Model Improvements

Practical Machine Learning (with R)

UC Berkeley

Spring 2016

Topics

- Administrativa
  - Role Call
  - Assignments due to github
- Review/Expectations
  - Readings
  - Previous Lecture
- New Topics

REVIEW AND EXPECTATIONS

Resampling Methods

- Get more accurate estimation of a statistic/value by resampling methods

→ Improves function estimate

Model Performance Evaluation

- Understand model performance metrics
- How they are calculated …

Classification

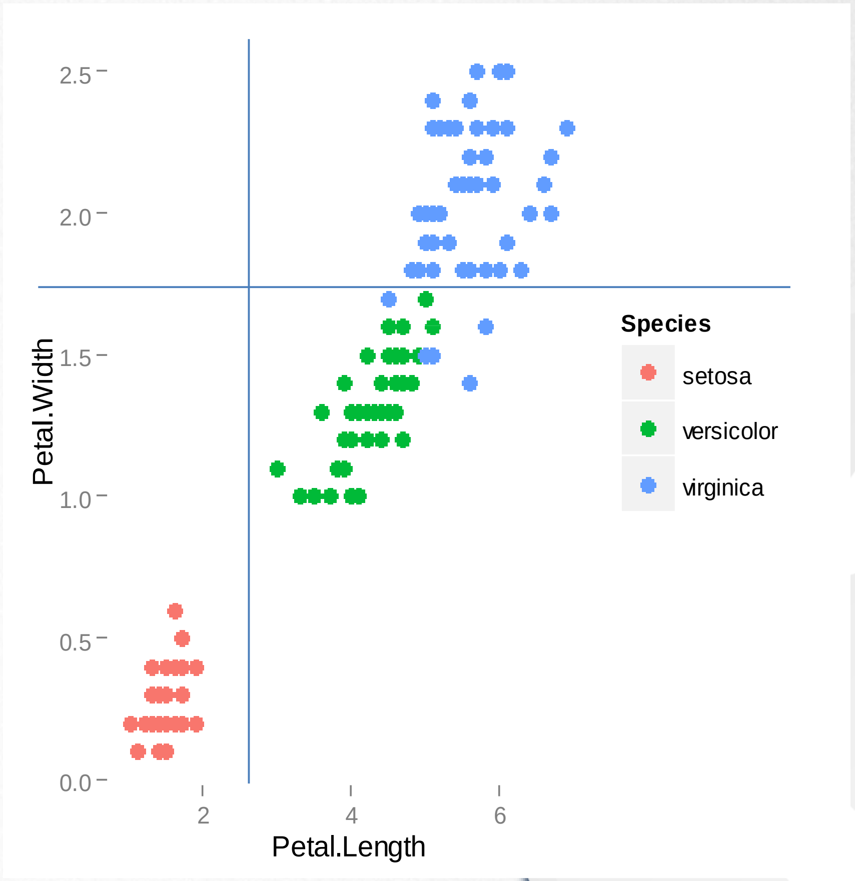
- Metrics: Accuracy, Kappa
- Graphical
  - `caret::confusionMatrix`
  - `pROC::ROC`

Regression

- RMSE, MAE, etc.
- Graphical
  - Histogram of errors
  - $y\ vs\ \hat{y}$ scatterplot

Decision Trees

- All about splitting
  - Different variants have different rules for evaluating the splits
- Tree = Ruleset = Partition of Space
  - Node = Rule = “box” (contiguous region of space)



Tree Variants

- There are many tree variants

- Tweaks
  - change how splits are determined
  - when to stop growing the tree
  - how the node value is determined

Rules

- As derived from trees often have repeated conditions

M5rules, C4.5Rules

```
NumCarbon > 3.777 &
SurfaceArea1 > 0.978 &
SurfaceArea1 > 8.404 &
FP009 <= 0.5 &
FP075 <= 0.5 &
NumRotBonds > 1.498 &
NumRotBonds > 1.701
```

Rules and their conditions live on their own, conditions can be adjusted to help bias-variance trade-off

Missing Data

- Missing values in predictors are common
- A split determines which observations go to the LHS and RHS. How to Handle `Nas`?
- `NA_Categorical`
  - Treat as separate category
- `NA` (in general)
  - Use **Surrogate Splits**

Surrogate Splits

- Tree is built ignoring missing data
  - Any record with incomplete data (response or predictor) is rejected -or-
  - Missing data is not used for split-point determinations

- Variables are often *collinear* → splits are similar and send variables down the same path.
  - Choose a surrogate (variable) split that best approximates the chosen split (accuracy)
  - Very often this is also a good split

Review and Expectation

Understand **Recursive Partitioning** :

- intrinsically how recursive partitioning models work; how splits are determined; what splitting accomplishes
- how model tuning parameters control for bias variance trade-offs
- what `Cp` is and how to use it to prune trees to the proper size

Tree Method Advantages

- List em

Review and Expectation

Use **`rpart`** and/or ctree

- Build Recursive Partitioning Models using `rpart`
- Prune trees to statistically relevant size
- Plot `rpart` trees using
  - `party::as.party`
  - `map.tree::drawtree`

Understand Caret

- Use the **caret** package and the `train` function to build models
- Understand the difference between using `caret` and building models manually. What `caret` provides.
- Control how models are built using the `train & trainControl` functions
- How to extract the final model
- How to plot the tuning parameters, performance curves

QUESTIONS

IMPROVING MODELS

Tree Disadvantages

- List em

Tree Disadvantages

- Model instability (sensitive to data)
  - Derives from each subsequent split is dependent on prior splits
- Less than optimal predictive performance
  - Rectangular regions
- Limited number of outcome values <= number of terminal nodes
- Intra-node high and low values not fit well
- Selection bias toward predictors with higher number of distinct values
- Tuning parameter, C_p
- Splits of correlated variables ambiguous
- Treatment of missing values

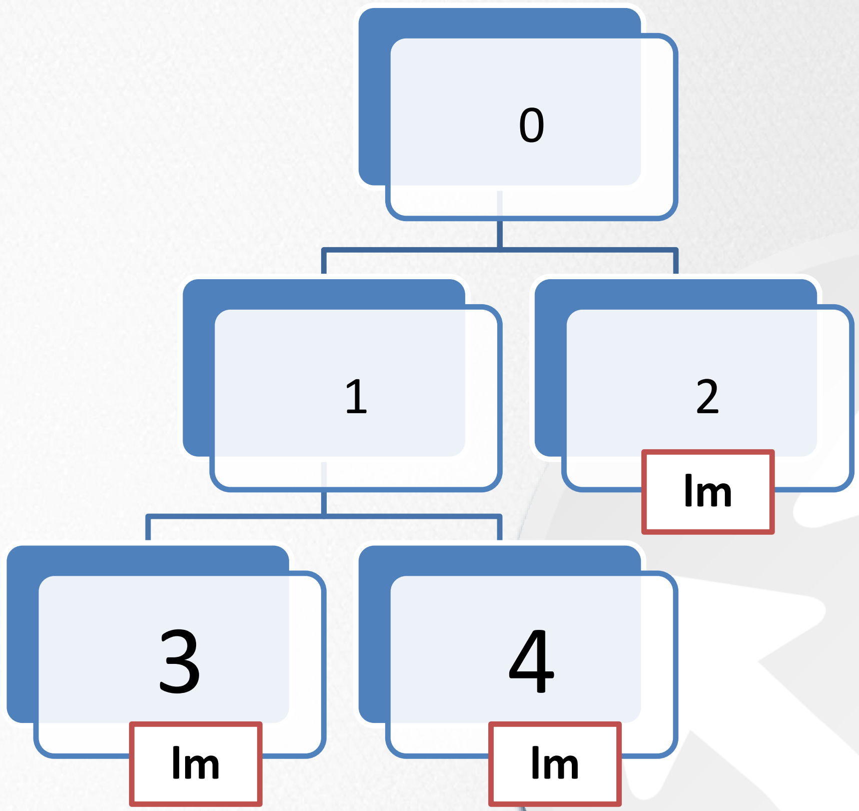
Two Big Ideas

- **Wisdom of the crowds**
  It is better to make estimates from multiple models (***ensembles***) than individual models
  - Better predictions
  - Lower variance for the same model

- **Greed is bad. Patience is good.**
  It is better to slowly approach your solution than arrive at an answer directly.
  - More accurate solutions

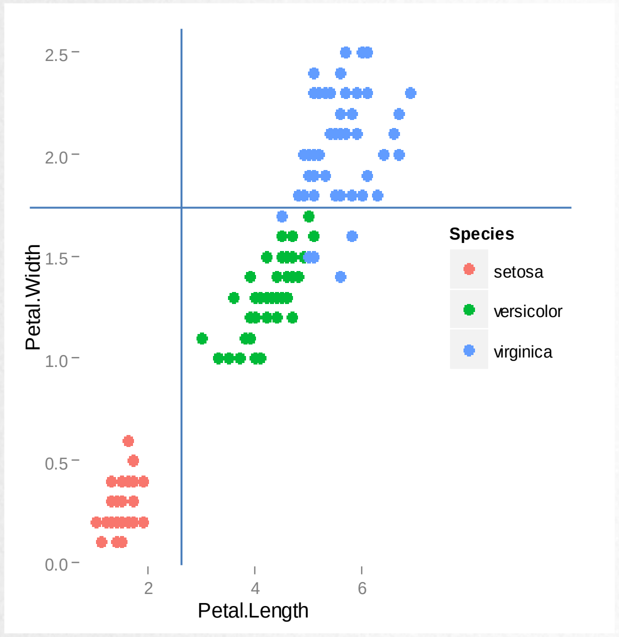
Tree Enhancement: M5

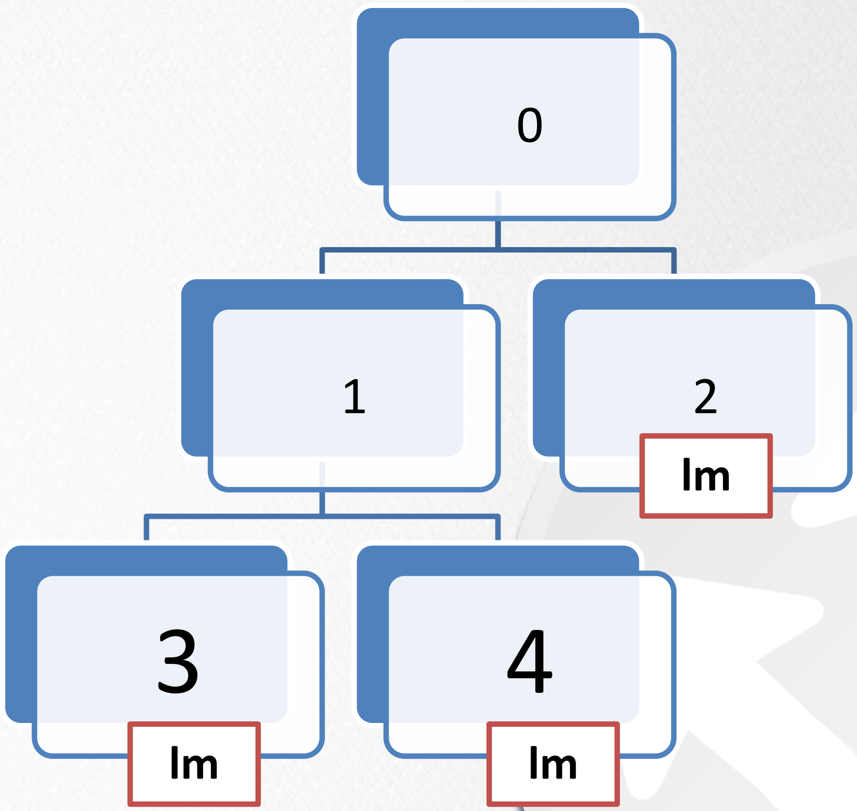
- **Wisdom of the Crowd!**
- Having one value represent the entirety of the node leaves information in the node.
- Function in the node is a simple average
- Use something better
  - **M5** put linear models in nodes of trees



M5 Tree Enhancement (cont.)

- **Greed is bad**
  - linear models are built on the residuals of the tree model.
  - Models are recursive



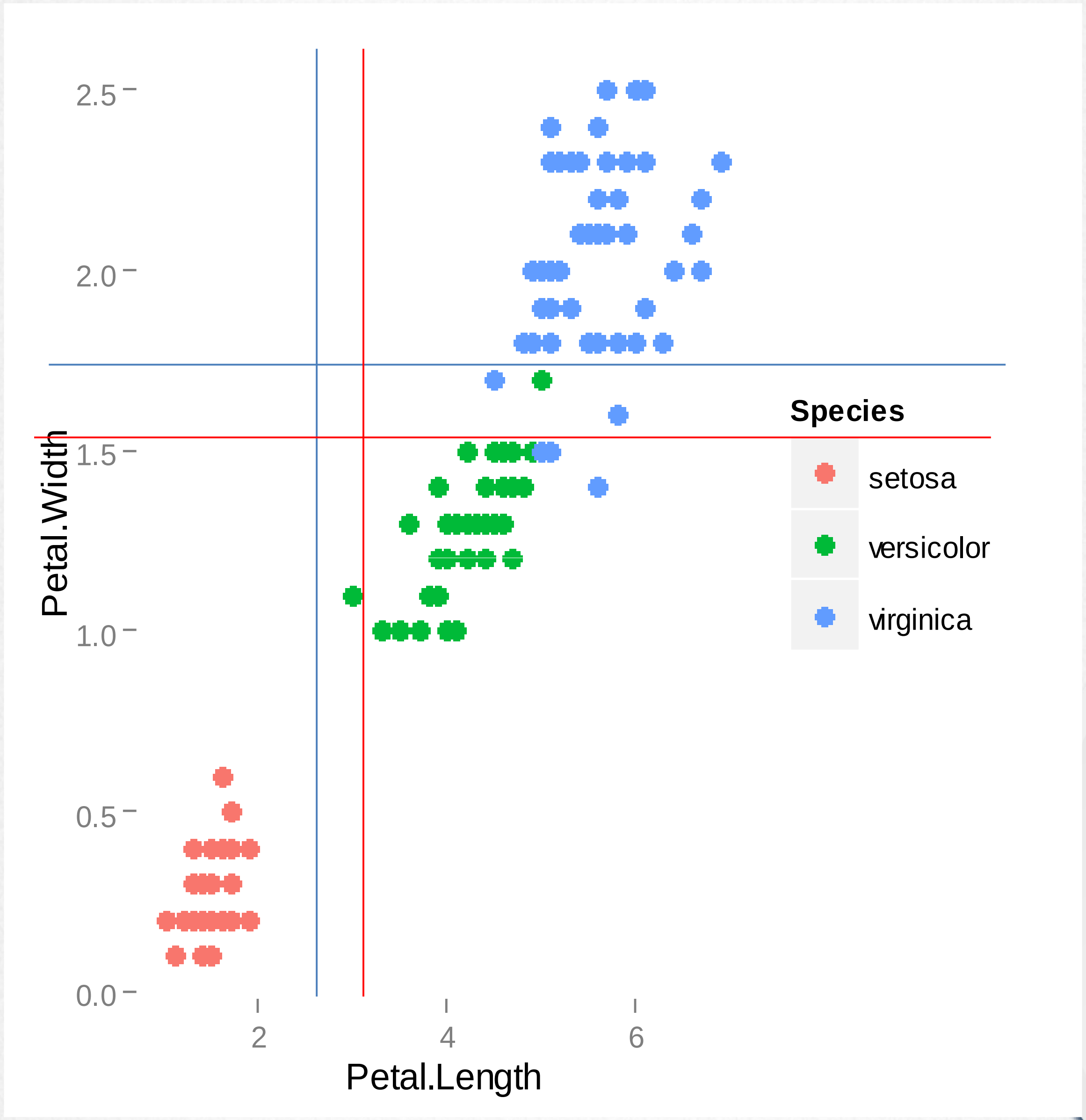


Bagging Models

- Brieman:
  "Bagging is a general approach that uses bootstrapping in conjunction with any regression (or classification) model to construct an ensemble.“

```
for $i = 1$ to $m$ do
    Generate a bootstrap sample of the original data
    Train an unpruned tree model on this sample
end
```

$$\hat{y} = \frac{\sum_i \hat{y}_i}{m}$$

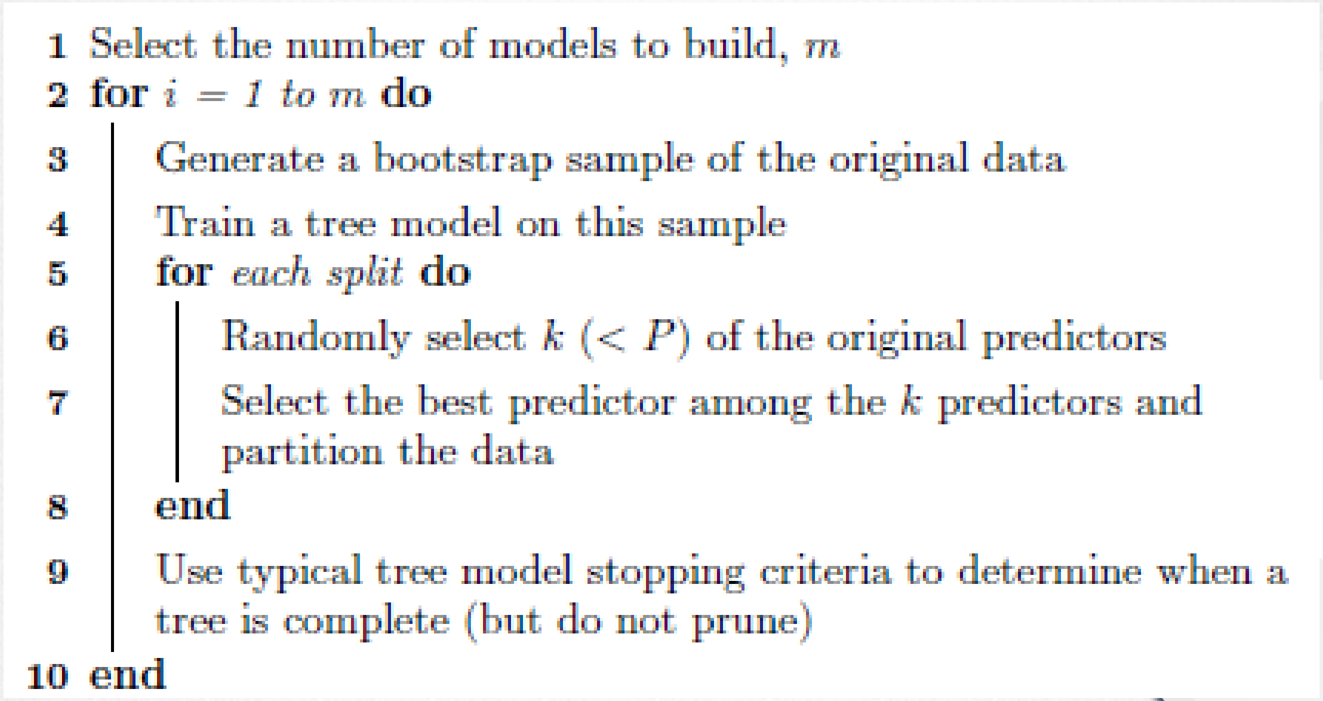

2.5
2.0
1.5
1.0
0.5
0.0
2
4
6
Petal.Width
Petal.Length
Species
setosa
versicolor
virginica

Bagging Notes

- Lowers variance
  - Increases stability
  - Has less effect on lower variance models (e.g. linear models)
  - More effect on weak learners
- Disadvantages
  - Computational cost → but parallelizable
  - Reduces Interpretability

Random Forest

- **Wisdom of the Crowds:** Bagging
- **Greed is bad: consider subset of predictors at each split**



```
Select the number of models to build, $m$
for $i = 1$ to $m$ do
    Generate a bootstrap sample of the original data
    Train a tree model on this sample
    for each split do
        Randomly select $k$ ($< P$) of the original predictors
        Select the best predictor among the $k$ predictors and
        partition the data
    end
    Use typical tree model stopping criteria to determine when a
    tree is complete (but do not prune)
end
```

Tuning Parameter

$\mathtt{m}_{\mathtt{try}}$: number of predictors to use at each split

- **regression** 1/3rd of number predictors
- **classification** sqrt(number of predictors)

➲ Kuhn: “Starting with five values of k that are somewhat evenly spaced across the range from 2 to P”.

Advantages

- No overfitting
- More trees better (limited by computation time/power only)
- In caret, parameters are considered independently
- Because each learner is selected independently of all previous learners, Random Forests is robust to a noisy response
- Computationally efficient -- each tree built on subset of predictors at each split.
- Use any tree variants as "base learner": CART, ctree, etc

Boosting

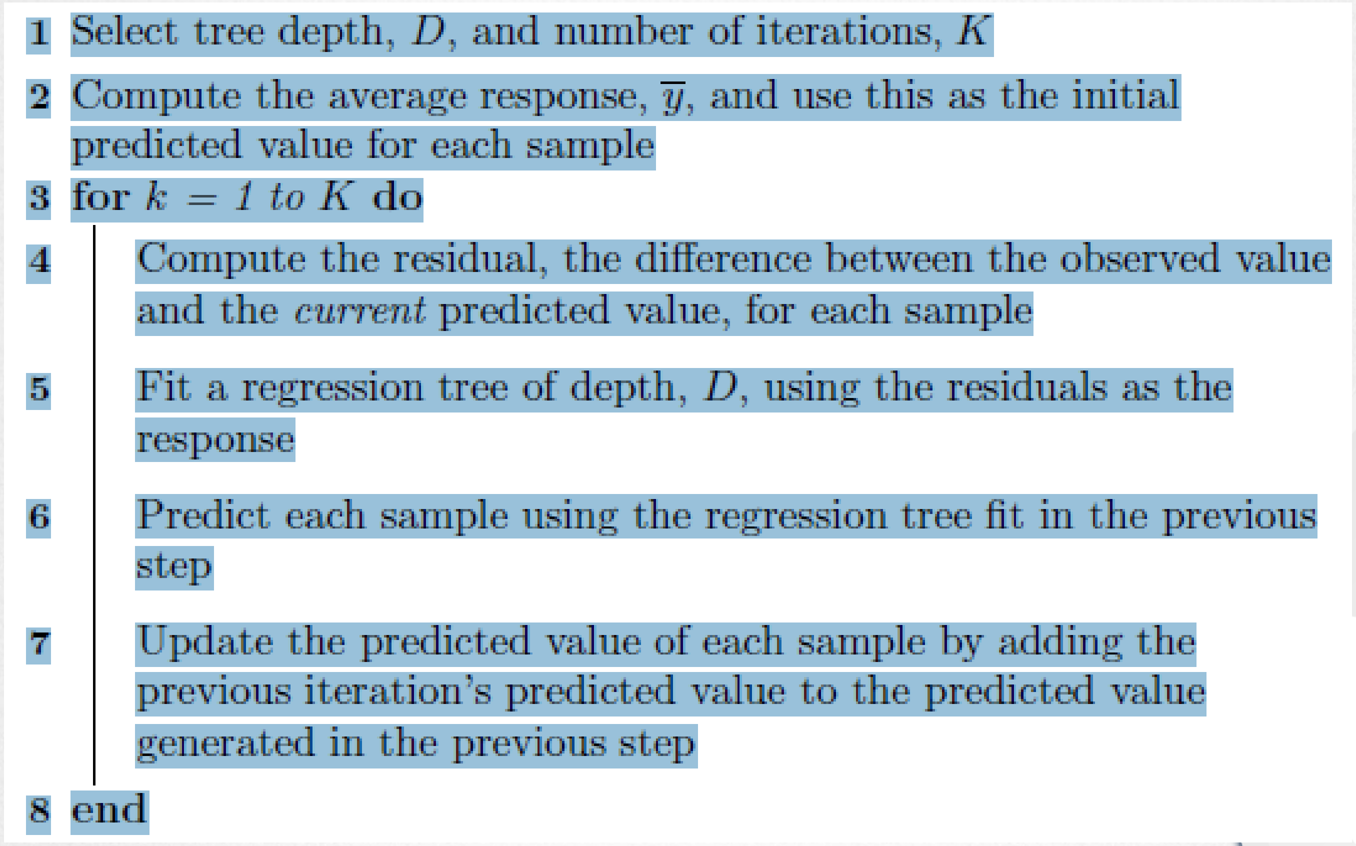
- Single models work;
  - Multiple models work better

- Idea is simple:
  - **Fit first** model: $\hat{y}_1 \sim f_1\,(x)$
  - **Fit** errors/residuals: $\hat{y}_2 = f_2(y - \hat{y}_1)$
    $= f_2\big(y - f_1(x)\big)$
    $= f_2\,(x)$
  - **Iterate:** $\hat{y}_i = (y - \hat{y}_{i-1}) \sim f_i\,(x)$
  - **Predict:** $\hat{y} \sim \sum_i f_i\,(x)$

Boosting Notes

- Additive models
- Works best with "weak learners"
  - i.e. ungreedy, low bias, low variance
  - ~~Any~~ Most models with a tuning parameter can be a weak learner
  - Trees are excellent weak learners
    - Weak → "restricted depth"
- Residuals or errors define a gradient
- Interpreted as forward step-wise regression with exponential loss

Simple Gradient Boosting



```
1 Select tree depth, $D$, and number of iterations, $K$
2 Compute the average response, $\overline{y}$, and use this as the initial
  predicted value for each sample
3 for $k$ = $1$ to $K$ do
4     Compute the residual, the difference between the observed value
      and the *current* predicted value, for each sample
5     Fit a regression tree of depth, $D$, using the residuals as the
      response
6     Predict each sample using the regression tree fit in the previous
      step
7     Update the predicted value of each sample by adding the
      previous iteration's predicted value to the predicted value
      generated in the previous step
8 end
```

Simple Gradient Boosting – Comparison To Random Forest

Similarities	Differences

Stochastic Gradient Boosting

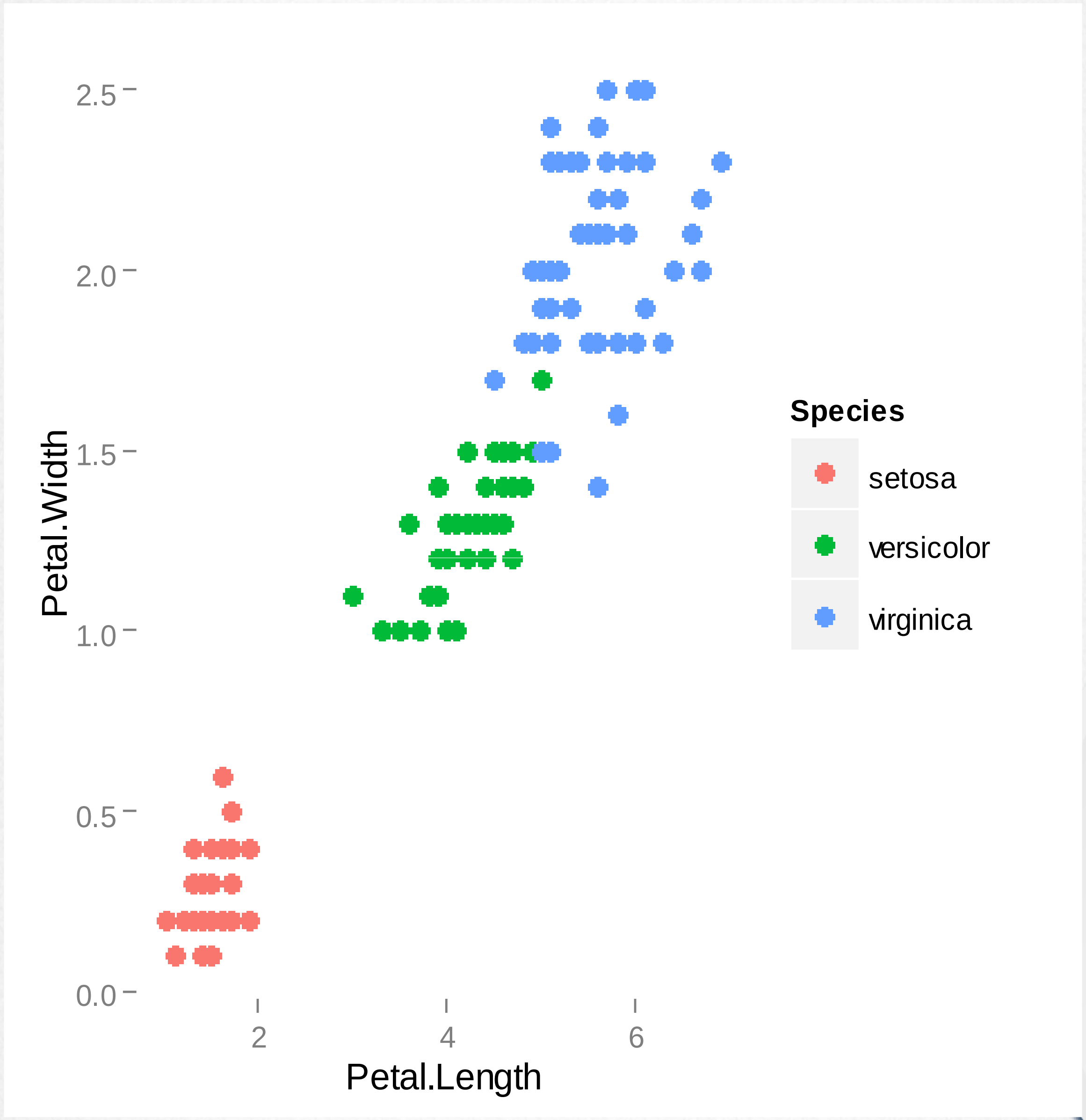
- Gradient Boosting Susceptible to Overfitting
  - Apply "regularization/shrinkage"
    - Use λ ("Learning Rate")
      Rather than add the entirety of the residuals, add a fraction of the residuals at each iteration.

$$\hat{y} \sim \lambda \sum_i f_i(x) \qquad 0 < \lambda \leq 1$$

    - Small values for λ (~0.01) work best
    - λ ~ 1/computational time ~ 1/storage time

- Use bagging, as well
  - Bagging Fraction: a sample of data in each loop iteration

APPENDIX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