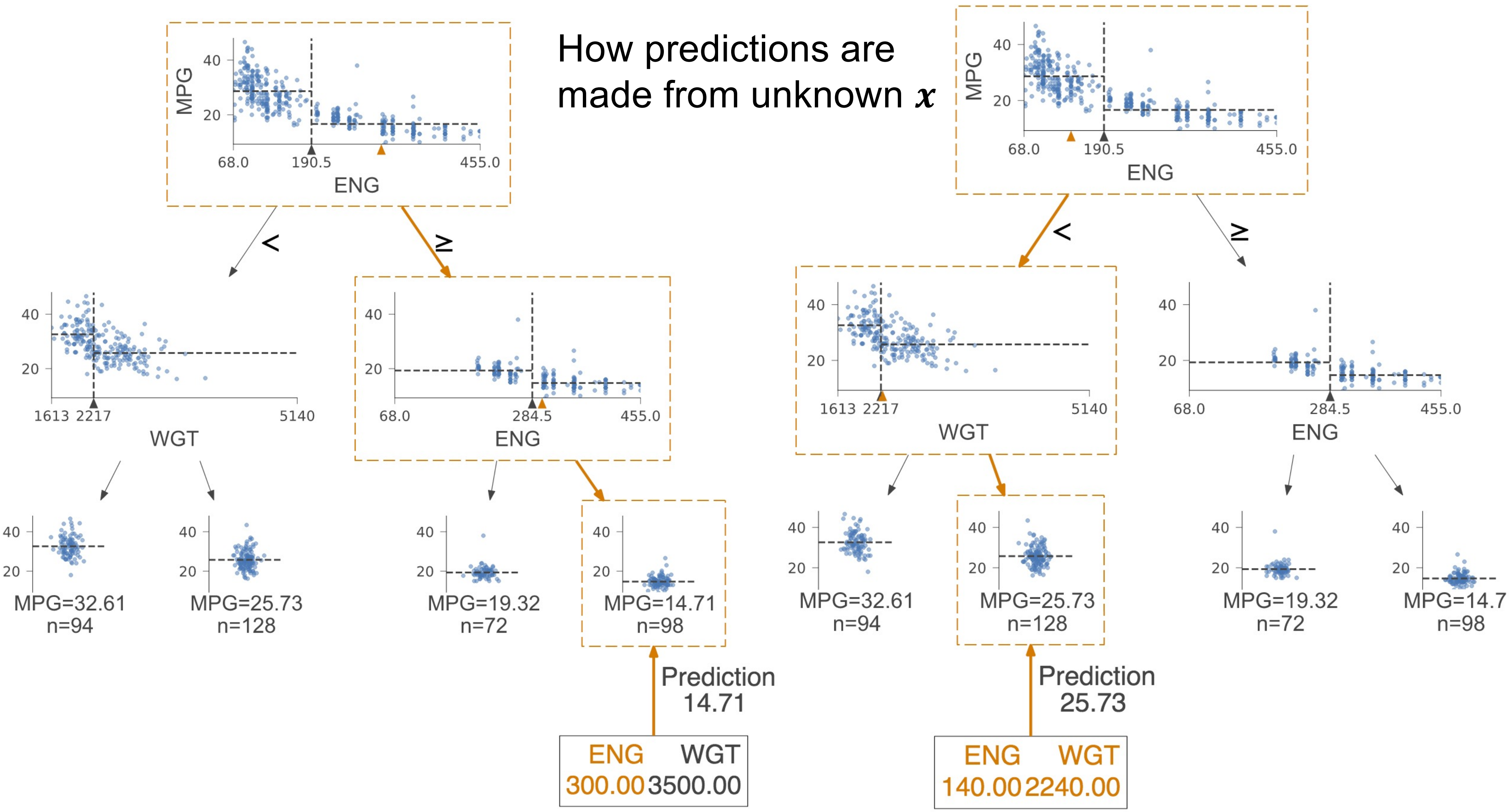
How predictions are made from unknown x



An aside: partitioning, tree viz done with custom library

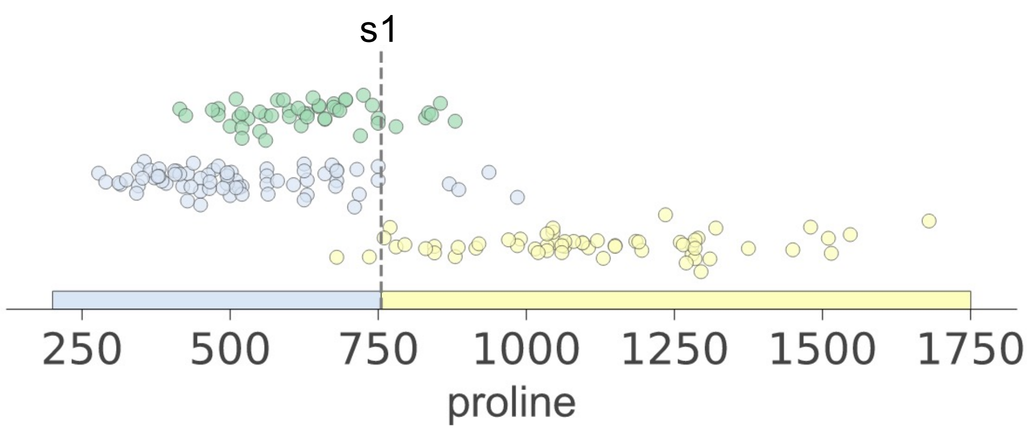
- Do "`pip install dtreeviz`"
- Partially built with Prince Grover, previous MSDS student
- See https://github.com/parrt/dtreeviz and the article for more detail: https://explained.ai/decision-tree-viz/index.html
- Advice: never accept status quo; always strive for more / better
- See "*How to lead a fulfilling life by being dissatisfied*" buried in my talk on decision tree viz https://twitter.com/the_antlr_guy/status/1120359898062000128

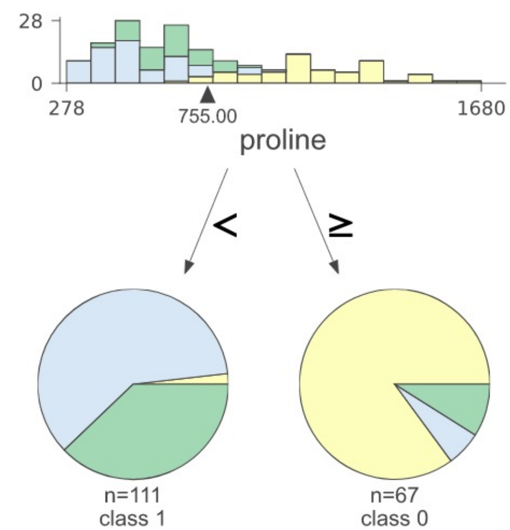
Classifiers

Classifiers split feature space too

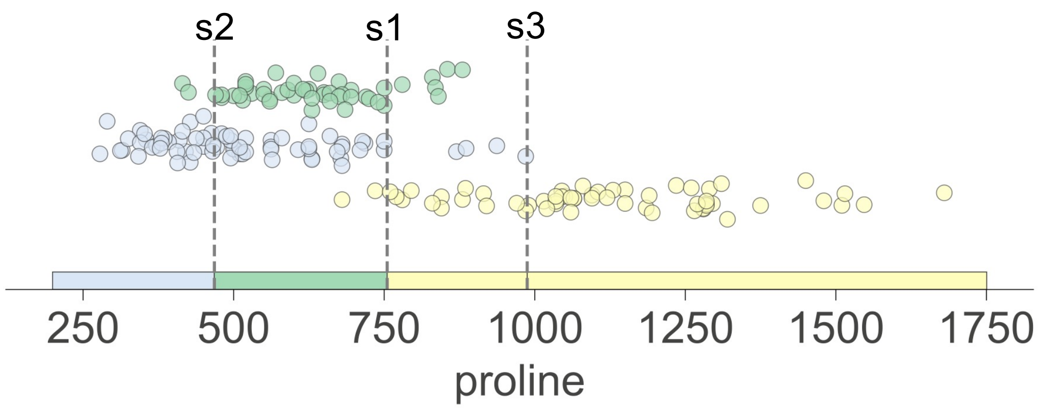
Predict wine from proline

- Internal decision nodes test features just like regressor trees
- Leaves predict most common target category (mode) not mean
- Find split that decreases average impurity of left/right subregions (we'll need a definition of impurity for categories)

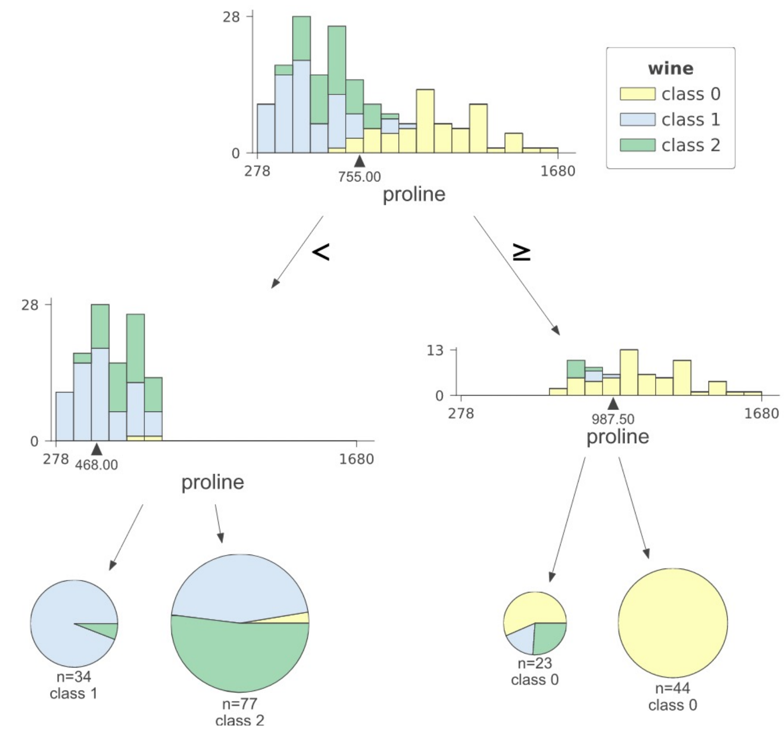




Split s1 subregions into more subregions



All splits use same proline variable



Still not very pure though

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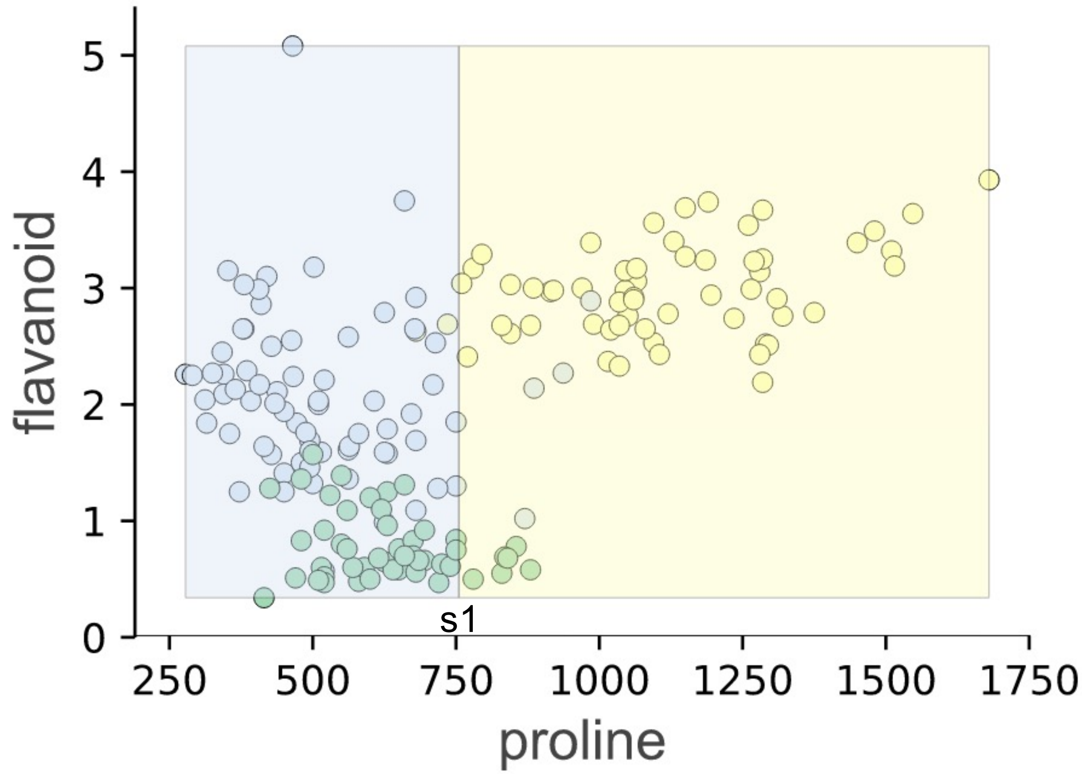
To improve predictions:
Use 2 features and
split 2D feature
space into regions



*Training looks for (feature, split point) combos giving more **pure** subregions.*

To test: decision nodes compare single feature value in subset of records to split point

To improve predictions:
Use 2 features and
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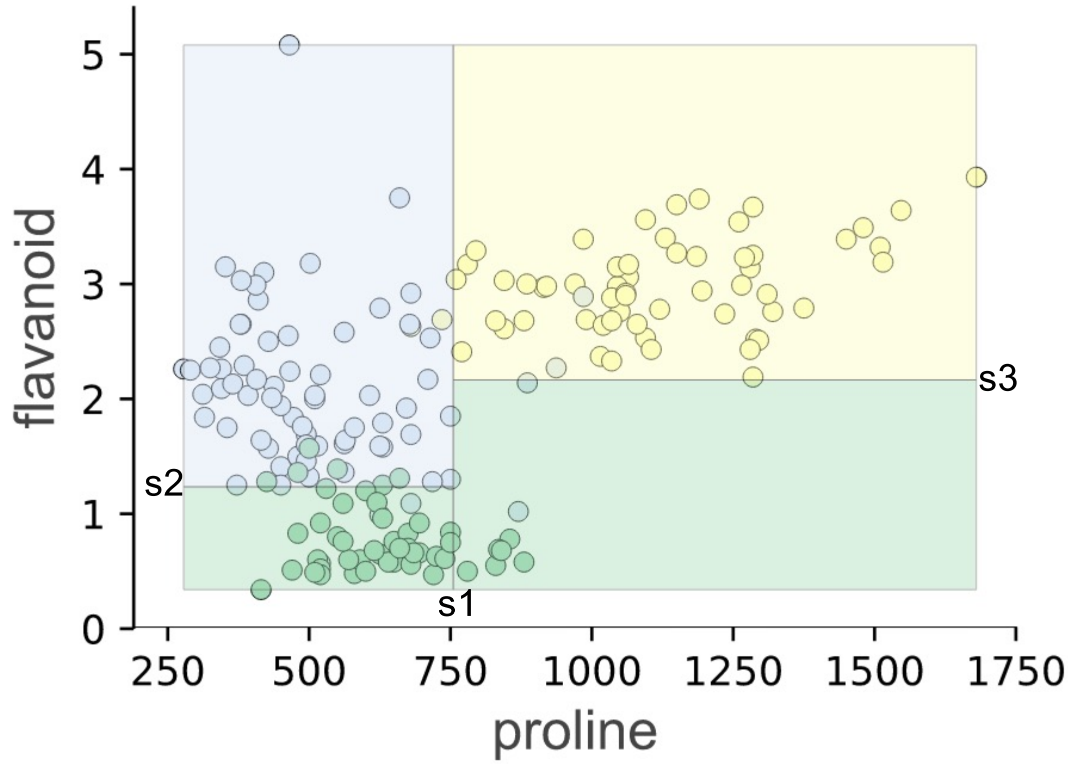
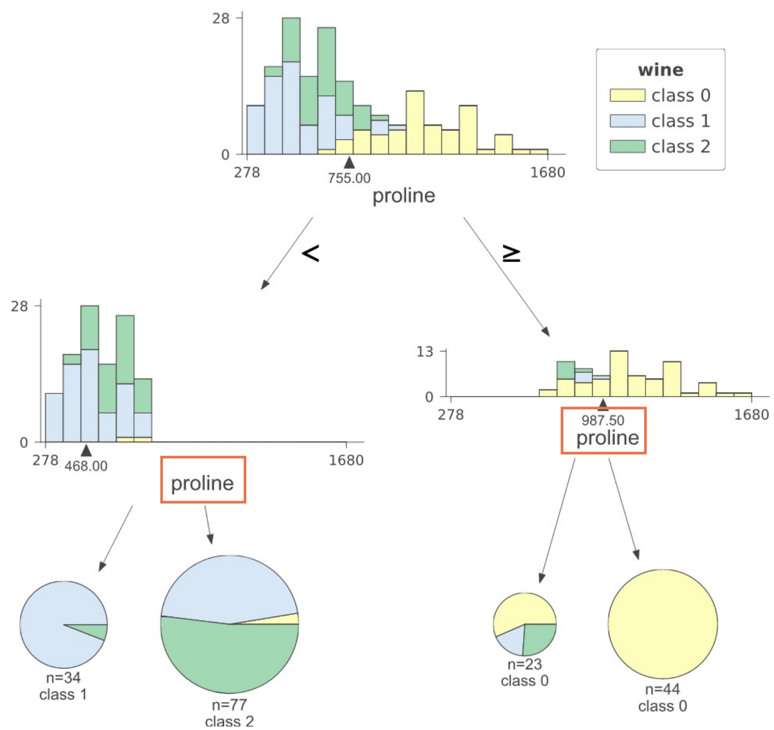


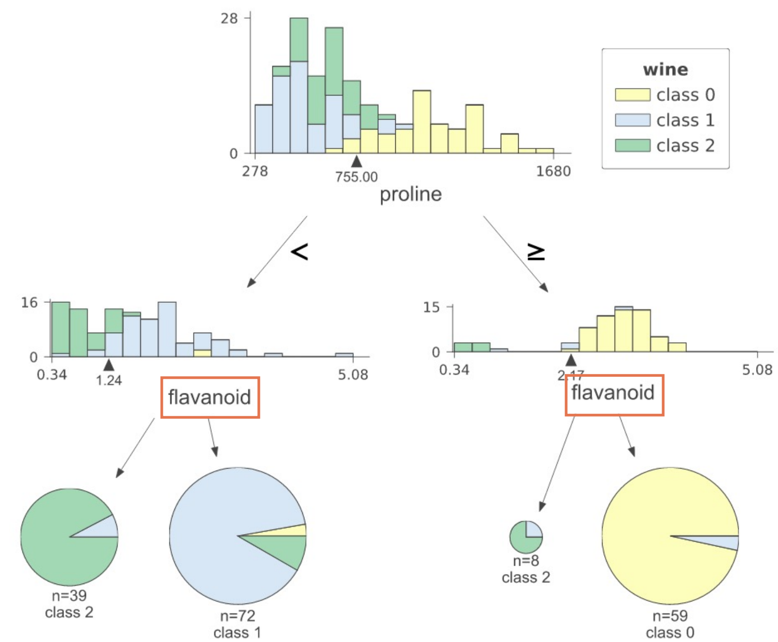
*Training looks for (feature, split point) combos giving more **pure** subregions.*

To test: decision nodes compare single feature value in subset of records to split point

Compare depth=2 trees for 1D, 2D vars



All splits use same proline variable



Splits use proline and flavanoid

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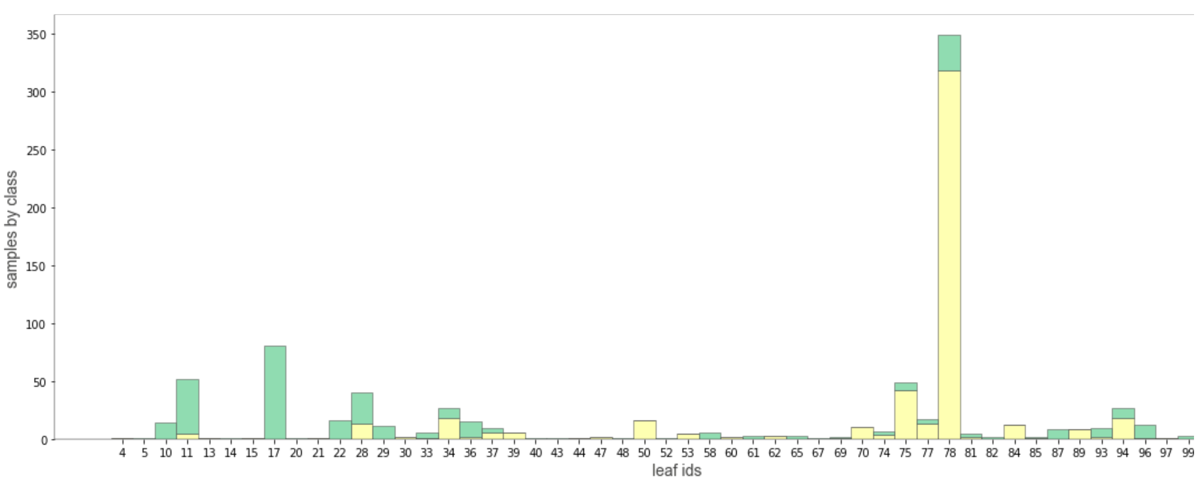
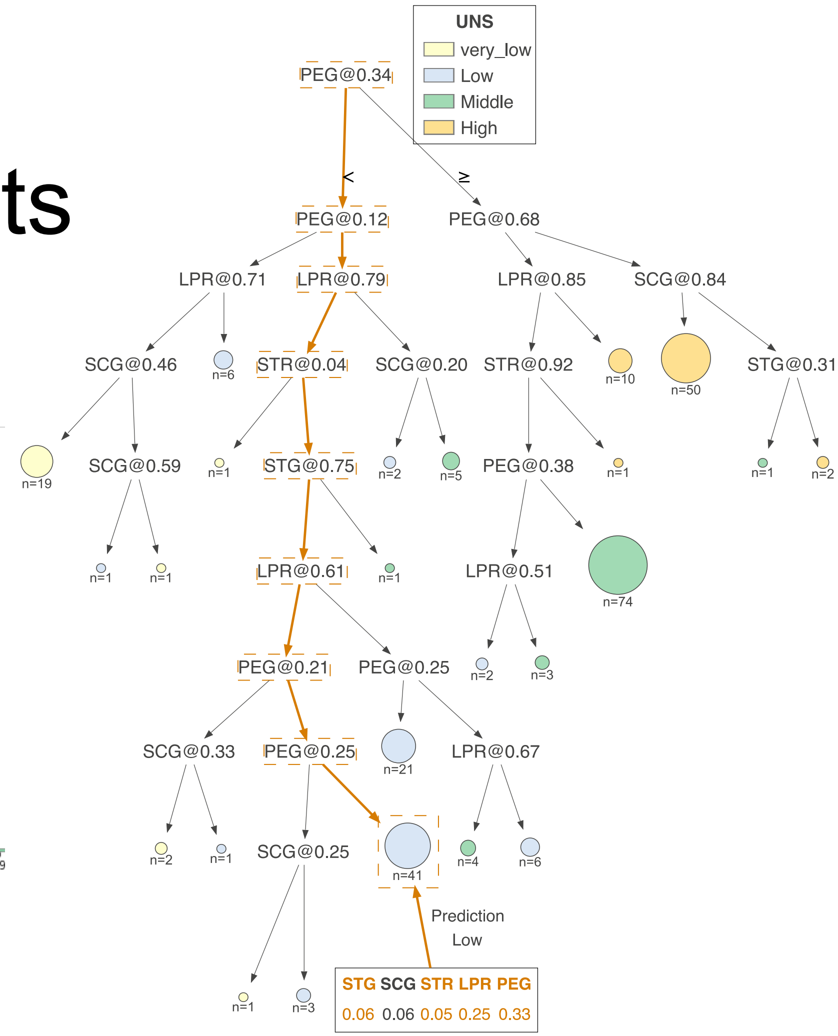
For bigger trees, can do nonfancy plot, leaf plots



Leaf stacked barcharts showing samples per class



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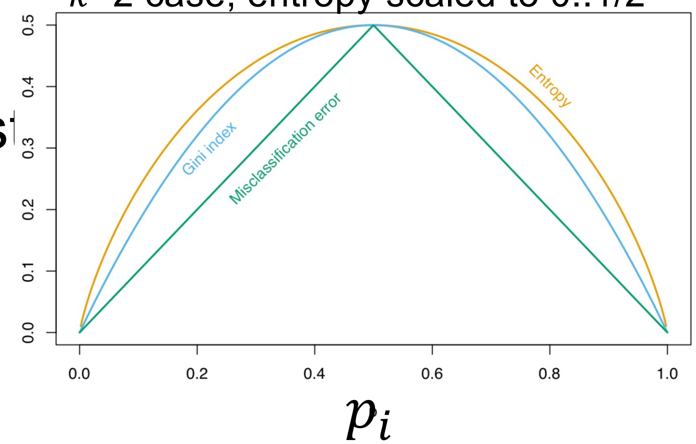
Node impurity: Gini impurity



- Measures y's uncertainty, like entropy but fast
- Minimize gini during node splitting
- Let p_i be the fraction of y values with class i and k = num of classes

$$Gini(y) = \sum_{i=1}^{k} p_i \left[\sum_{j \neq i}^{k} p_j \right] = \sum_{i=1}^{k} p_i(1 - p_i) = 1 - \sum_{i=1}^{k} p_i^2$$

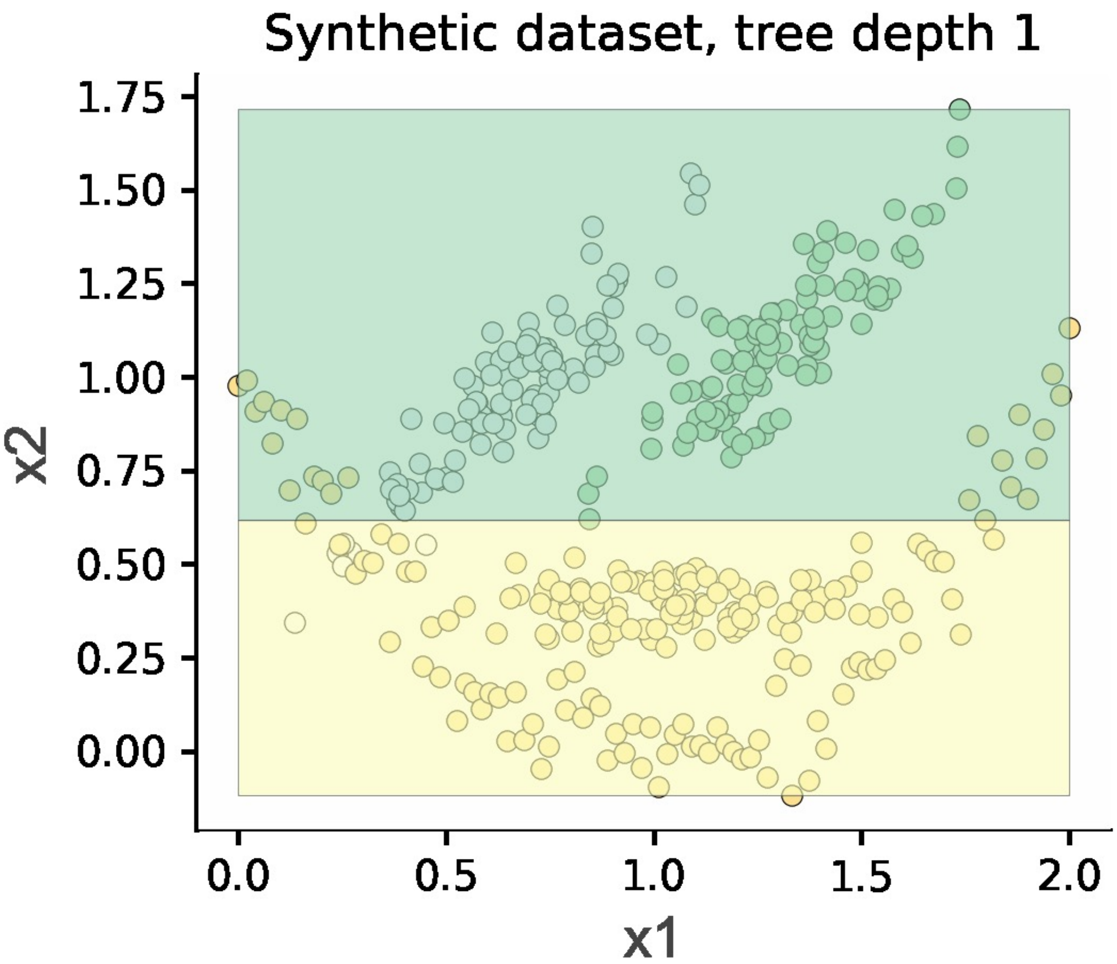
- Gini range is 0..(k-1)/k
- Max uncertainty is when all $p_i = p_j$:
  $p_i = 1/k$ so gini = $1 - \sum_{i=1}^{k} \frac{1}{k^2}$ = $1 - 1/k$ = $(k-1)/k$
- Min uncertainty is when a single $p_i = 1$ and other $p_j = 0$

See https://github.com/parrt/msds621/blob/master/notebooks/trees/gini-impurity.ipynb

Tree structure's effect on prediction error

Hyperparameter max_depth

Restricts how many splits tree can make, preventing tree from getting too specific to training set (zeroing in on outliers)



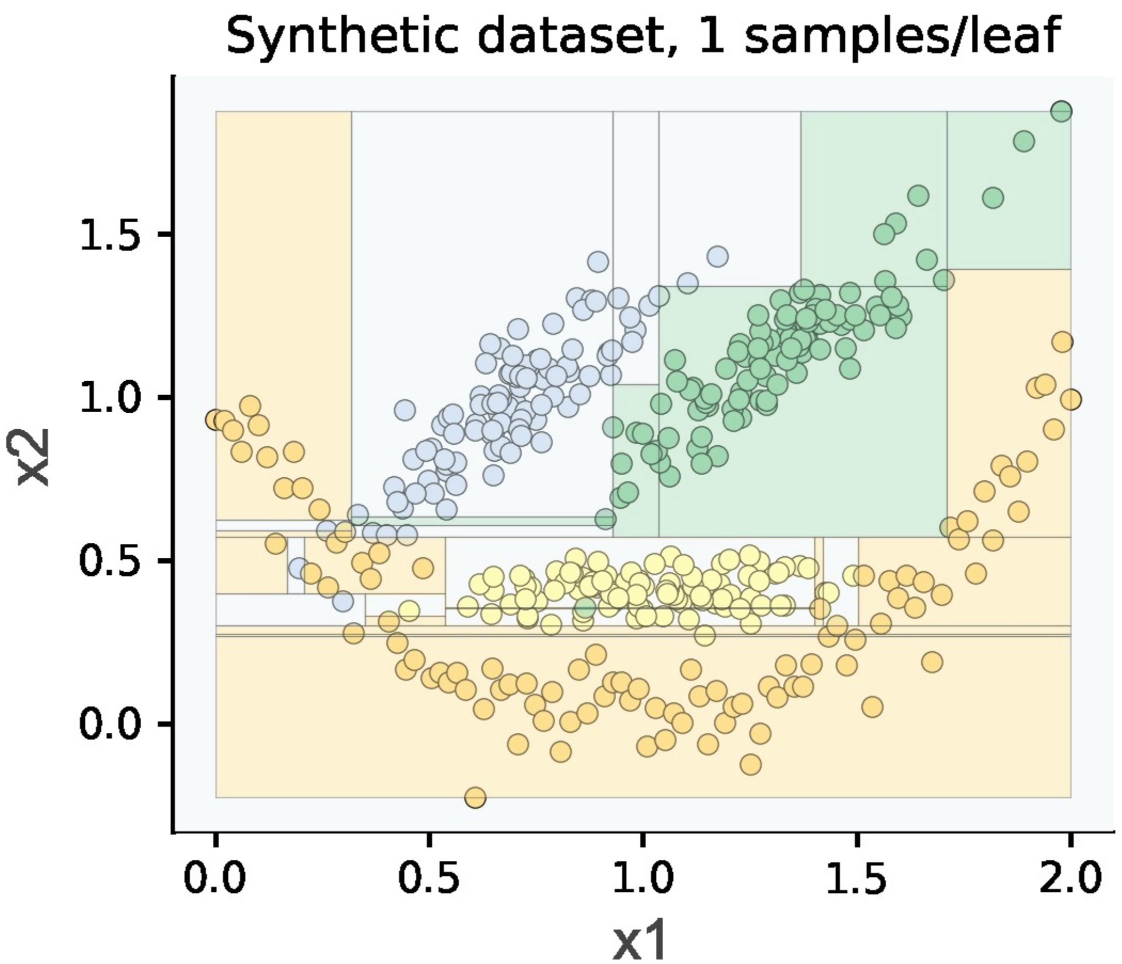
Hyperparameter min_samples_leaf

- Idea: don't split regions w/less than min_samples_leaf records
- Similar to limiting height of tree but finer granularity of control
- More direct control of generality than tree height
- Degenerate case where min_samples_leaf=n
  - What does such a regressor predict?
  - What does such a classifier predict?
  - Describe accuracy of this extreme model
  - If we trained on many different training sets pulled from same data distribution, how stable would the test set prediction error be? (What does that say about variance/generality?)

https://github.com/parrt/msds621/blob/master/notebooks/trees/decision-trees.ipynb

2D tesselation varying min samples/leaf in action

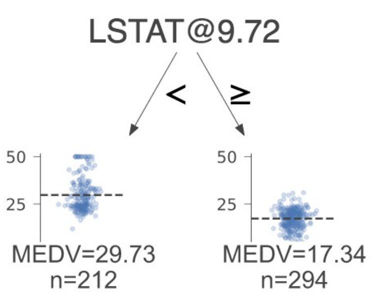
As min leaf size gets bigger, more general but less accurate

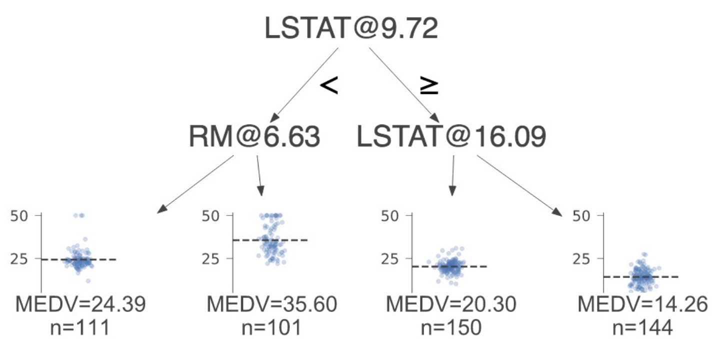


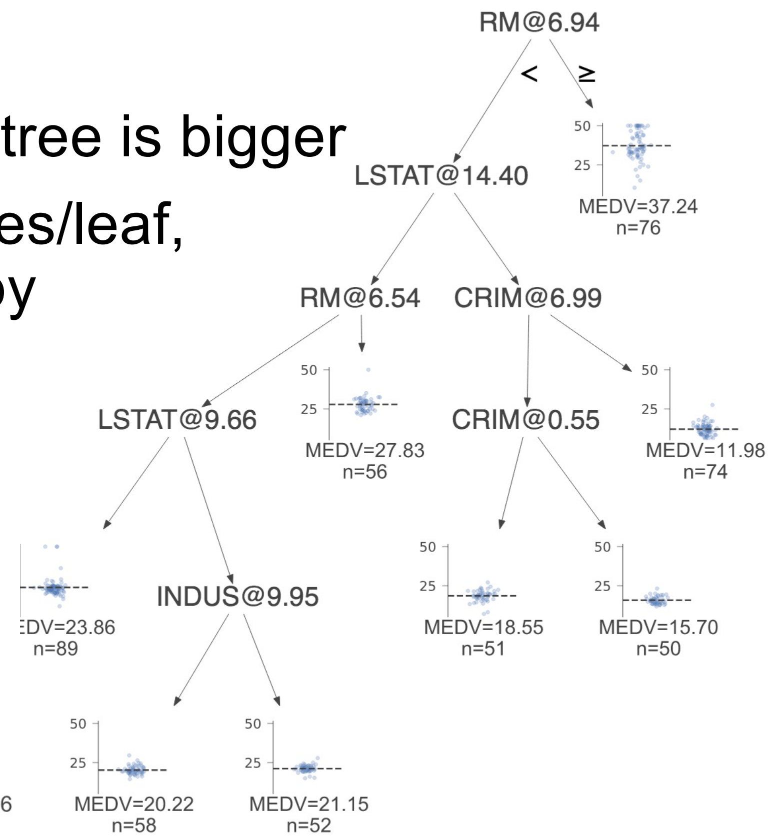
Trees for 200,100,50 samples per leaf

(Boston housing data, n=506 records)

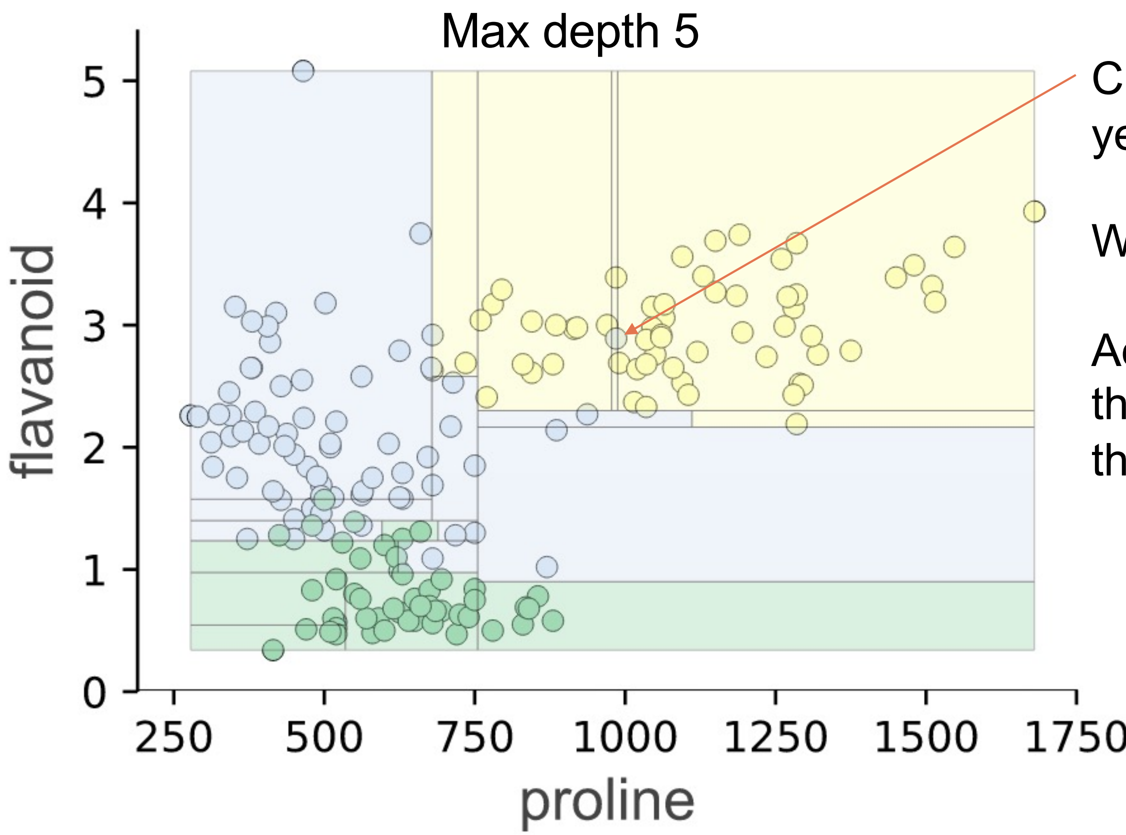
- Leaves have fewer & fewer elements, but tree is bigger
- Variance of y in leaves shrinks with samples/leaf, which is training goal; increase accuracy by reducing impurity







What happens with very small leaves?



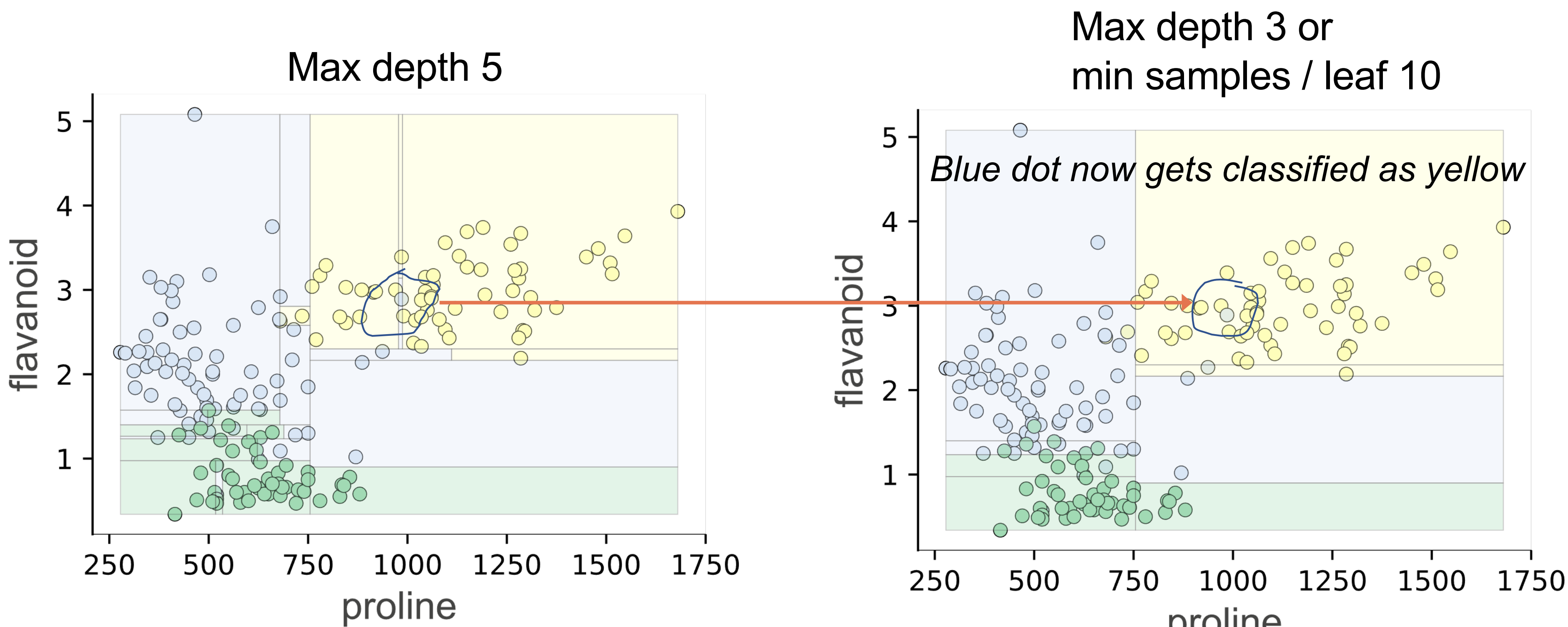
Check out that lonely blue dot in sea of yellow! (let's assume tiny region is blue)

We let model get overly specific; it's overfit

Accuracy on training set is very high, but at the cost of generality; test set error is higher than necessary

(Wine data set)

How could we (likely) improve generality?



(Wine data set)

Key takeaways

- Trees partition feature space into rectangular hypervolumes of similar features but also with pure/similar y values for records in that hypervolume
- Decision trees have internal decision nodes that test variables at split points and leaf nodes that make predictions
- Leaves predict mean (regressor) or mode (classifier) of samples
- Partitioning subject to reducing MSE (y variance) or Gini impurity
- Limiting tree height or increasing leaf size reduces accuracy but improves generality
- (We'll have whole lecture on training these beasts)

Lab time

- Partitioning feature space
  https://github.com/parrt/msds621/blob/master/labs/trees/partitioning-feature-space.ipynb