Model Building:
Ensemble Methods

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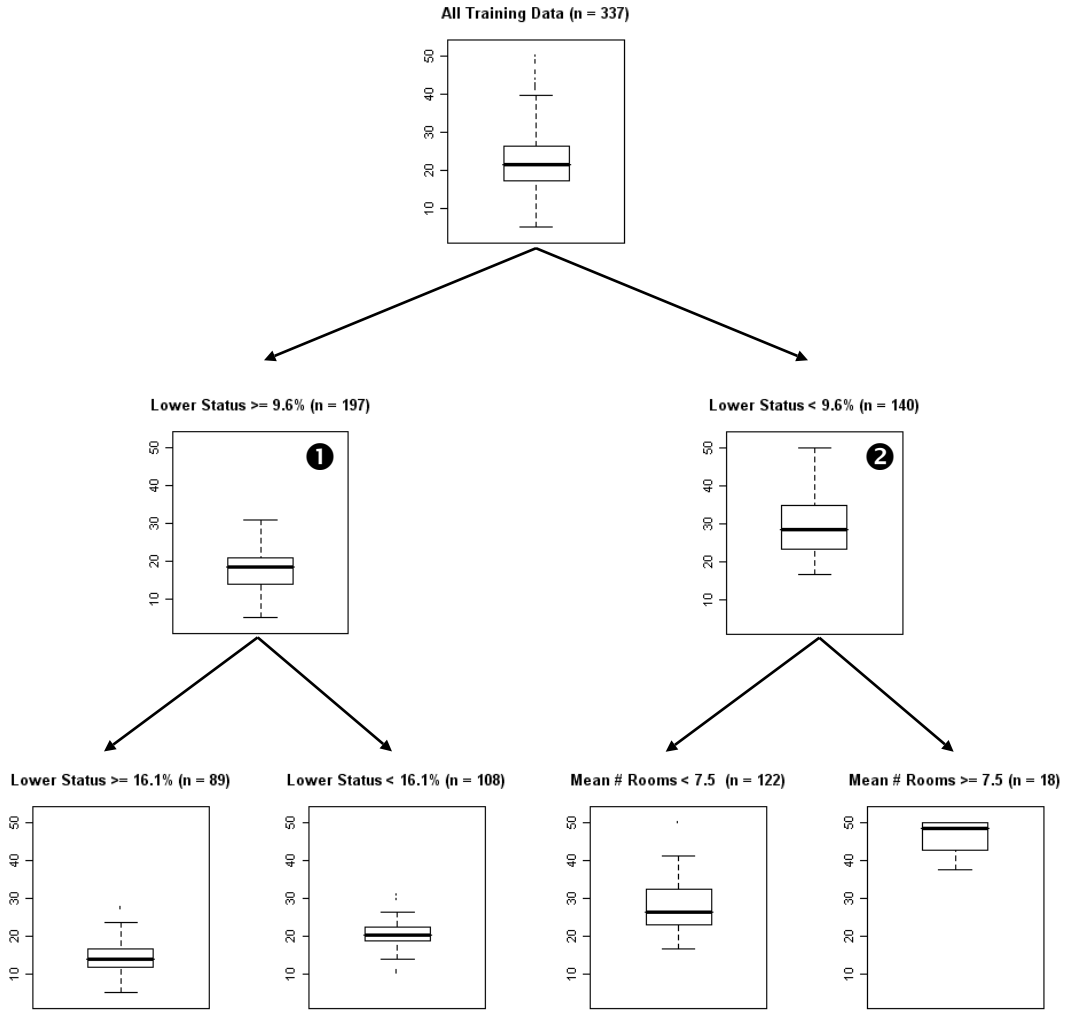
Splitting Example – Boston Housing

- Searching though the first left split (❶), the best split again uses the lower status %
- In the initial right split (❷), the split was based on the mean number of rooms
- Now, there are 4 possible predicted values



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Single Trees

- Advantages
  - can be computed very quickly and have simple interpretations.
  - have built-in predictor selection: if a predictor was not used in any split, the model is completely independent of that data.
- Disadvantages
  - instability due to high variance: small changes in the data can drastically affect the structure of a tree
  - data fragmentation
  - high order interactions

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Ensemble Methods

- Ensembles of trees have been shown to provide more predictive models than individual trees and are less variable than individual trees

- Common ensemble methods are:
  - Bagging
  - Random forests, and
  - Boosting

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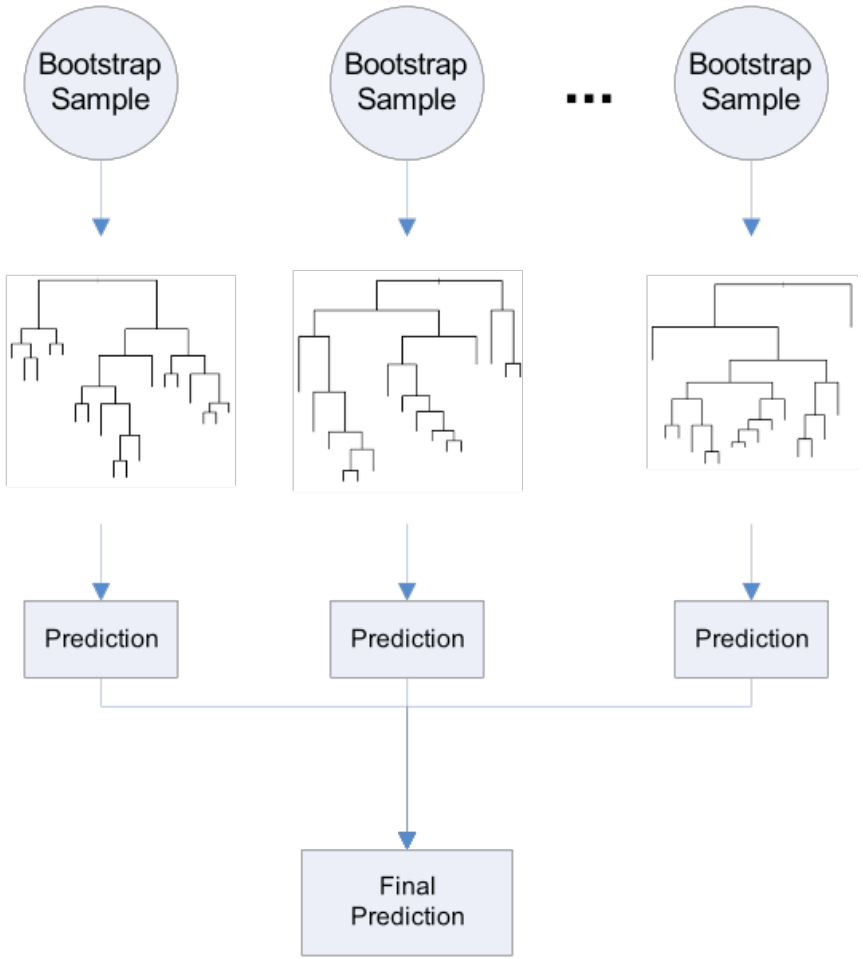
Bagging Trees

- Bootstrap Aggregation
  - Breiman (1994, 1996)
  - Bagging is the process of
    1. creating bootstrap samples of the data,
    2. fitting models to each sample
    3. aggregating the model predictions
  - The largest possible tree is built for each bootstrap sample



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Bagging Model

Prediction of an observation, x:

$$F(x) = \frac{\sum_{m=1}^{M} f_m(\mathrm{x})}{M}$$

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Comparison

- Bagging can significantly increase performance of trees
  - from resampling:

	Training Data (bootstrap)		Test	
	RMSE	**Q^2**	**RMSE**	**R^2**
Single Tree	5.18	0.700	4.28	0.780
Bagging	4.32	0.786	3.69	0.825

- The cost is computing time and the loss of interpretation
- One reason that bagging works is that single trees are unstable
  - small changes in the data may drastically change the tree

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Random Forests

- Random forests models are similar to bagging
  - separate models are built for each bootstrap sample
  - the largest tree possible is fit for each bootstrap sample
- However, when random forests starts to make a new split, it only considers a random subset of predictors
  - The subset size is the (optional) tuning parameter
- Random forests defaults to a subset size that is the square root of the number of predictors and is typically robust to this parameter

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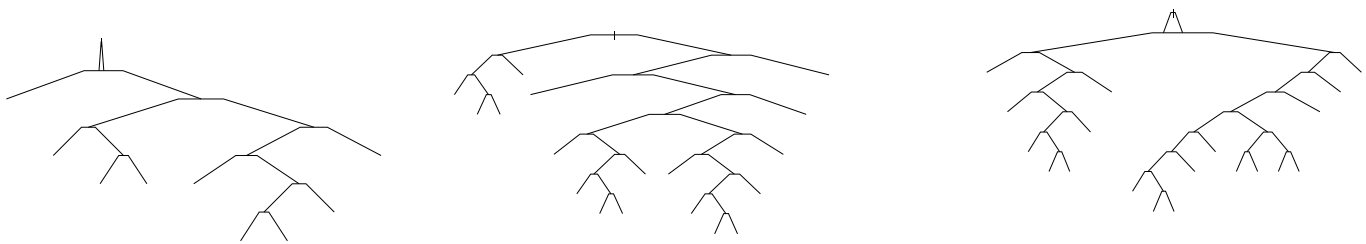
Random Predictor Illustration

Randomly select a subset of variables from original data

Dataset 1 | Dataset 2 | Dataset *M*

Build trees



Predict | Predict | Predict

Final Prediction

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Random Forests Model

Prediction of an observation, x:

$$F(x) = \frac{\sum_{m=1}^{M} f_m(\mathrm{x})}{M}$$

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Properties of Random Forests

- Variance reduction
  - Averaging predictions across many models provides more stable predictions and model accuracy (Breiman, 1996)
- Robustness to noise
  - All observations have an equal chance to influence each model in the ensemble
  - Hence, outliers have less of an effect on individual models for the overall predicted values

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Comparison

- Comparing the three methods using resampling:

	Training Data (bootstrap)		Test	
	RMSE	**Q^2**	**RMSE**	**R^2**
Single Tree	5.18	0.700	4.28	0.780
Bagging	4.32	0.786	3.69	0.825
Rand Forest	3.55	0.857	3.00	0.885

- Both bagging and random forests are “memoryless”
  - each bootstrap sample doesn’t know anything about the other samples

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Boosting Trees

- A method to “boost” weak learning algorithms (small trees) into strong learning algorithms
  - Kearns and Valiant (1989), Schapire (1990), Freund (1995), Freund and Schapire (1996a)

- Boosted trees try to improve the model fit over different trees by considering past fits

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Boosting Trees

- First, an initial tree model is fit (the size of the tree is controlled by the modeler, but usually the trees are small (depth < 8))
  - if a sample was not predicted well, the model residual will be different from zero
  - samples that were predicted poorly in the last tree will be given more weight in the next tree (and vice-versa)
- After many iterations, the final prediction is a weighted average of the prediction form each tree

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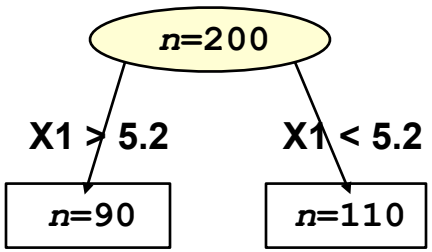
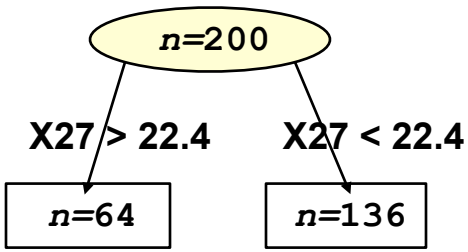
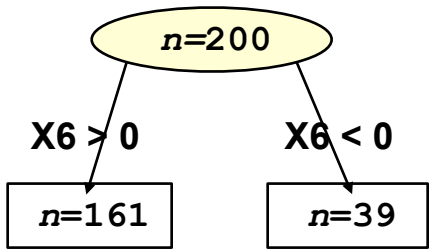
Boosting Illustration

Stage	**1**	**2**	**. . .**	***M***
Build weighted tree				
Compute error	$\sum_{i=1}^{n} e_i^2 = 32.9$	$\sum_{i=1}^{n} e_i^2 = 26.7$		$\sum_{i=1}^{n} e_i^2 = 29.5$
Compute stage weight	$\beta_{\text{stage 1}} = f(32.9)$	$\beta_{\text{stage 2}} = f(26.7)$		$\beta_{\text{stage M}} = f(29.5)$
Reweigh observations (w_i=1,2,..., n)	Determine weight of i^{th} observation: The larger the error, the higher the weight	Determine weight of i^{th} observation		

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Boosting Trees

- Boosting has three tuning parameters:
  - number of iterations (i.e. trees)
  - complexity of the tree (i.e. number of splits)
  - learning rate: how quickly the algorithm adapts

- This implementation is the most computationally taxing of the tree methods shown here

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Final Boosting Model

Prediction of an observation, x:

$$F(x) = \sum_{m=1}^{M} \left(\beta_m f_m \left(\mathrm{x} \right) \right)$$

where the β_m are constrained to sum to 1.

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Properties of Boosting

- Robust to overfitting
  - As the number of iterations increases, the test set error does not increase
  - Schapire, et al. (1998), Friedman, et al. (2000), Freund, et al. (2001)
- Can be misled by noise in the response
  - Boosting will be unable to find a predictive model if the response is too noisy.
  - Kriegar, et al. (2002), Wyner (2002), Schapire (2002), Optiz and Maclin (1999)

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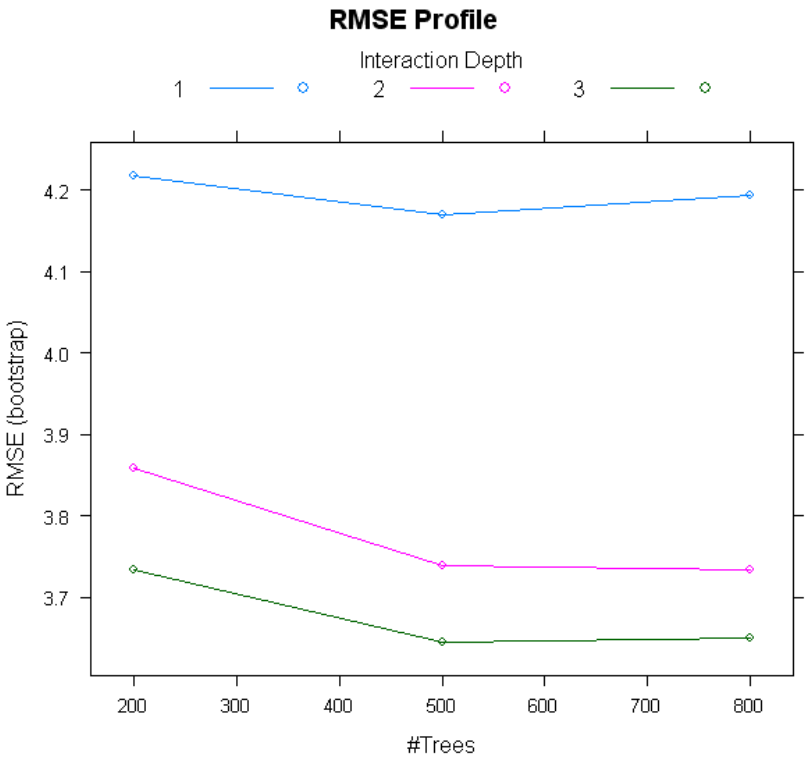
Boosting Trees

- One approach to training is to set the learning rate to a high value (0.1) and tune the other two parameters
- In the plot to the right, a grid of 9 combinations of the 2 tuning parameters were used to optimize the model
- The optimal settings were:
  - 500 trees with high complexity



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Comparison Summary

- Comparing the four methods:

	Training Data (bootstrap)		Test	
	RMSE	**Q^2**	**RMSE**	**R^2**
Single Tree	5.18	0.700	4.28	0.780
Bagging	4.32	0.786	3.69	0.825
Rand Forest	3.55	0.857	3.00	0.885
Boosting	3.64	0.847	3.19	0.870

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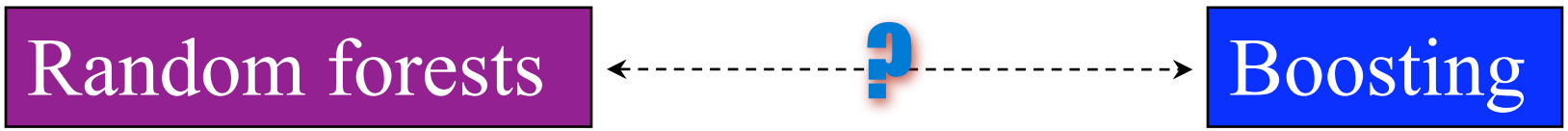
Current Research at Pfizer: The best of both worlds?

- Random forests are robust to noise
- Boosting is robust to overfitting
- Can we create a hybrid ensemble that takes advantage of both of these properties?



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Contrasts

- Random forests
  - Prefer large trees
  - Use equally weighted data
  - Use randomness to build the ensemble
- Boosting
  - Prefers small trees
  - Uses unequally weighted data
  - Does not use randomness to build the ensemble
- How to combine these methods?

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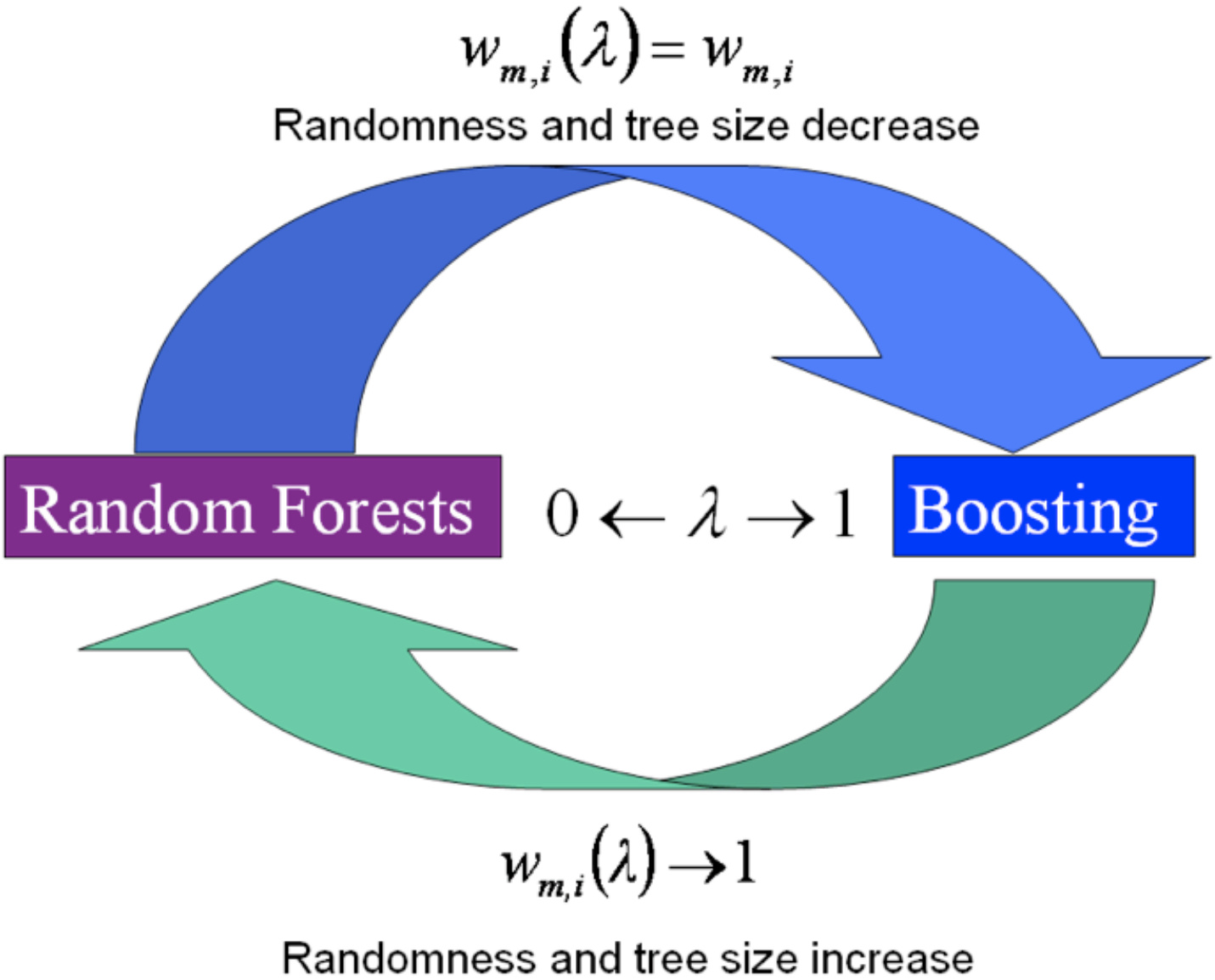
Connecting Random Forests and Boosting



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Multivariate Adaptive Regression Splines

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Multivariate Adaptive Regression Splines

- MARS is a nonlinear statistical model
- The model does an exhaustive search across the predictors (and each distinct value of the predictor) to find the best way to sub-divide the data
- Based on this “split” value, MARS creates new features based on that variable
- These artificial features are used to model the outcome

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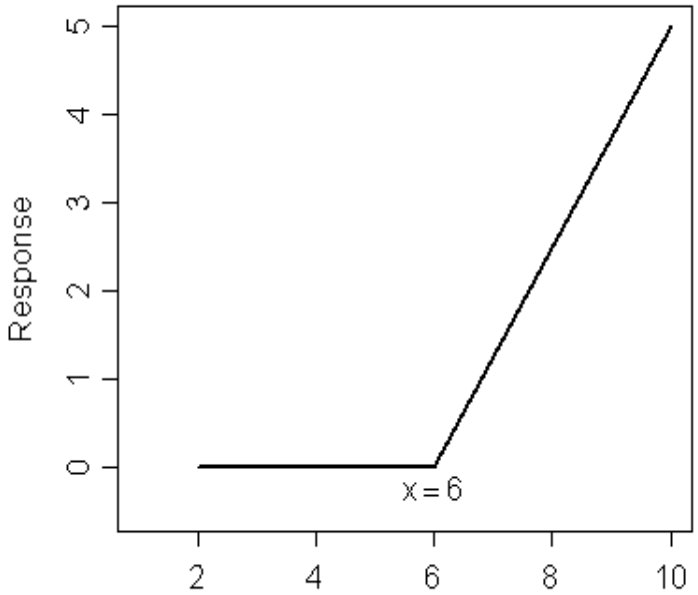
MARS Features

- MARS uses “hinge” functions that are two connected lines
- For a data point x of a predictor, MARS creates a function that models the data on each side of x:

$$h(u) = \begin{cases} u & \text{if } u > 0 \\ 0 & \text{otherwise} \end{cases}$$

- These features are created in sets of two (switching which side is “zeroed”)



x	h(x-6)	h(6-x)
2	0	2
4	0	4
8	8	0
10	10	0

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Prediction Equation and Model Selection

- The model iteratively adds the two new features and uses ordinary regression methods to create a prediction equation. The process then continues iteratively.

- MARS also includes a built-in feature selection routine that can remove model terms
  - the maximum number of retained features (and the feature degree) are the tuning parameters

- The Generalized Cross-Validation statistic (GCV) is used to select the most important terms

$$GCV = penalty \times \sum_{i=1}^{n} \left[y_i - \widehat{f_i(M)} \right]^2$$

$$M = \text{candidate model}$$

$$penalty = \left(1 - \frac{r + 3K}{n}\right)^{-2}$$

$$r = \text{number of basis functions}$$

$$K = \text{number of knots}$$

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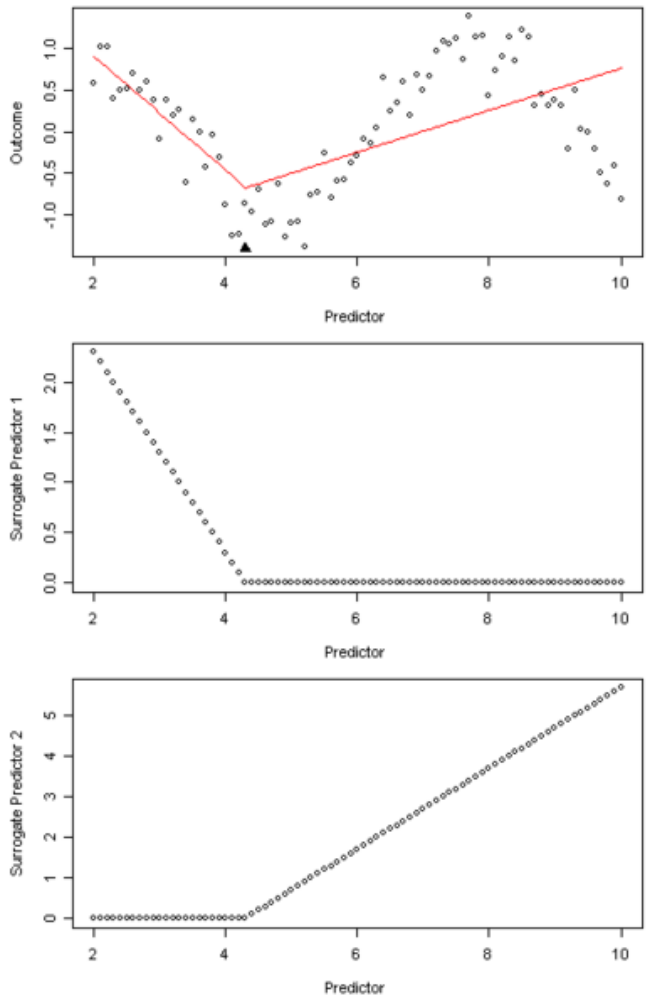
Sine Wave Example

- As an example, we can use MARS to model one predictor with a sinusoidal pattern
- The first MARS iteration produces a split at 4.3
  - two new features are created
  - a regression model is fit with these features
  - the red line shows the fit



$$\hat{y}_i = \beta_0 + \beta_1\, h(x_i - 4.3) + \beta_2\, h(4.3 - x_i)$$

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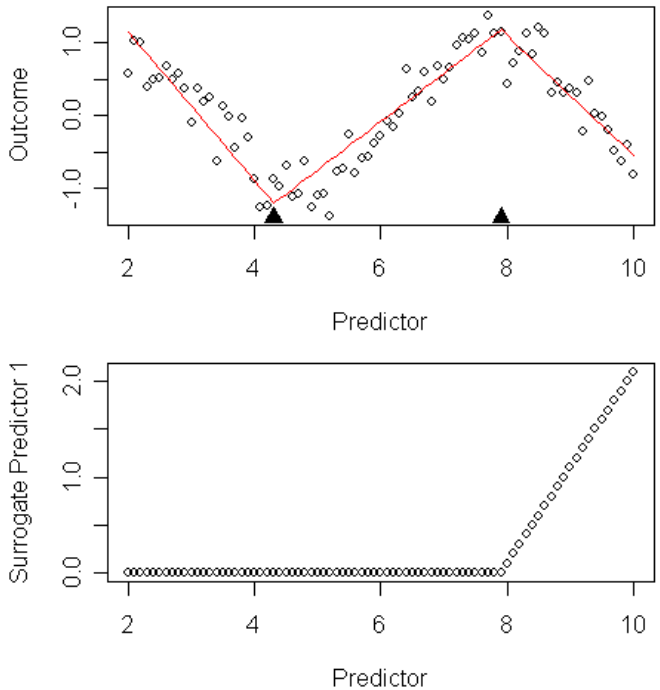
Sine Wave Example

- On the second iteration, a split was found at 7.9
  - two new features are created
- However, the model fit on the left side was already pretty good
  - one of the new surrogate predictors was removed by the automatic feature selection
- The model now has three features



$$\hat{y}_i = \beta_0 + \beta_1\, h(x_i - 4.3) + \beta_2\, h(4.3 - x_i) + \beta_3\, h(x_i - 7.9)$$

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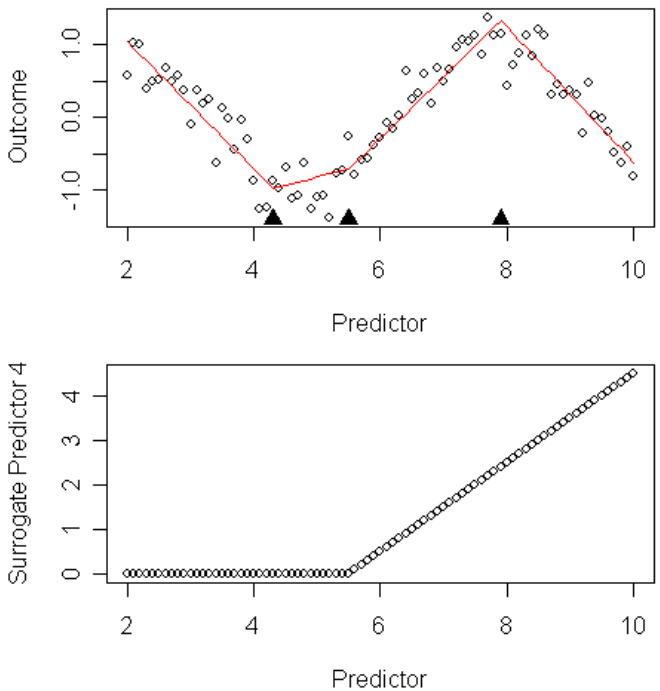
Sine Wave Example

- The third split occurred at 5.5
- Again, only the “right-hand” feature was retained in the model
- This process would continue until
  - no more important features are found
  - the user-defined limit is achieved



$$\hat{y}_i = \beta_0 + \beta_1\, h(x_i - 4.3) + \beta_2\, h(4.3 - x_i) + \beta_3\, h(x_i - 7.9) + \beta_4\, h(x_i - 5.5)$$

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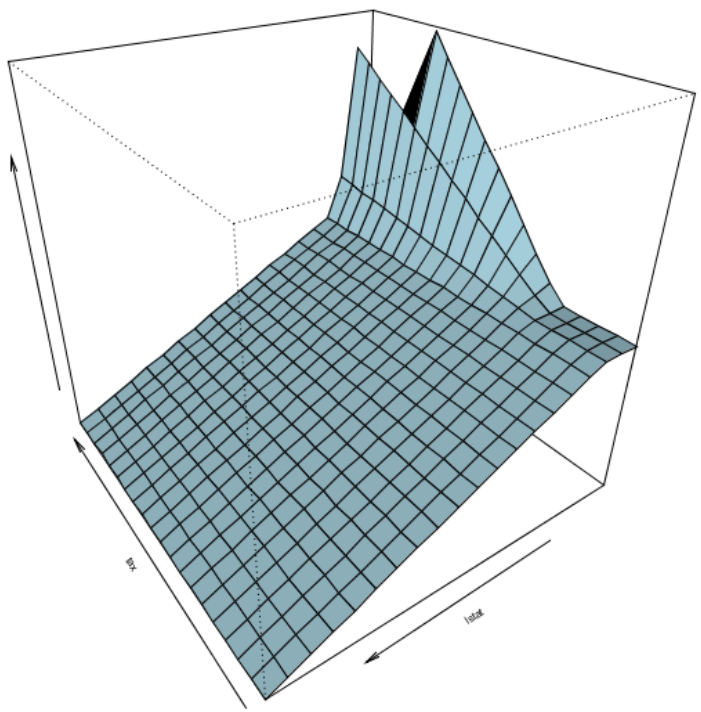
Higher Order Features

- Higher degree features can also be used
  - two or more hinge functions can be multiplied together to for a new feature
  - in two dimensions, this means that three of four quadrants of the feature can be zero if some features are discarded



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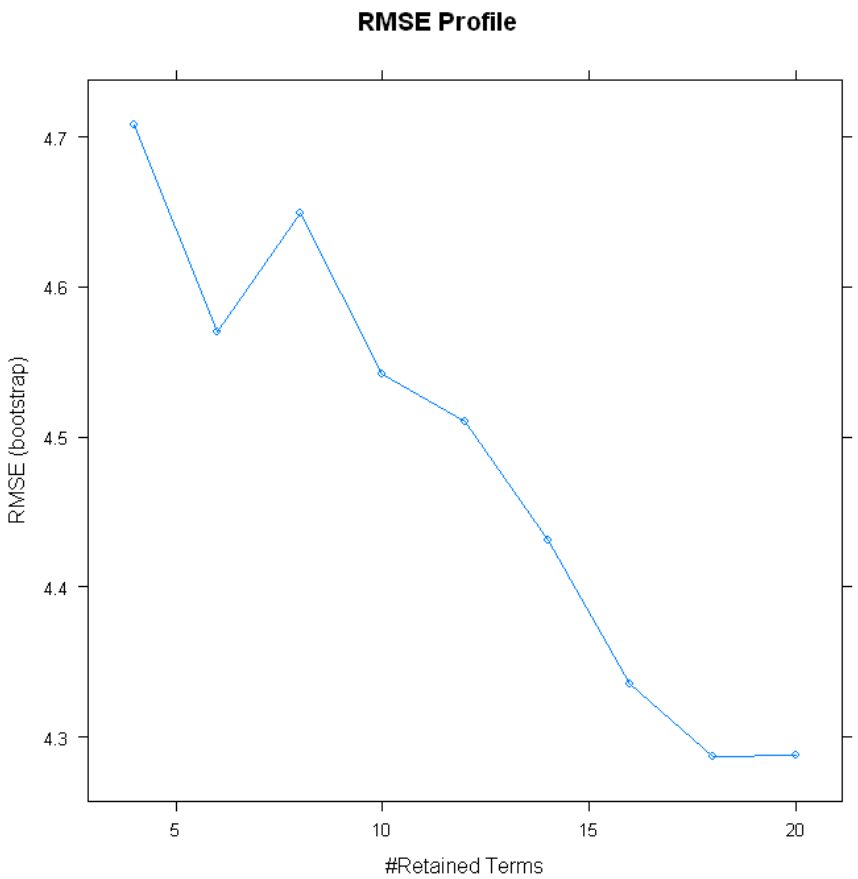
Boston Housing Data

- We tried only additive models
  - the model could retain from 4 to 36 model terms
- The “best” model used 18 terms



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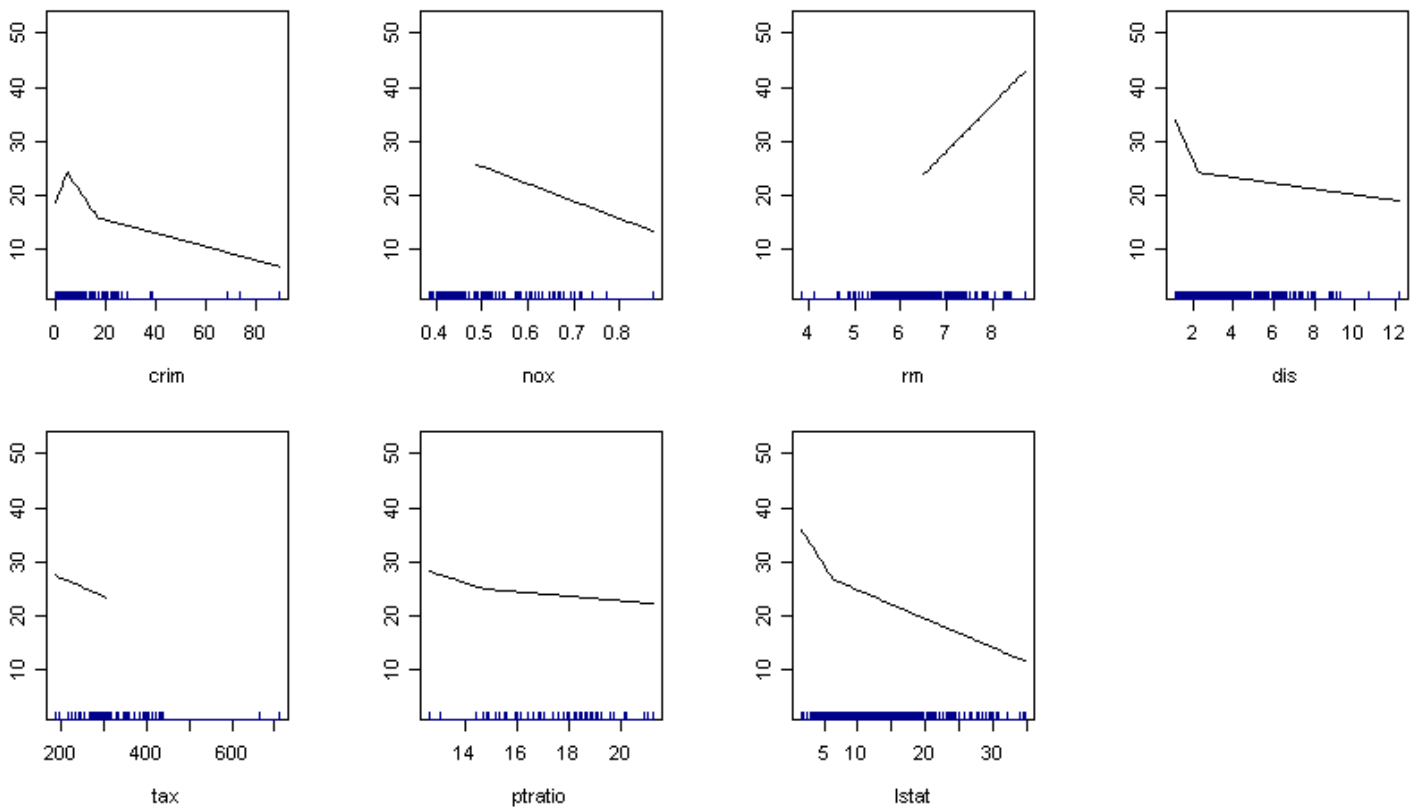
Boston Housing Data

- Since the model is additive, we can look at the prediction profile of each factor while keeping the others constant



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Summary

- SVMs are still optimal, but the respectable performance and interpretability of MARS might make us reconsider

	Training Data (bootstrap)		Test Data	
	RMSE	**Q^2**	**RMSE**	**R^2**
Linear Reg	5.23	0.691	4.53	0.742
PLS	5.25	0.689	4.56	0.739
Neural Net	4.60	0.757	4.20	0.780
SVM (radial)	3.79	0.834	3.28	0.861
MARS	4.29	0.791	3.98	0.804

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Model Building Training

Model Comparisons

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Which Model is Best?

- The “No Free Lunch Theorem”:
  - over the set of all possible problems, each algorithm will do on average as well as any other

  or, in other words,

  - if one model is better than another, it is because of the particular problem at hand; no one method is uniformly best

- Despite this statement, the next slide has some (subjective) ratings of models

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Top Level Comparisons

Model	Speed	Performance	Interpretability	Robustness
Boosted Tree				
Random Forest				
Linear Model				
PLS				
MARS				
Neural Net				
SVM				
RDA				
FDA				
Naïve Bayes				

 Excellent Very Good Average Fair Poor

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Top Level Comparisons

Model	#Param	Pre-Process	P > N ?	Missing Data ?
Boosted Tree	2-3	None	Yes	Yes*
Random Forest	0-1	None	Yes	Yes*
Linear Model	0	ZV, NZV, HCP	No	No
PLS	1	CS	Yes	No
MARS	2	ZV, NZV, HCP	Yes	Yes
Neural Net	2	ZV, CS, HCP	Yes	No
SVM	2-3	CS	Yes	No
RDA	2	ZV	No	No
FDA	2	None	Yes	Yes
Naïve Bayes	0-1	ZV	Yes	Yes

ZV = zero var predictor, NZV = near-zero var predictor,
CS = center+scale, HCP = highly correlated predictor
* Depends on implementation

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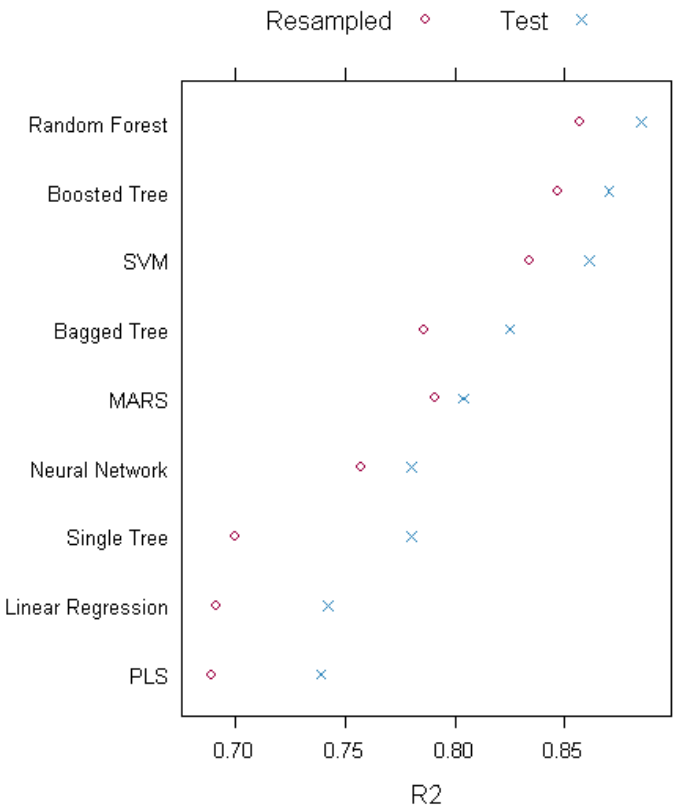
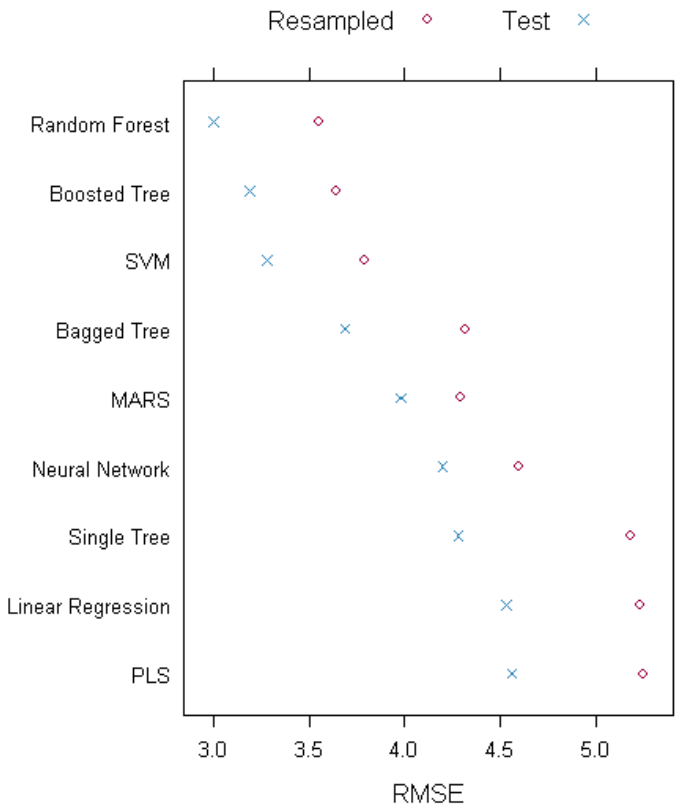
Boston Housing Data





- The correlation between the results on the training set (n=337) via cross-validation and the results from the test set (n=169) were 0.971 (RMSE) and 0.965 (R^2)

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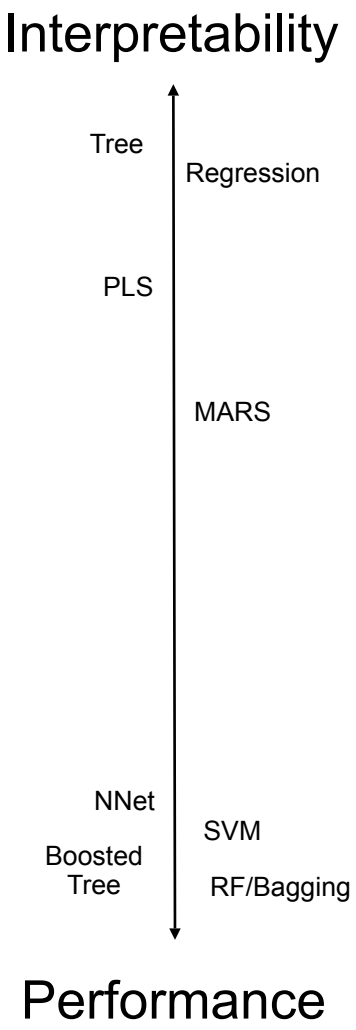
Some Advice

- There is an inverse relationship between performance and interpretability
- We want the best of both worlds: great performance and a simple, intuitive model
- Try this:
  - Fit a high performance model to get an idea of the best possible performance
  - Move up the line and see if a less complex model can keep performance up with some interpretability



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