Ensemble Methods (Part I)
Bagging and Random Forests

Schwartz

August 1, 2017

Objectives

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- What is "out of bag error" (OOB) relative to K-folds?
- How can one interpret variables in tree ensembles?

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  Do we think a prediction from a single tree is good?

Ensemble Challenge

Suppose you are trying to predict the election...

You have 5 expert opinions, each with a 70% chance of being right, and each expert pick is *independent* of the other expert picks.

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```
1 - stats.binom.cdf(26,n=53,p=.7) < .5
< 1 - stats.binom.cdf(27,n=55,p=.7)
```

Averaging Multiple Predictors/Estimators

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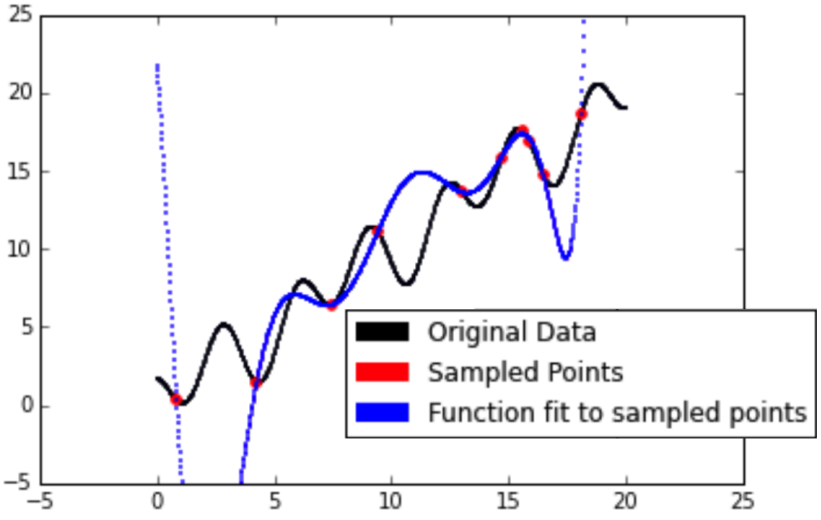
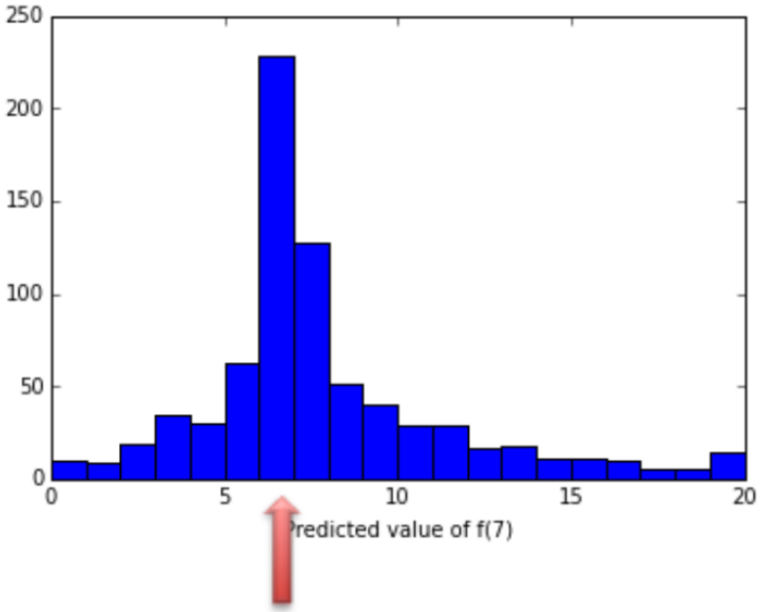
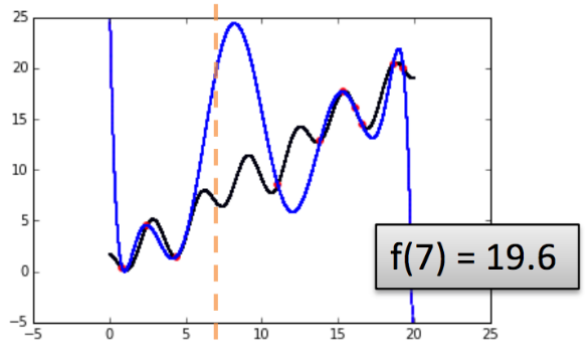
  So even if $\hat{f}^{(j)}$ is a high variance predictor the variance of the *averaged* predictor $\frac{1}{m}\sum_{j=1}^{m}\hat{f}^{(j)}$ decreases with m

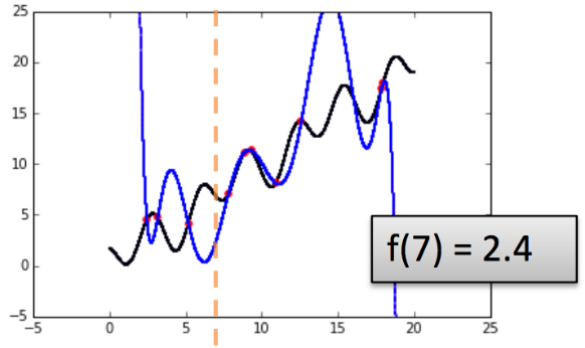
What is happening?

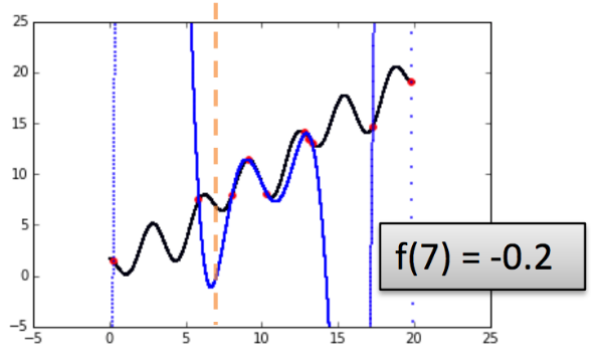




Actual value: f(7) = 6.8







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* *Bagging is a general ensemble procedure often used with trees*

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(j)	Y_1	Y_2	Y_3	Y_4	Y_5	Y_6	Y_7	Y_8	Y_9	$\cdots$
(1)	■	■	■	□	□	■	■	□	■	
(2)	□	□	■	■	■	□	■	■	■	
(3)	■	□	■	■	■	□	■	□	■	
⋮	Bootstrapped samples of size n leave out $\sim \frac{1}{3}$ of the data									

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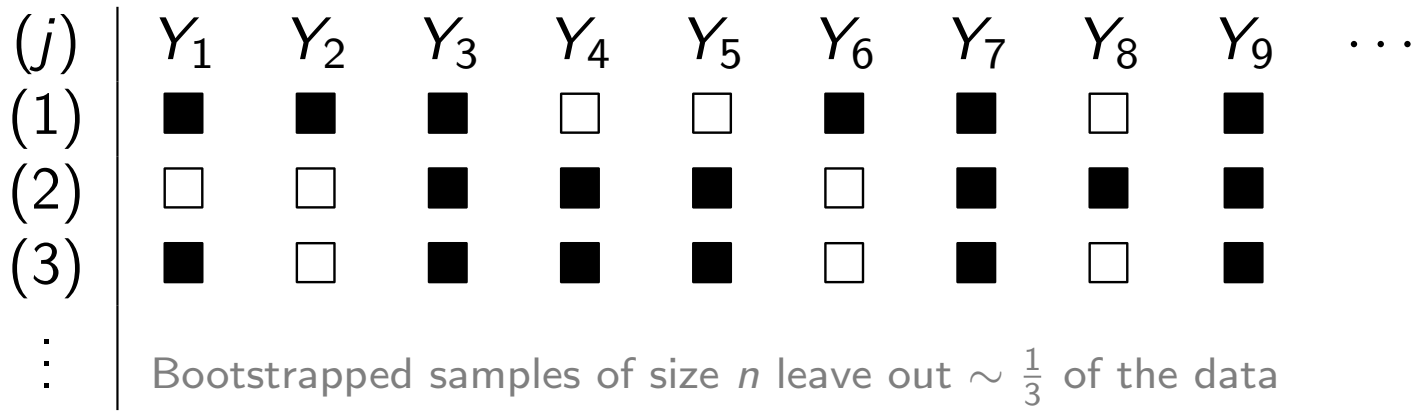

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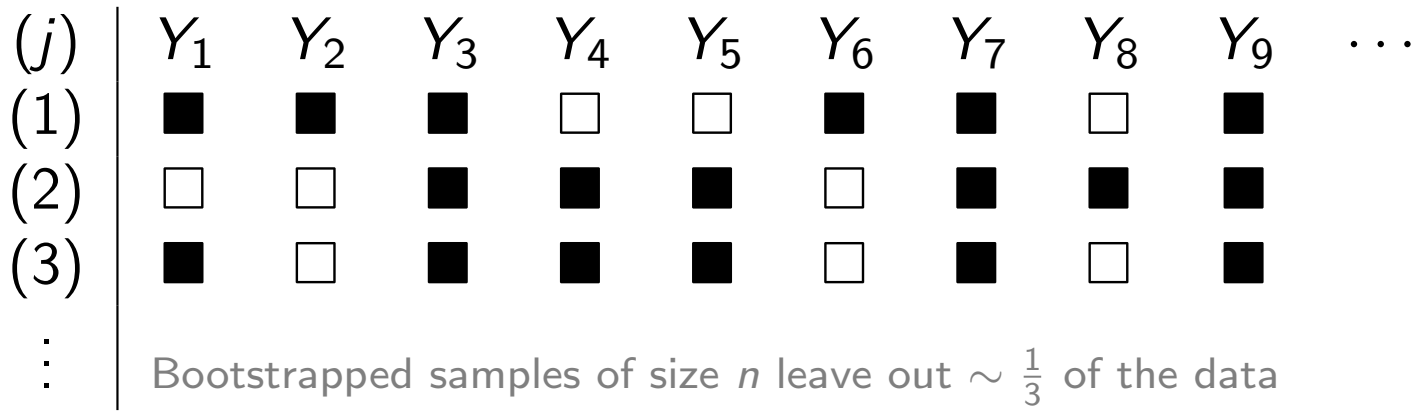

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- Parameter tuning can be done "for free" when model fitting

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- Why?

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I.e.,

$$\text{Var}\left[\hat{f}^{(j)}(\boldsymbol{x}_0) + \hat{f}^{(k)}(\boldsymbol{x}_0)\right] = \text{Var}\left[\hat{f}^{(j)}(\boldsymbol{x}_0)\right] + \text{Var}\left[\hat{f}^{(k)}(\boldsymbol{x}_0)\right] + 2\text{Cov}\left[\hat{f}^{(j)}(\boldsymbol{x}_0), \hat{f}^{(k)}(\boldsymbol{x}_0)\right]$$

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$\hat{f}^{(j)}$ and $\hat{f}^{(k)}$ are correlated: they're predicting the same thing from bootstrapped samples $\boldsymbol{x}^{(j)}/\boldsymbol{Y}^{(j)}$ & $\boldsymbol{x}^{(k)}/\boldsymbol{Y}^{(k)}$ from $\boldsymbol{x}/\boldsymbol{Y}$!

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- So is there any way to get ρ close to 0?

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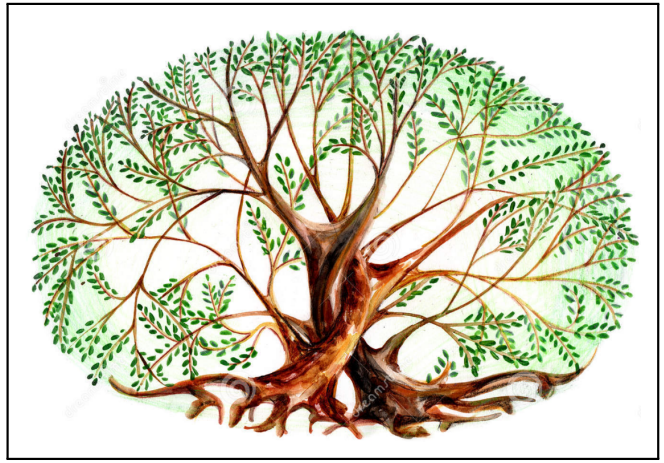

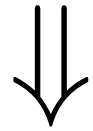

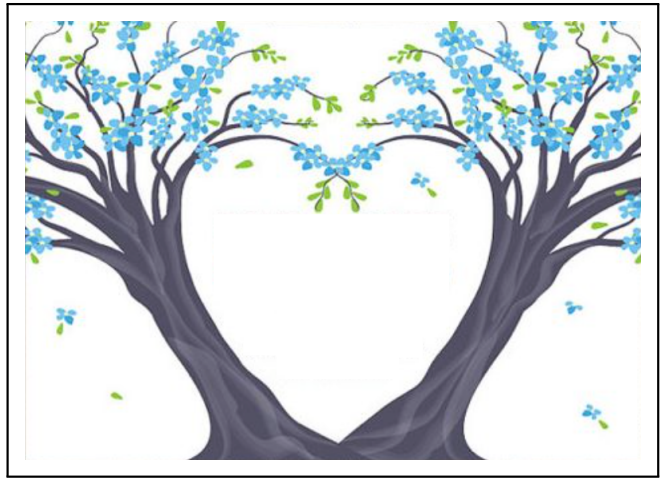

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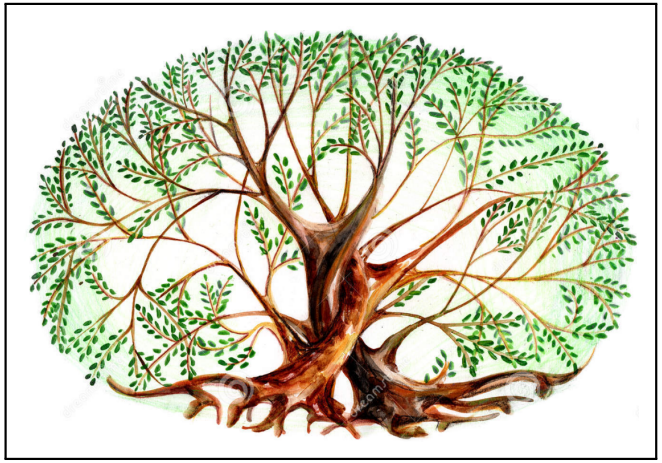
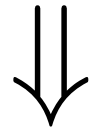
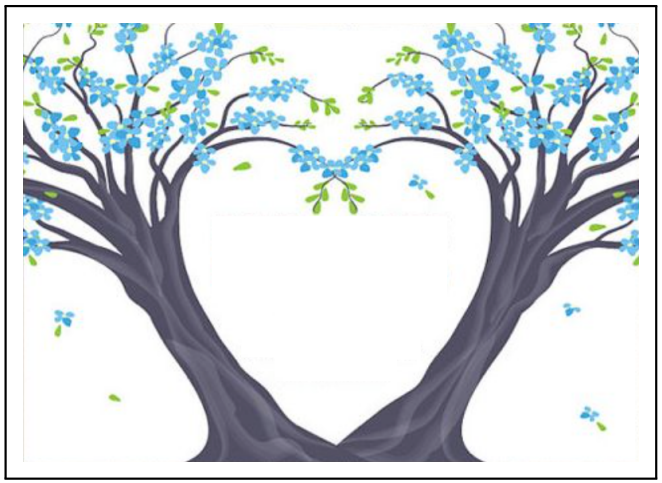
Trees are "correlated" because







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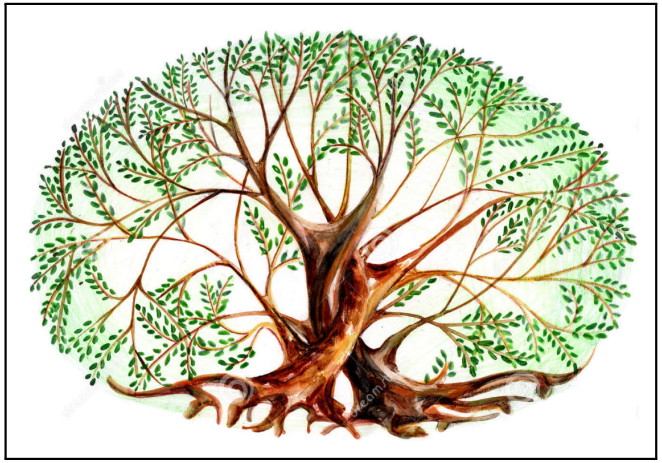

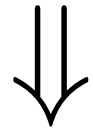

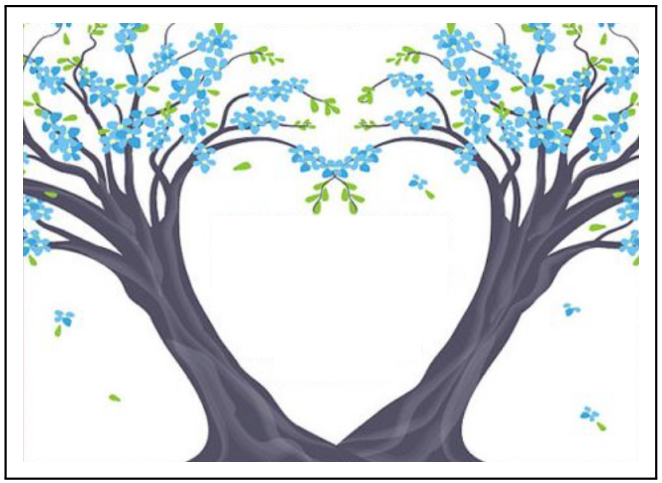

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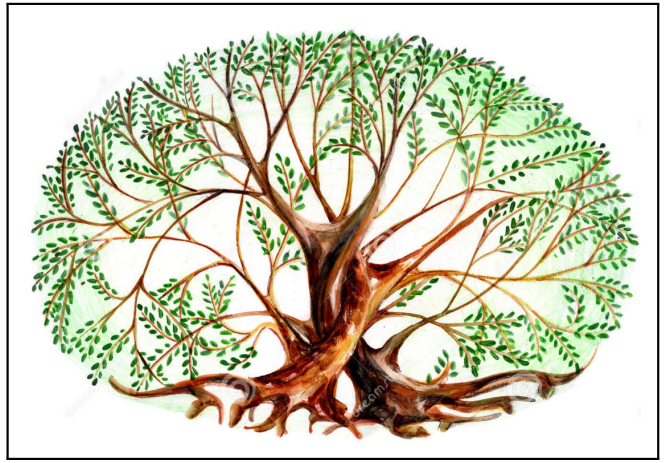

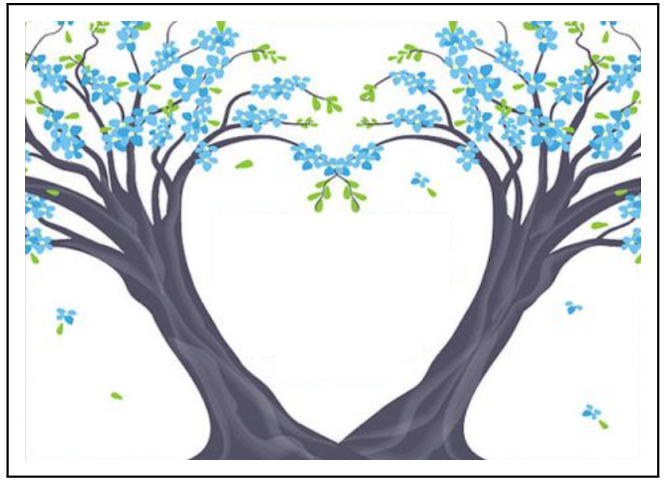

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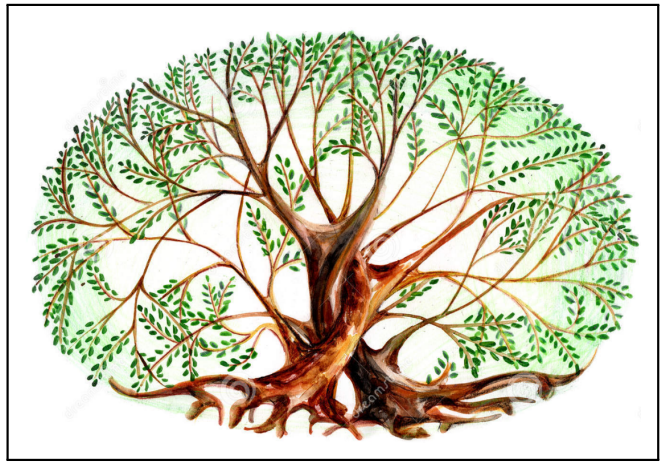
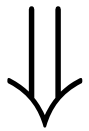
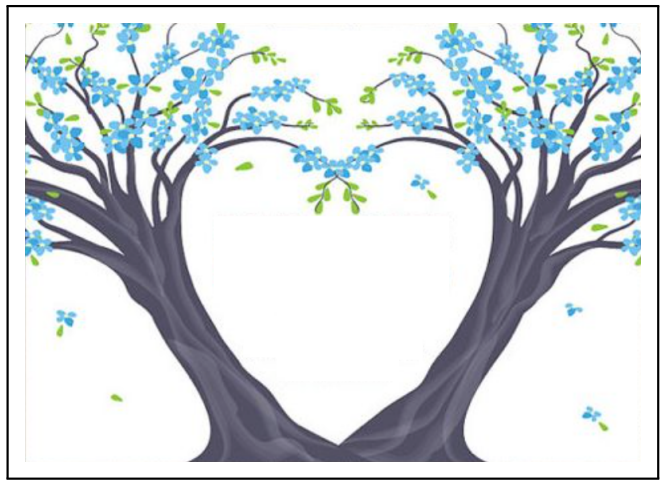
How can we make constructed tree not exactly the same?







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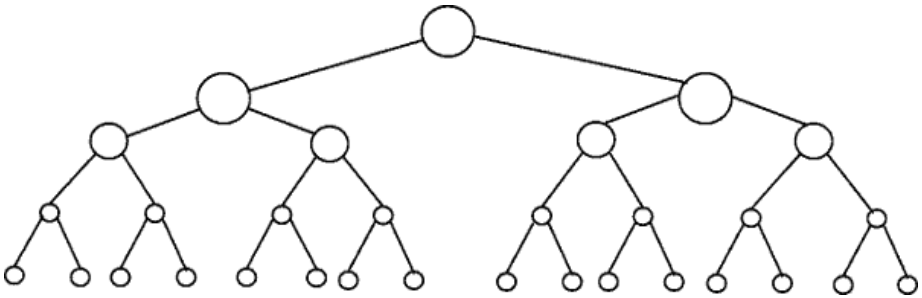

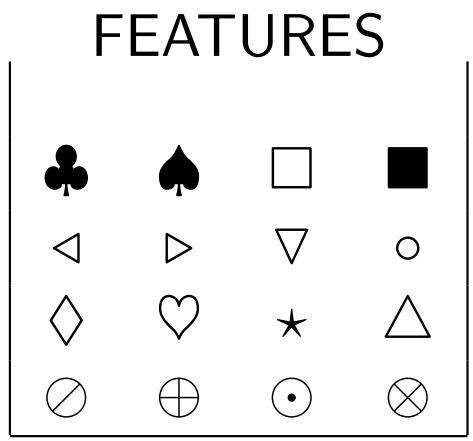

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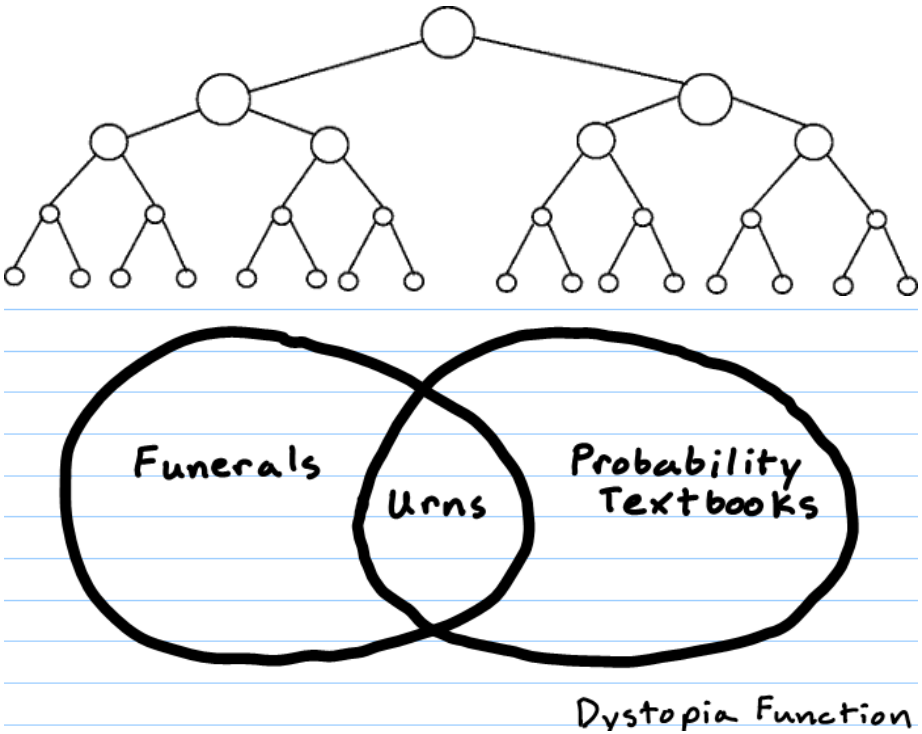

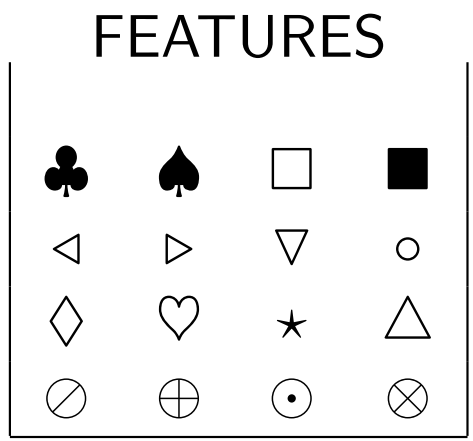

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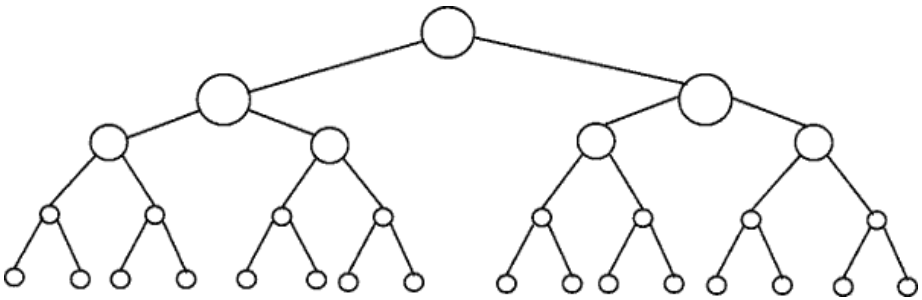

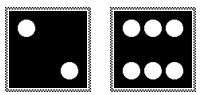

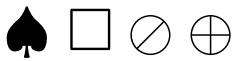

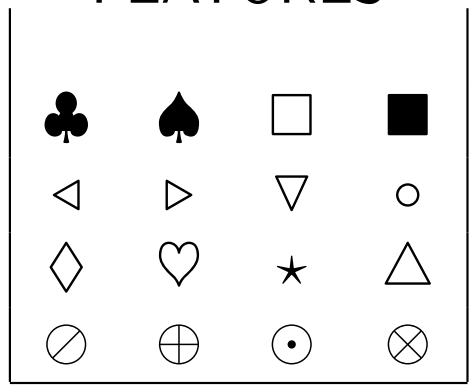

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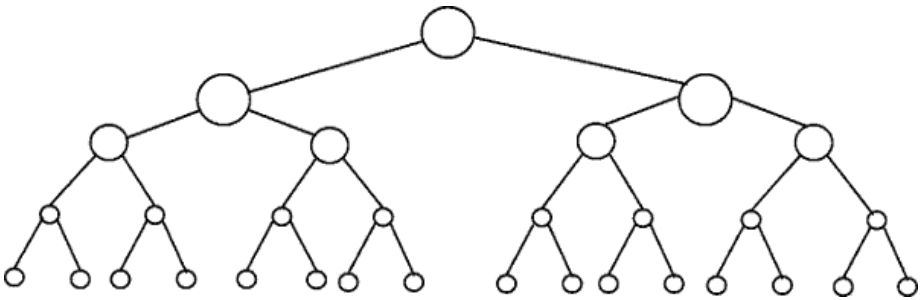

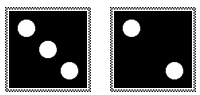

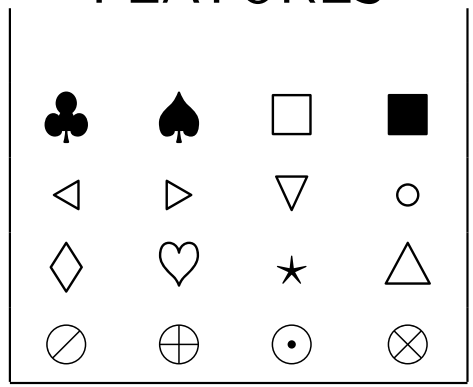

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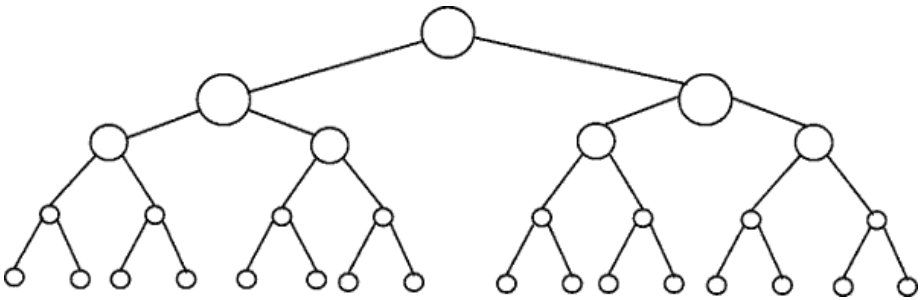

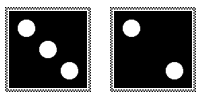

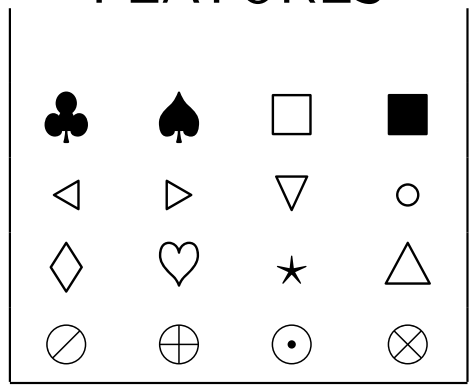

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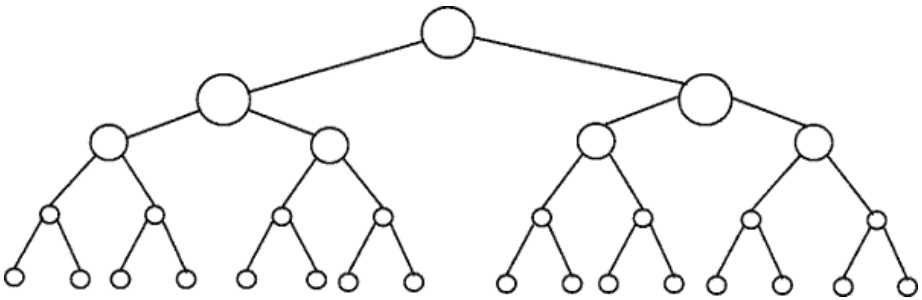

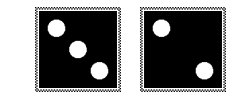

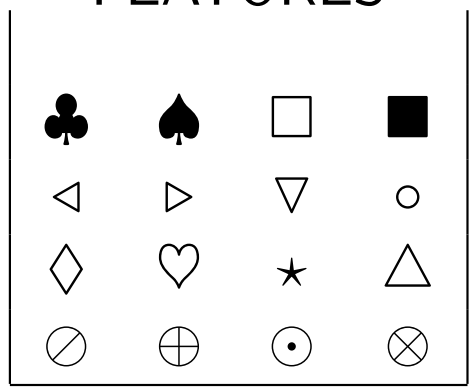

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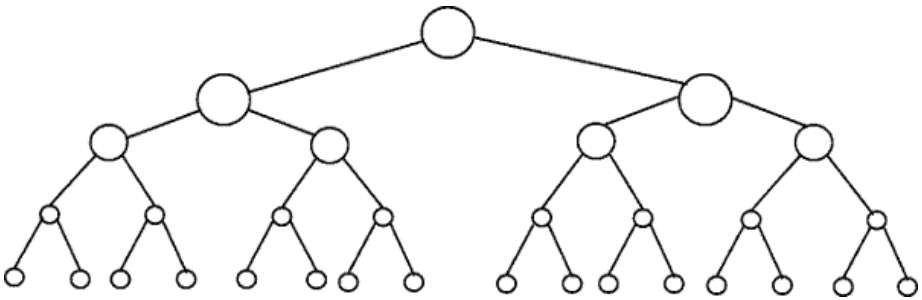

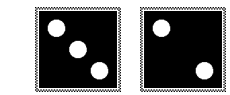

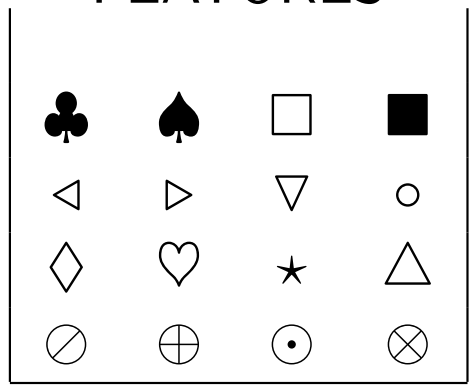

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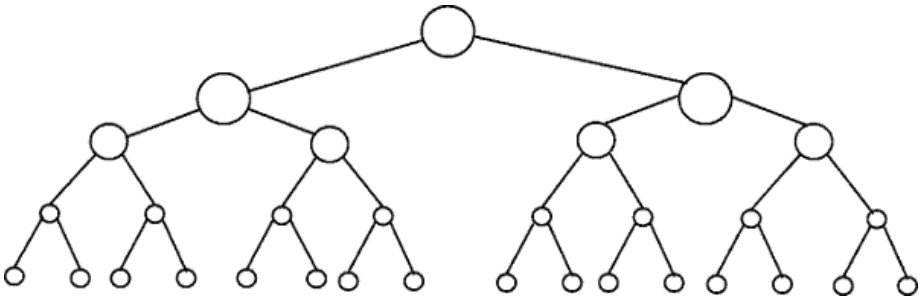

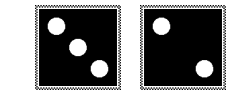

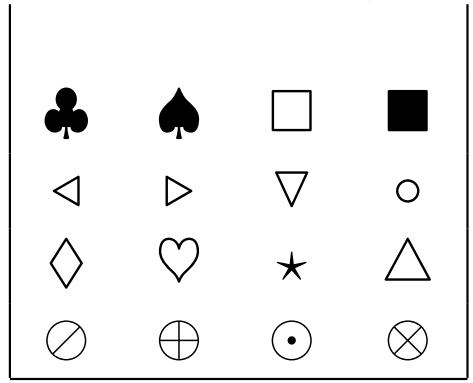

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- More features means stronger but also more correlated trees...

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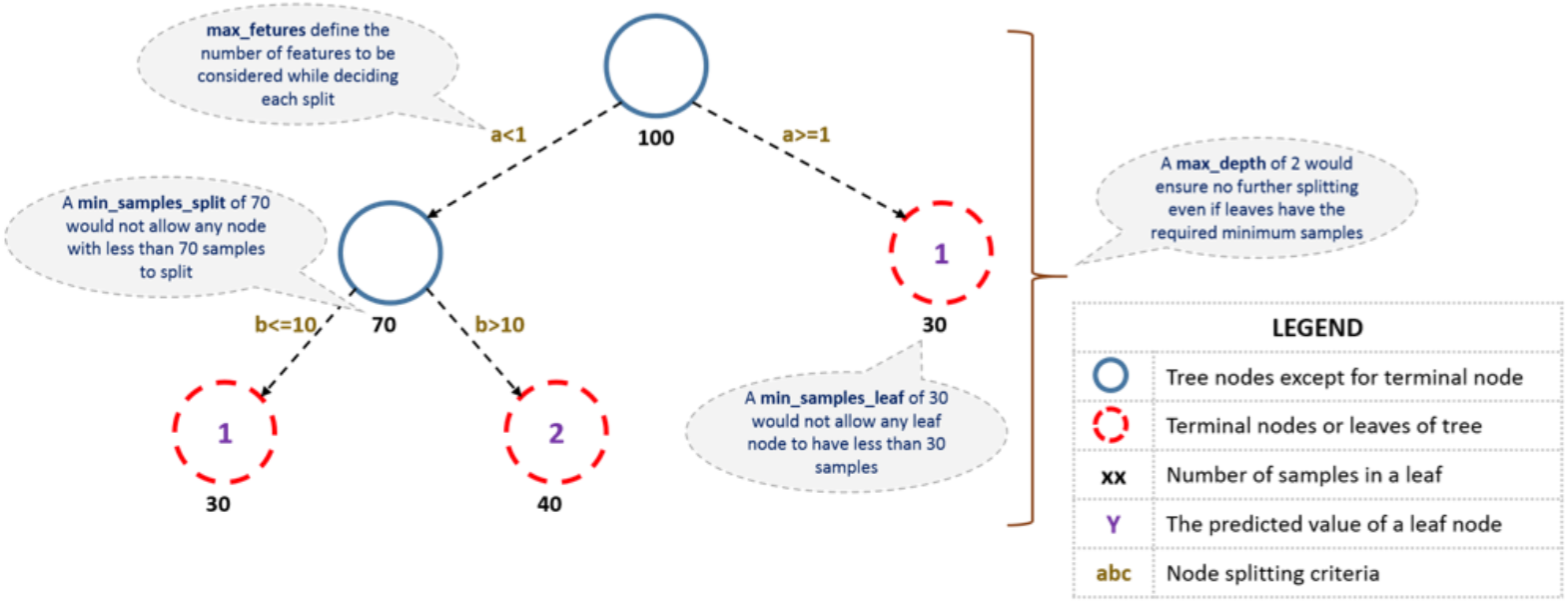

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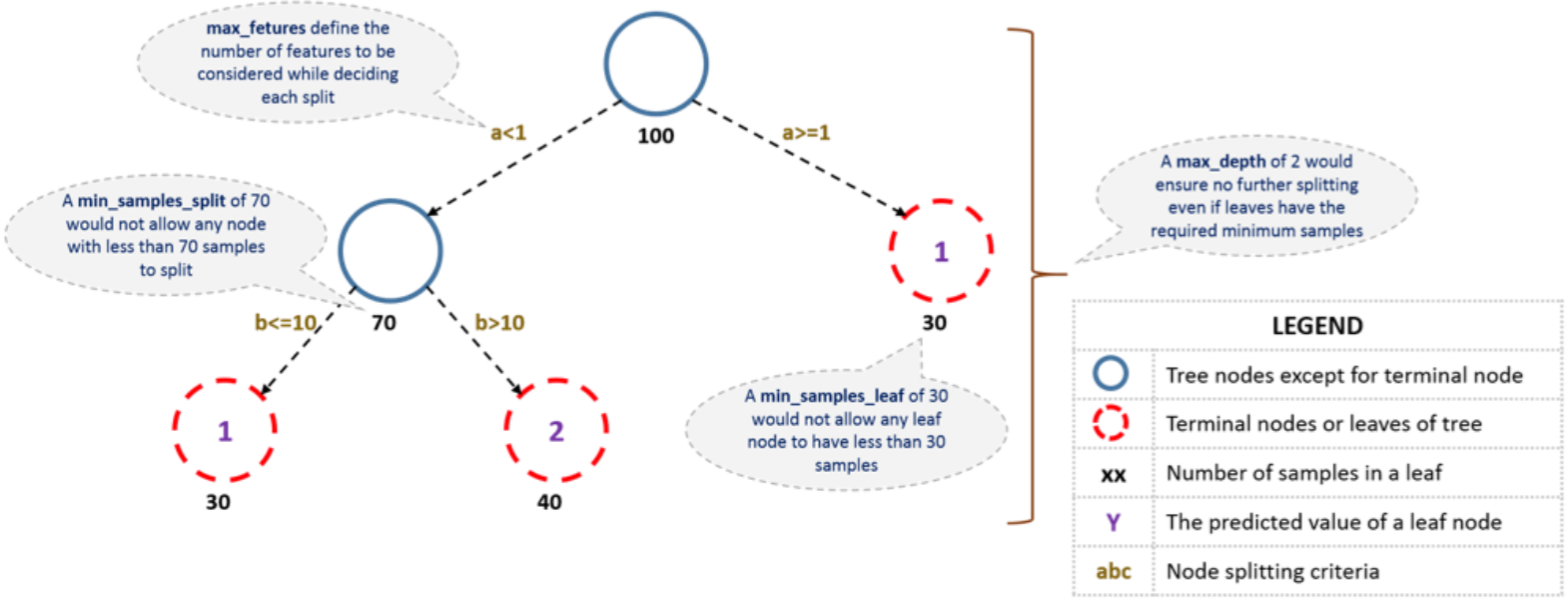

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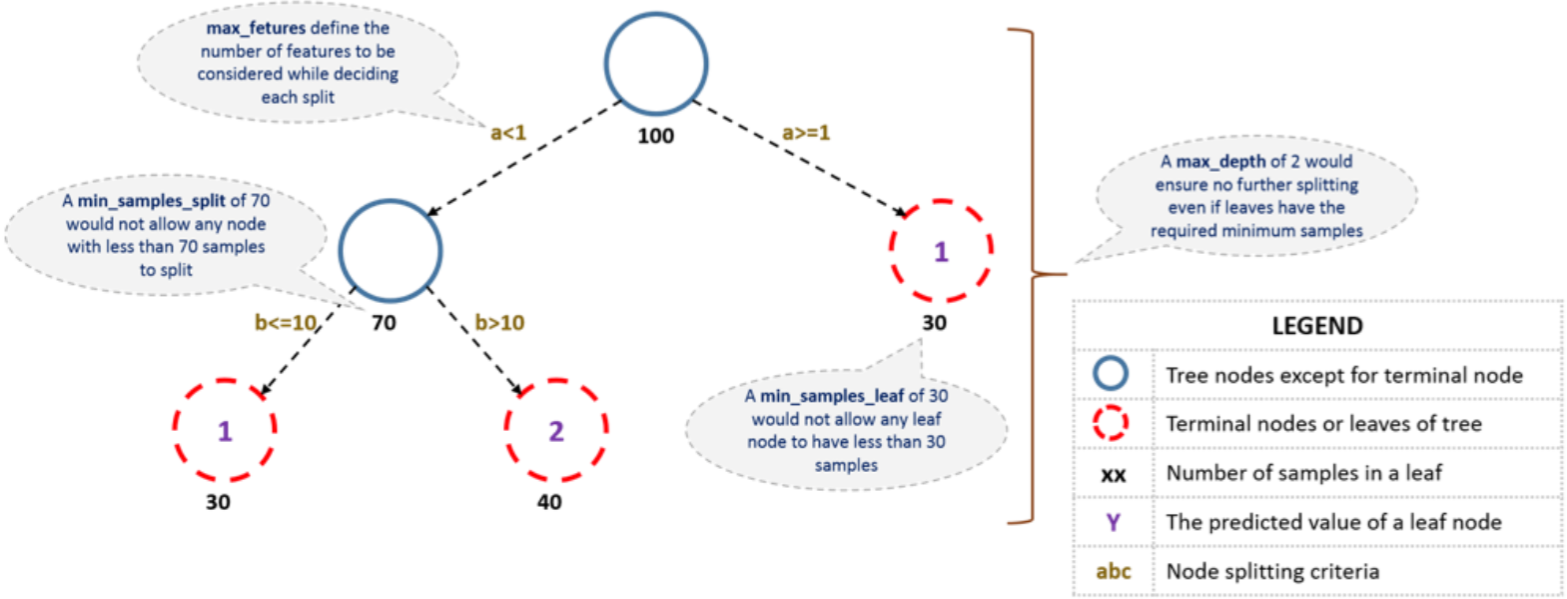

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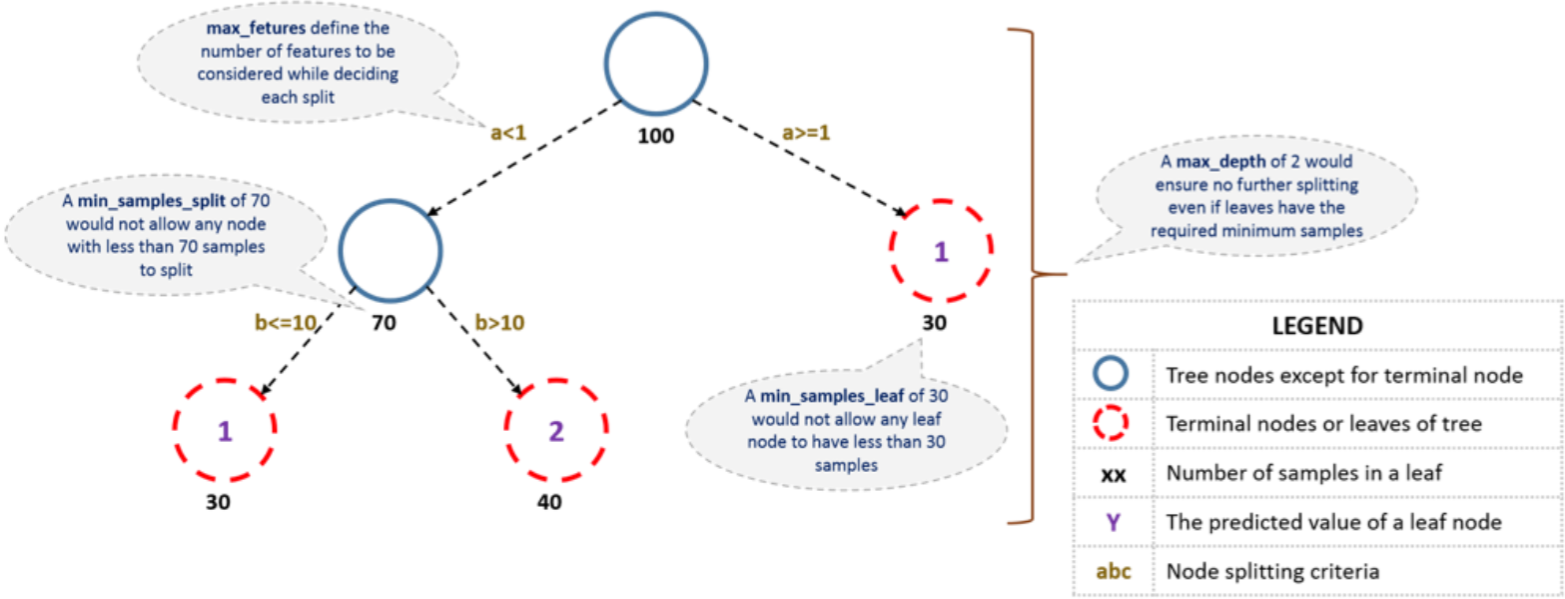

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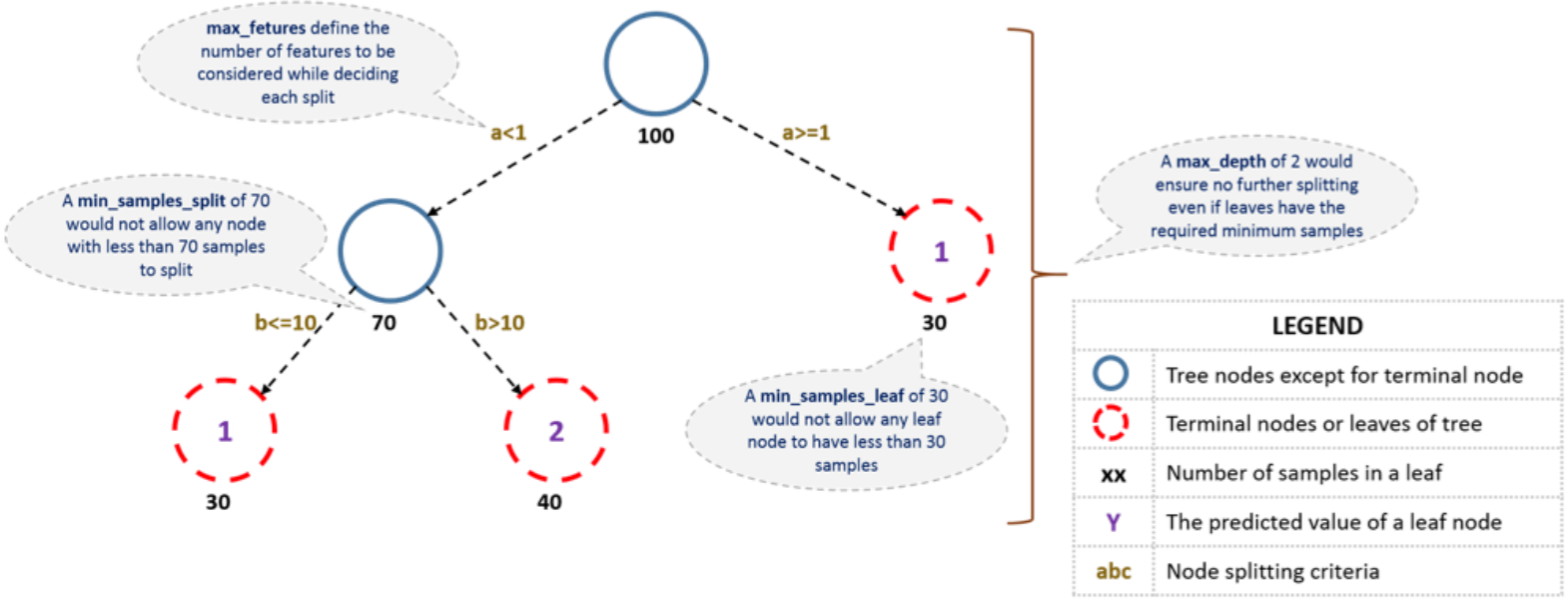

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  - Cross-validation is still needed for methodology comparisons...

    OOB samples don't appear in other model fitting contexts – so you still need a common "out of sample" set to compare on...

Change X_j and see what happens

It's just really not that hard...

Interpreting Models

Change X_i and see what happens

It's just really not that hard...

That's all your doing in a linear model:

$$\beta_0 + \beta_1 X_1 + \beta_1 X_1 + \beta_2 X_2 + \cdots$$

Partial Dependency Plots

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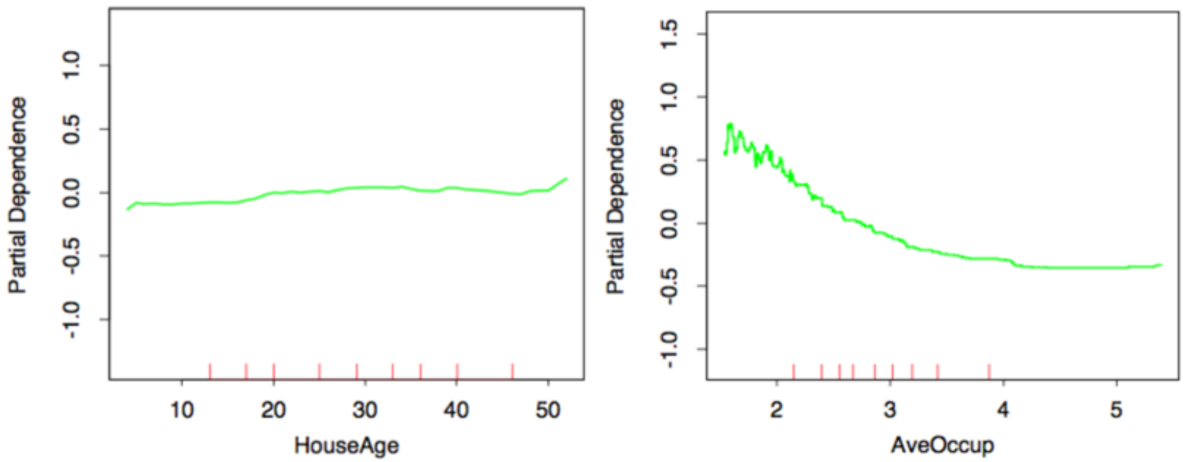

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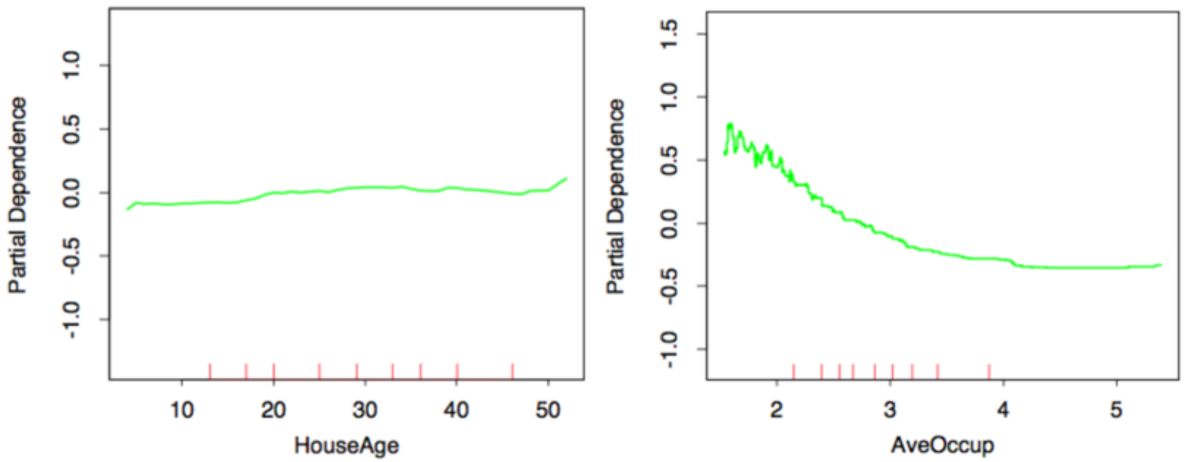

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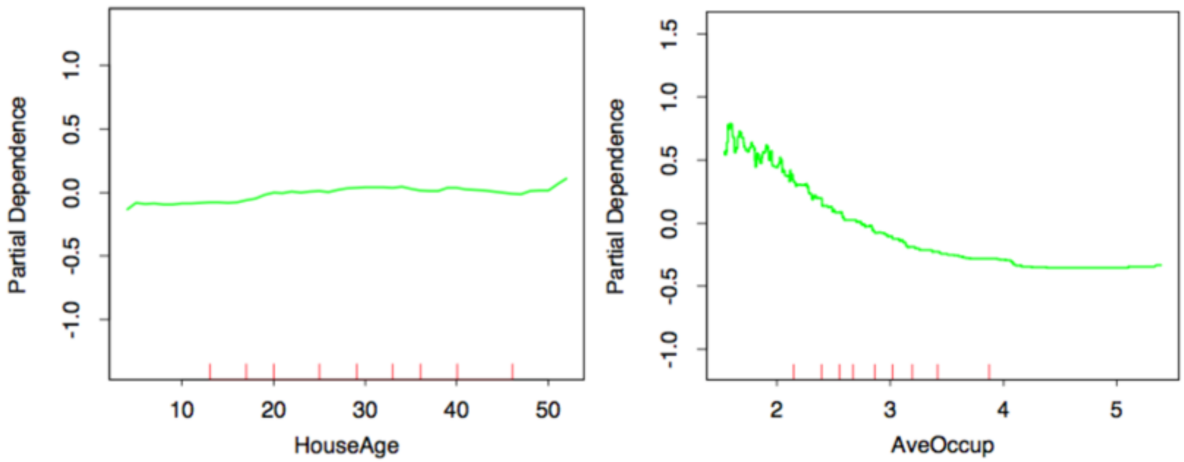
3. Plot $\frac{1}{n}\sum_{i=1}^{n} \hat{Y}_i^{(v)}$ at v



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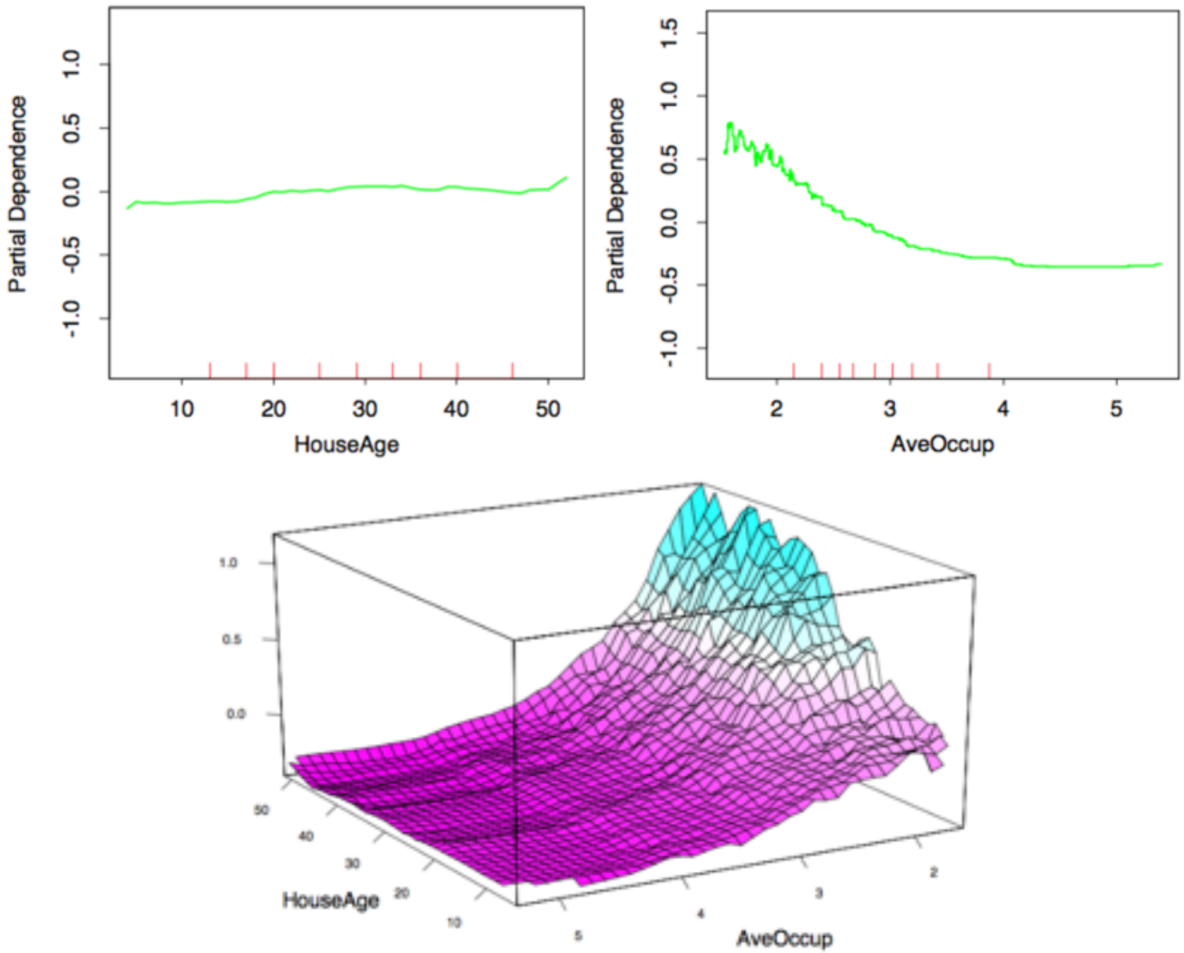

Variable Importance

But there are some other *Very Cool* model interpretation options available in tree based contexts as well...

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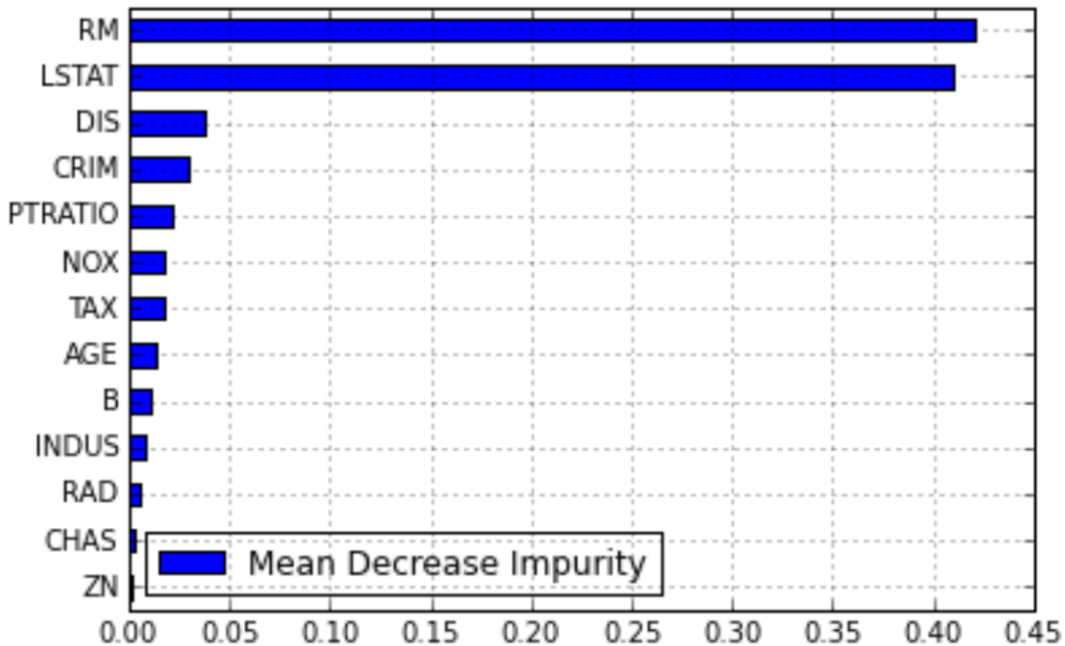

In Boston, the most relevant associations with neighborhood home values are (1) number of rooms and (2) proportion of low income households in the neighborhood

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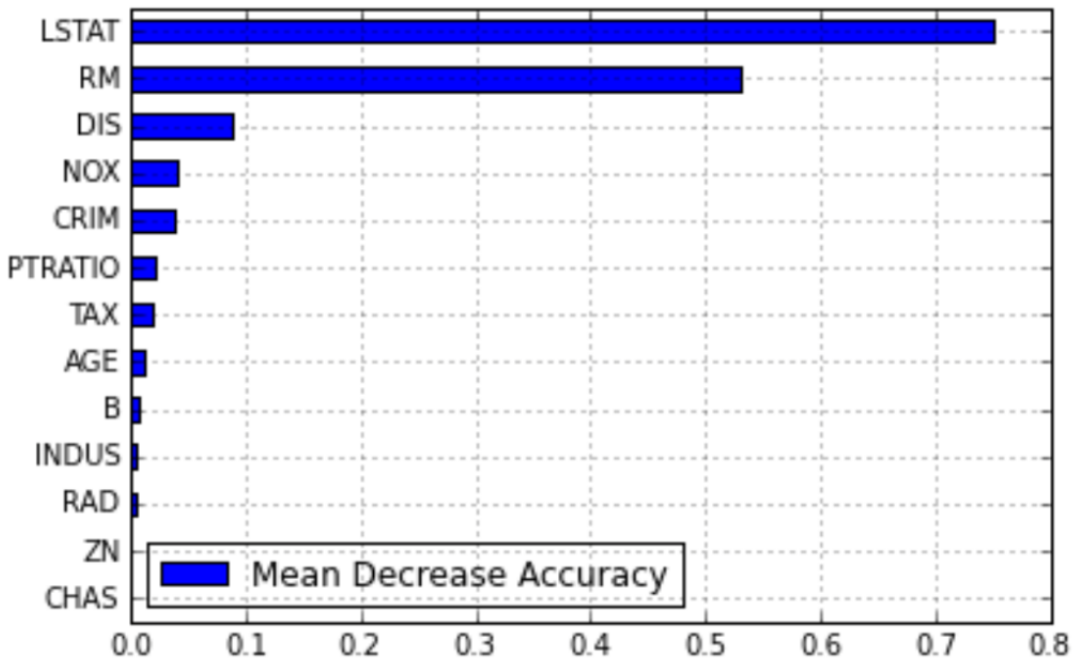

This approach suggests prediction is more sensitive to (1) low income proportion rather than (2) room number

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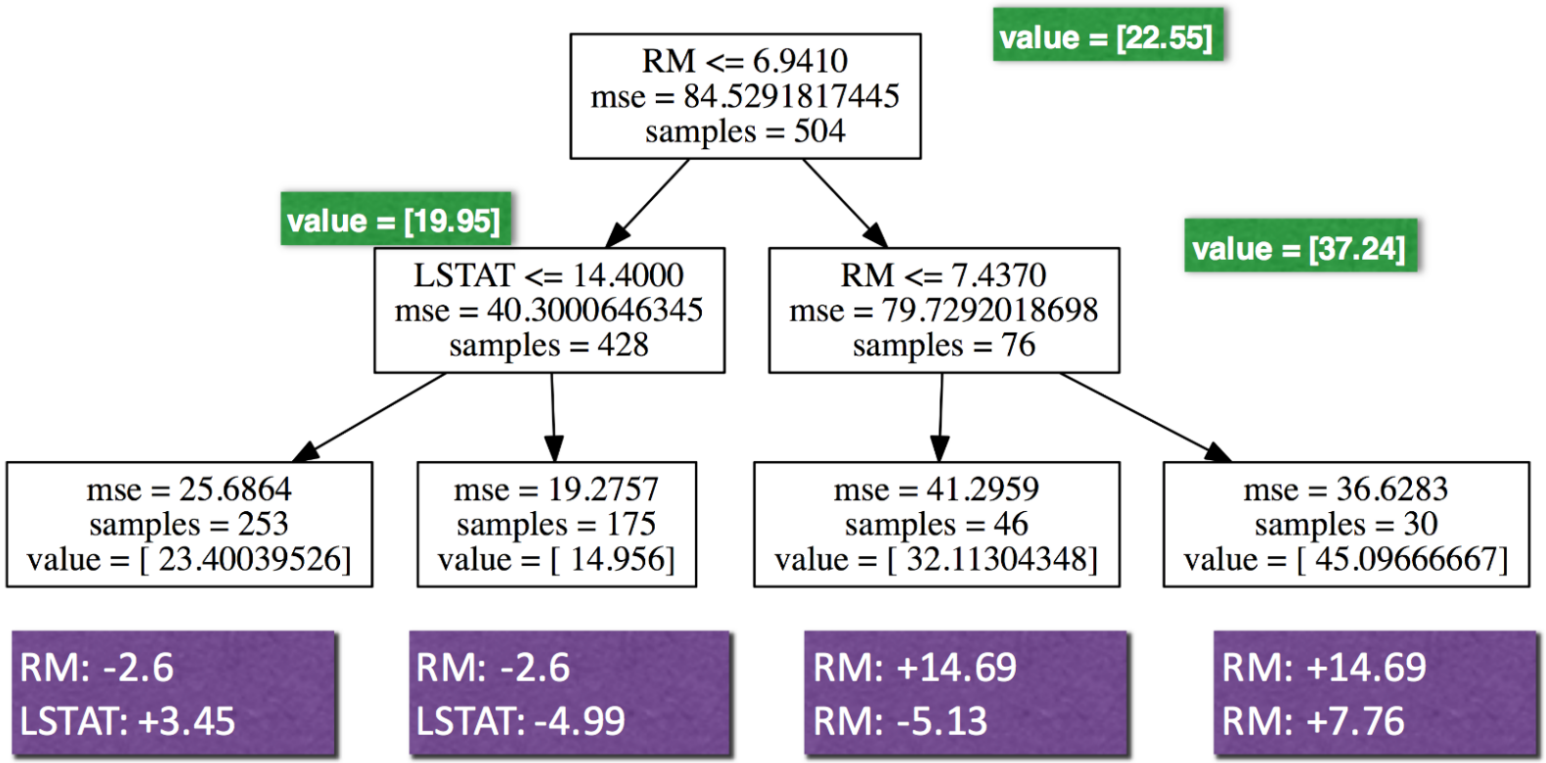

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Distance from city-center

Fraction of lower-class residents

Average number of rooms

	DIS	INDUS	LSTAT	NOX	PTRATIO	RAD	RM	TAX	ZN
Prediction 1	6.11	0.10	2.67	-0.02	-0.19	0.06	-2.63	-0.20	0.03
Prediction 2	6.22	0.16	2.56	-0.01	-0.19	0.06	-3.15	-0.16	0.03
Prediction 3	-0.70	0.04	7.42	-0.11	0.42	-0.02	1.10	-0.14	-0.05
Prediction 4	-0.53	0.25	3.50	0.16	1.46	0.13	2.21	-0.24	0.11
Prediction 5	-0.68	0.15	7.86	0.03	0.85	0.01	-1.14	-0.16	0.18
Prediction 6	0.18	-0.26	8.62	-0.19	-0.02	-0.07	-1.83	-0.34	-0.05

Features effects can be characterized on individual samples (!)

Variable Importance (v4.0): "what the tree predicts with"

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2. Average the "proportion of samples visited" across all trees

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Now:

Tree $<$ **Bagging** $<$ **Random Forests** $<$ **_____?**