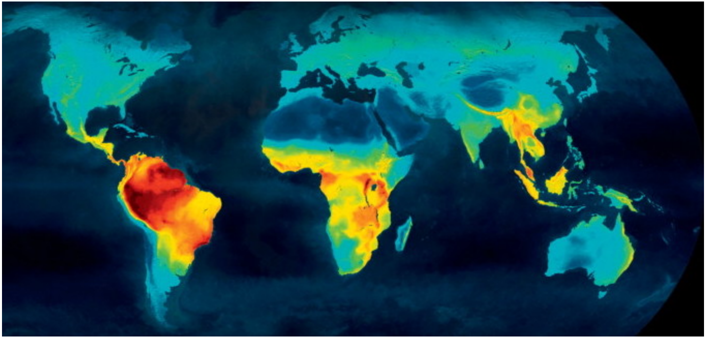
Ensemble Methods (Part I)
Bagging and Random Forests

Schwartz

August 1, 2017

Trees!

A recent study published in the Proceedings of the National Academy of Sciences estimates that there are somewhere between 40,000 to 50,000 unique tree species in the American neotropics and Indo-Pacific tropics, respectively, and that tropical Africa includes an additional approximately 10,000 species. This amount of tree diversity far outpaces tree diversity in temperate regions. For example, temperate forests in Europe have only 124 unique tree species and there are only approximately 1,000 tree species in North America. Another recent study published in Nature estimates that there are 3.04 trillion trees on earth – 422 per person – and that 45% of the trees are in the tropics. Tropical forests make up 2% of the earth's landmass. By area then, tropical jungles produce tree diversity at a rate of 5000:1 and tree density at a rate of 40:1 compared the rest of the earth's dry landmasses.



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

Single Predictors/Estimators

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

Ensemble Challenge

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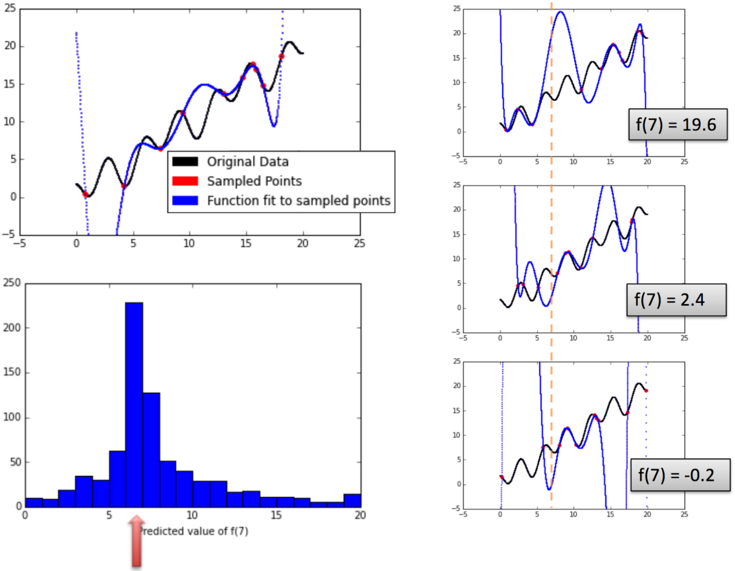
So even if $\hat{f}^{(j)}$ is a high variance predictor the variance of the *averaged* predictor $\frac{1}{m}\sum_{j=1}^{m}\hat{f}^{(j)}$ decreases with m

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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- Parameter tuning can be done “for free” when model fitting

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I.e.,

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

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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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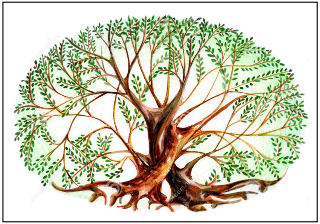

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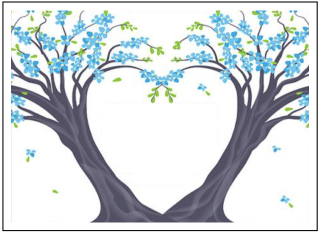

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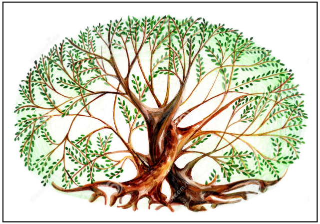

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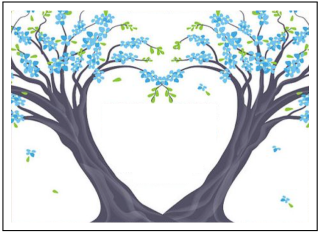

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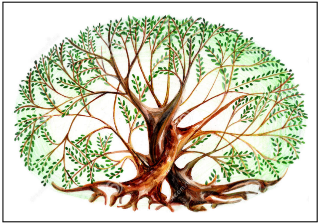

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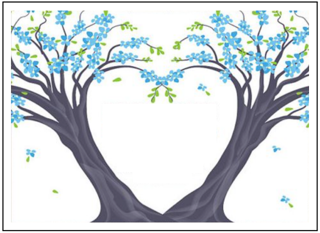

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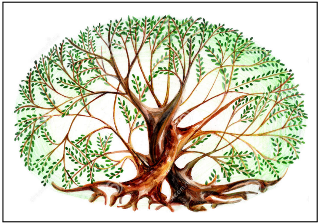

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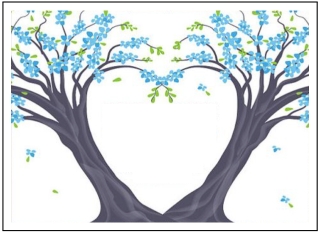

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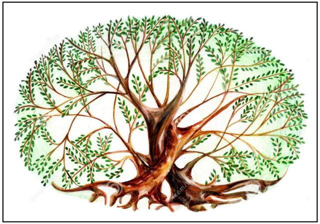
How can we make constructed tree not exactly the same?



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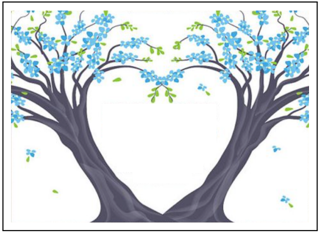

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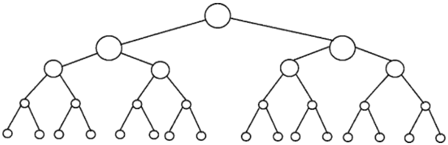
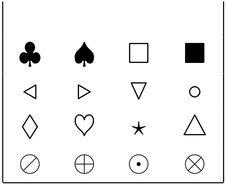


FEATURES



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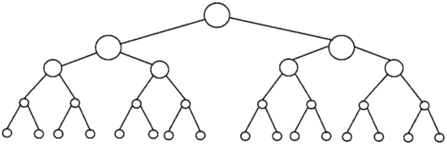

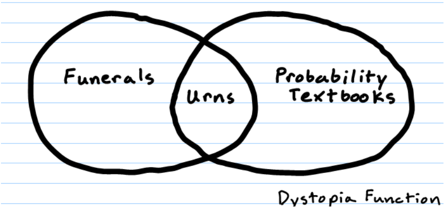

FEATURES

$\clubsuit$	$\spadesuit$	$\square$	$\blacksquare$
$\triangleleft$	$\triangleright$	$\triangledown$	$\circ$
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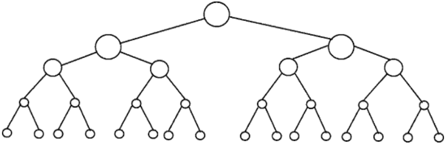

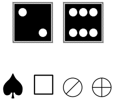

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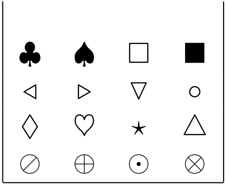

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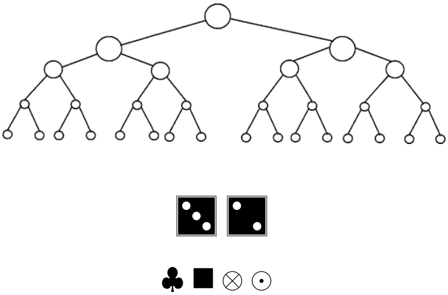

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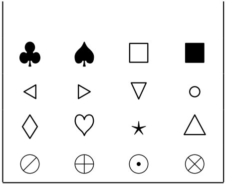

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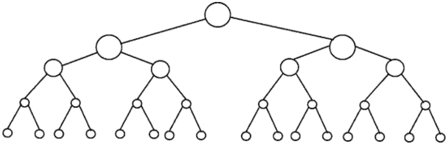

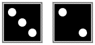

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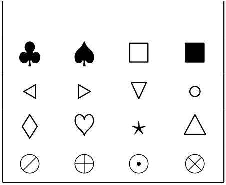

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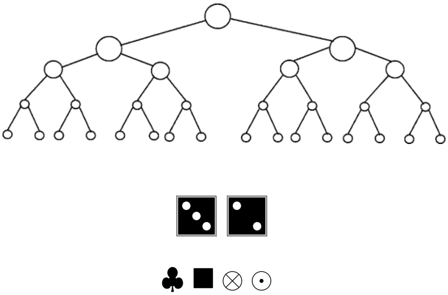

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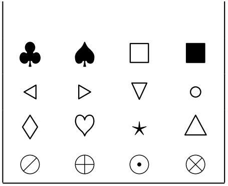

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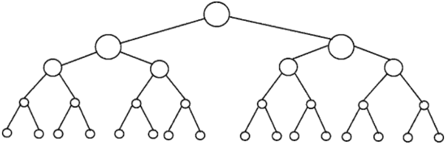

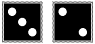

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FEATURES

♣	♠	□	■
◁	▷	▽	○
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⊘	⊕	⊙	⊗

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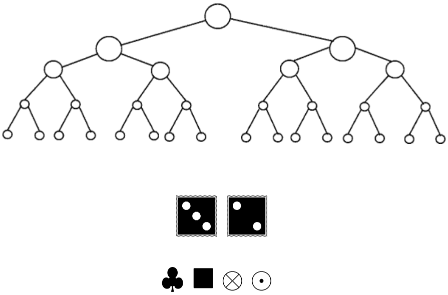

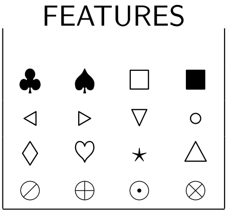

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- More features means stronger but also more correlated trees...

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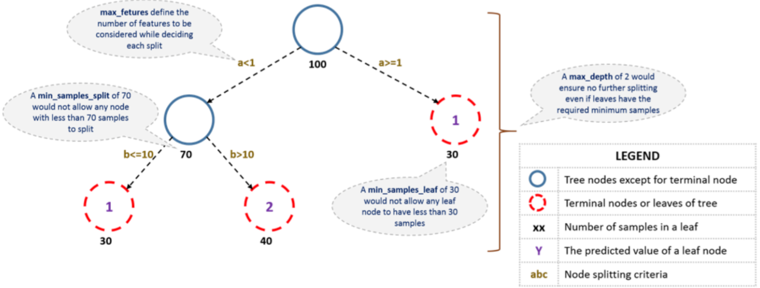

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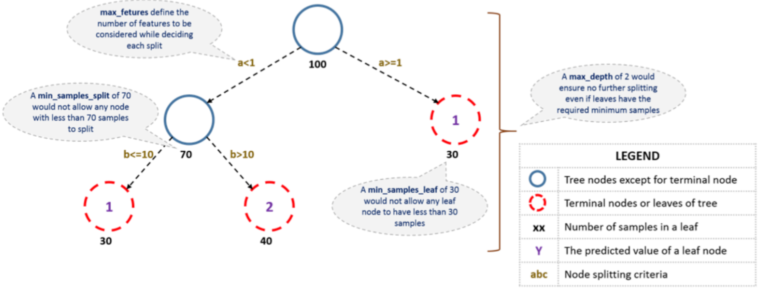

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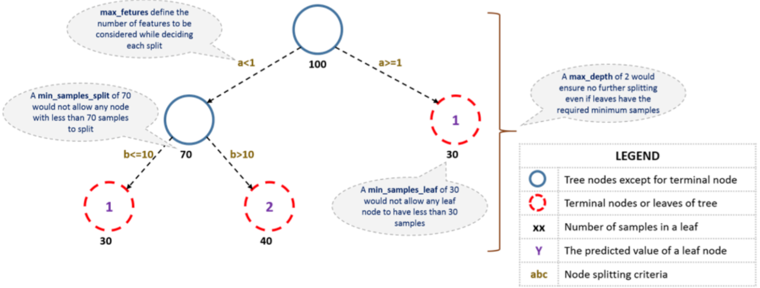

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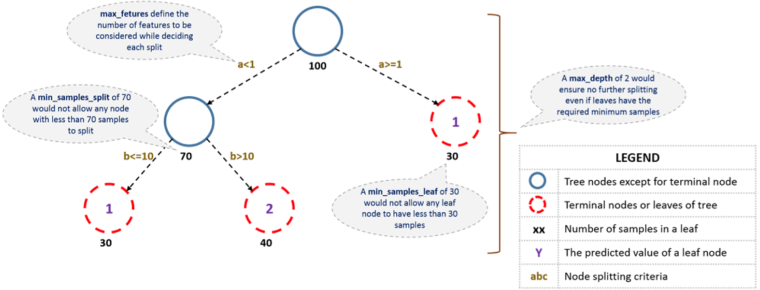

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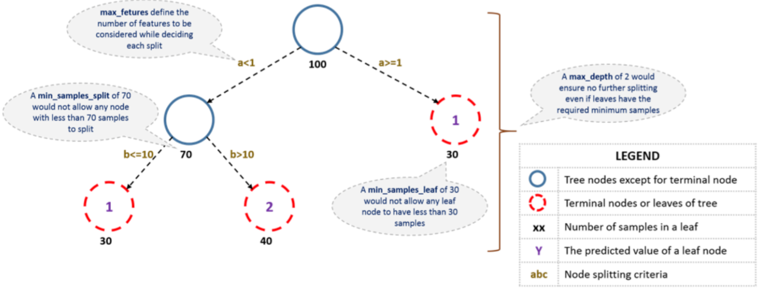

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    You have built-in test samples so you don't need K-folds – you score a model right when it's fit at a specific tuning parameter!

  - 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...

Interpreting Tree Ensembles

"Plentie is nodeintie, ye see not your owne ease. I see, ye can not see the wood for trees."

– J. Heywood (1546)

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"I find that people be all like,

'Machine learning models are "Black Boxes" and you can't interpret them...',

and I be like, 'Damn you people have some back-ass wackwards ideas...'"

– S. Schwartz (Yesterday)

Interpreting Models

Change X_i and see what happens

It's just really not that hard...

Change X_i and see what happens

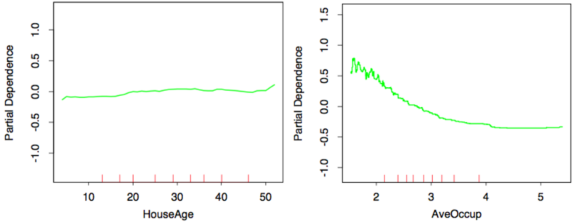
It's just really not that hard...

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

1. Set feature $V = v$ for a single values v



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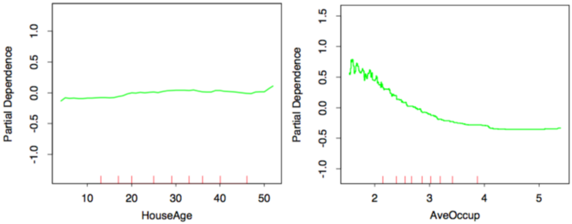

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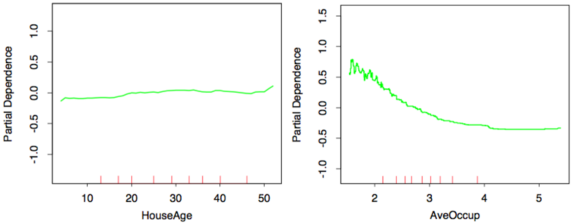

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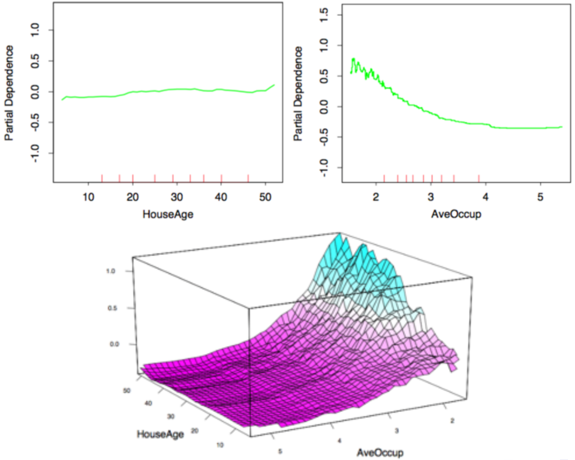

But there are some other *Very Cool* model interpretation options available in tree based contexts as well...

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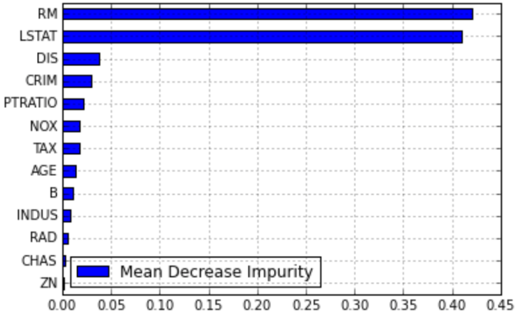

In Boston, the most relevant associations with neighborhood home values are (1) number of rooms and (2) proportion of low income households in the neighborhood

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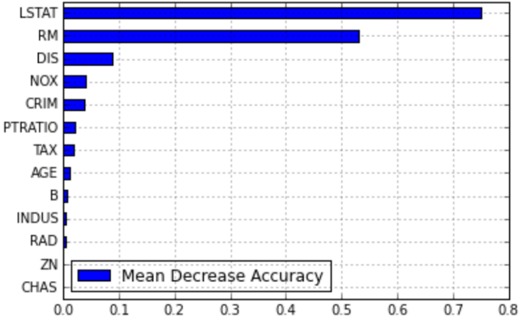

This approach suggests prediction is more sensitive to (1) low income proportion rather than (2) room number

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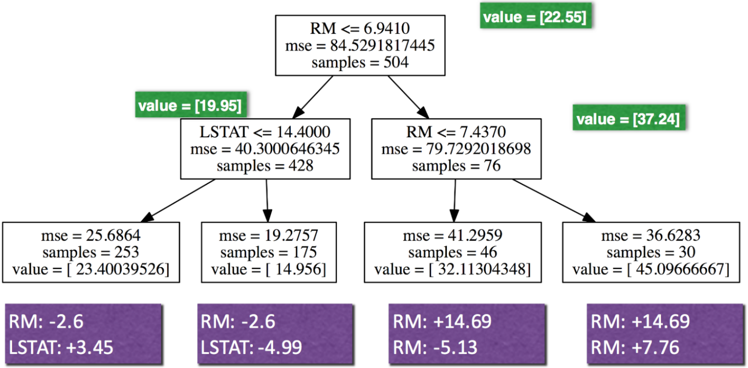

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Distance from city-center

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 (!)

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2. Average the “proportion of samples visited” across all trees

Fine

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Now:

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