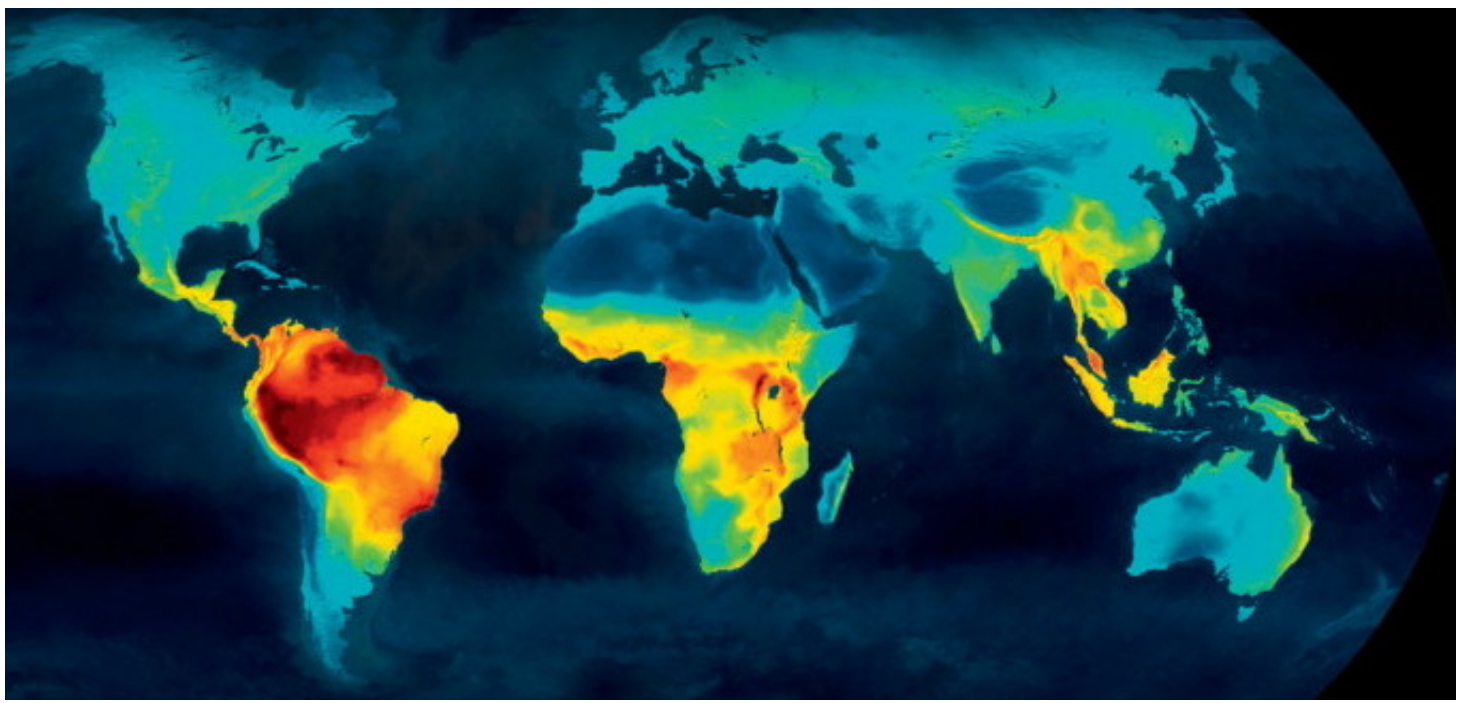
Ensemble Methods (Part I)
Bagging and Random Forests

Schwartz

January 3, 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 Estimators

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  Do we think a tree prediction is a good one?

Ensemble Challenge

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

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

How could you leverage expert picks to improve accuracy and how often would you be right?

How many independent predictors would you need to have a 99.9% of being correct?

Averaging Multiple Estimators

- Let $\hat{f}^{(j)}(\boldsymbol{x}_0)$ be an estimator of outcome $f(\boldsymbol{x}_0)$ constructed from a training set with features $\boldsymbol{x}^{(j)}$ and outcomes $\boldsymbol{Y}^{(j)}$

- If each $\hat{f}^{(j)}(\boldsymbol{x}_0)$ is an unbiased estimator of $f(\boldsymbol{x}_0)$ then

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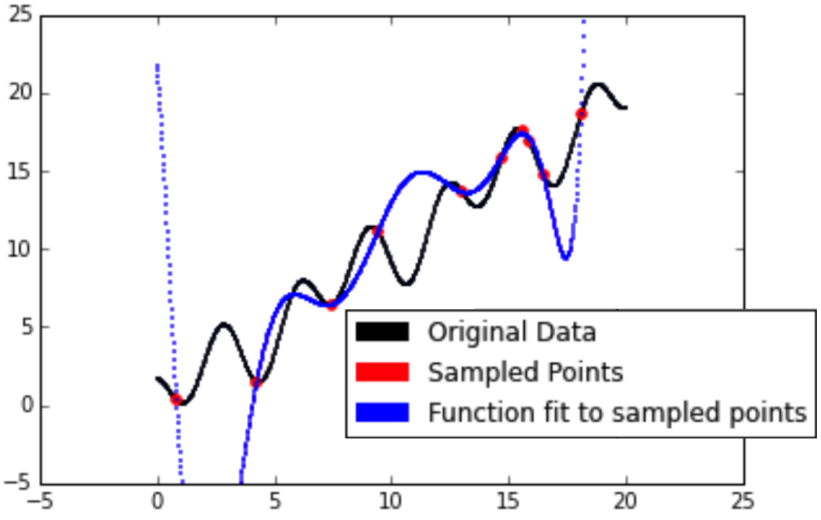
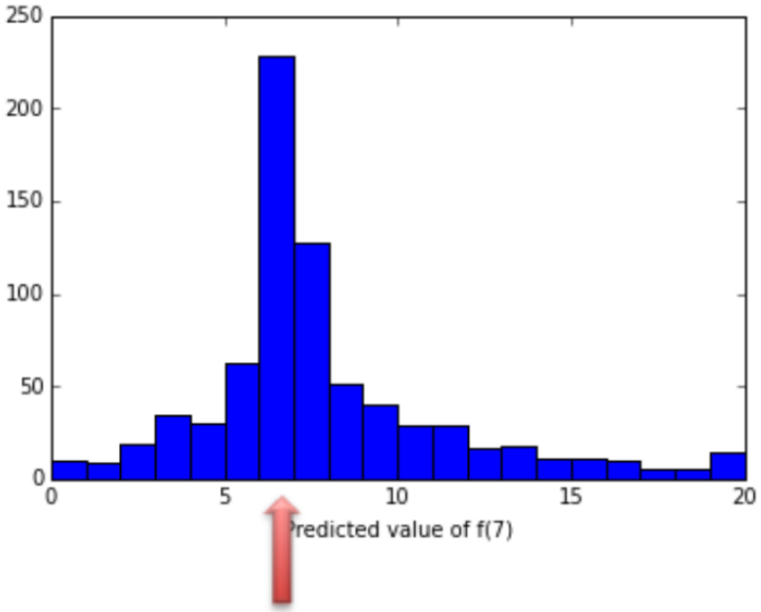
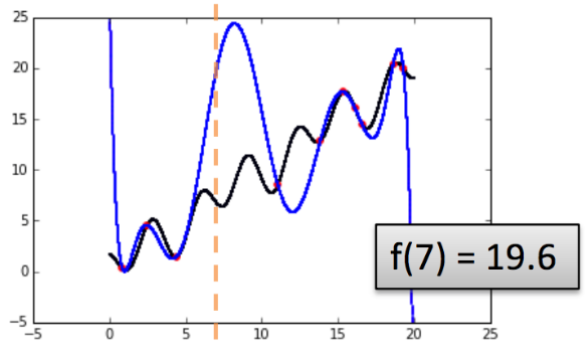
  So even if $\hat{f}^{(j)}$ is a high variance estimator the variance of the *average* estimator $\frac{1}{m}\sum_{j=1}^{m}\hat{f}^{(j)}$ decreases with m

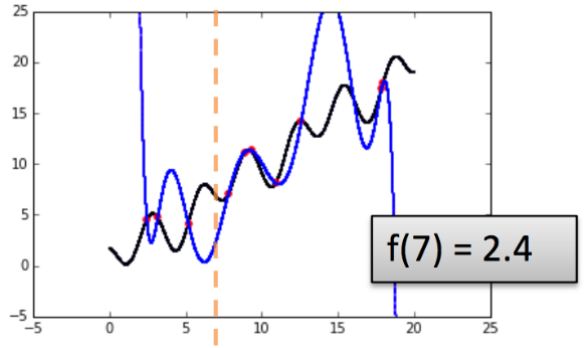
What is happening?

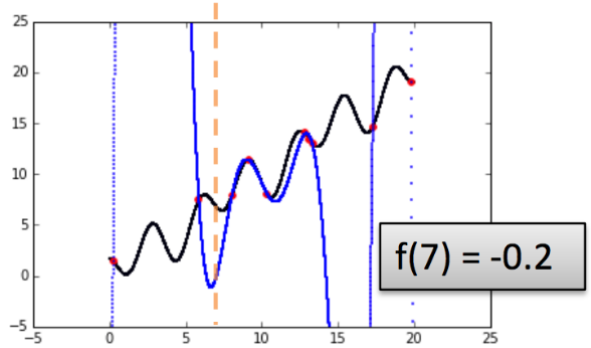




Actual value: f(7) = 6.8







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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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- Why?

$$\text{Var}\left[X + Y\right] = \text{Var}\left[X\right] + \text{Var}\left[Y\right] + 2\text{Cov}\left[X, Y\right]$$

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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- So $\hat{f}^{(j)}$ and $\hat{f}^{(k)}$ are expected to be correlated

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

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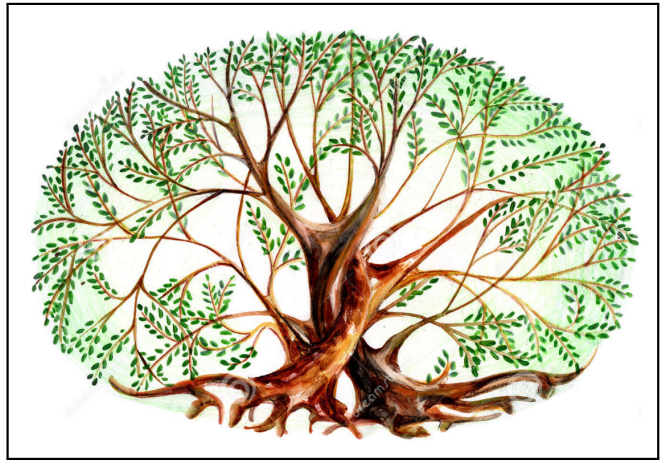

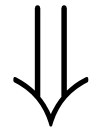

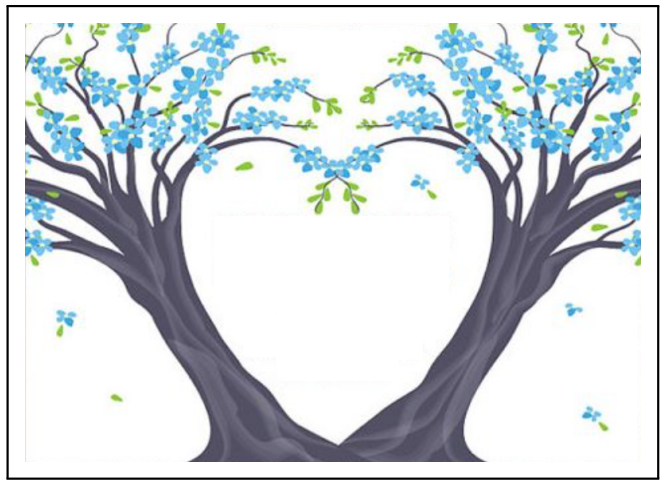

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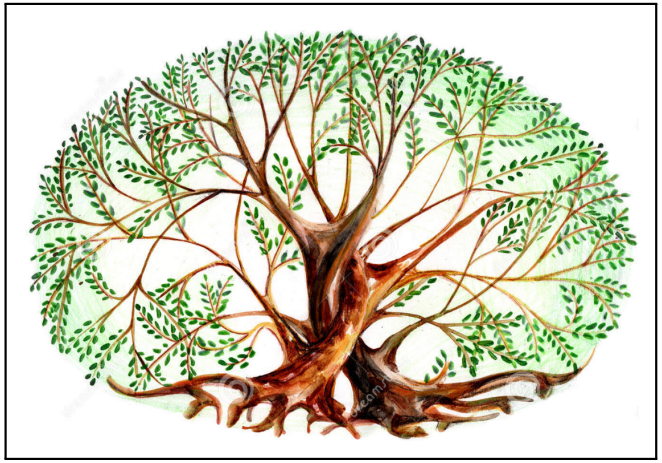

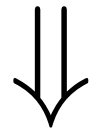

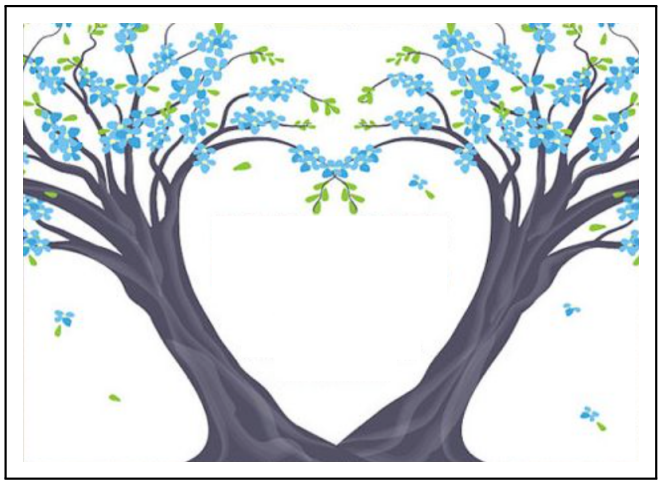

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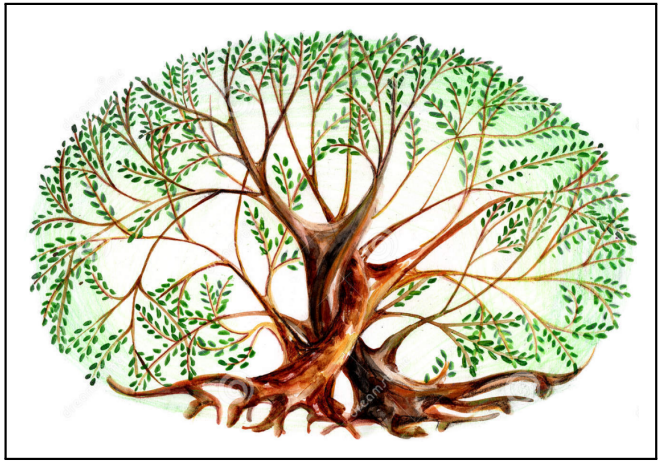

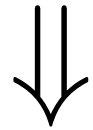

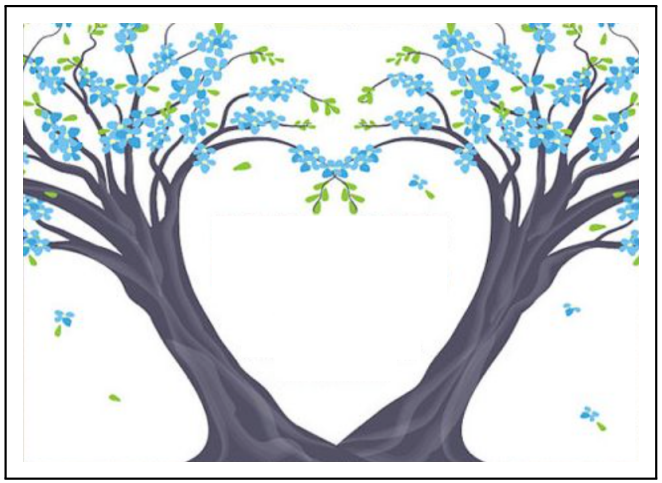

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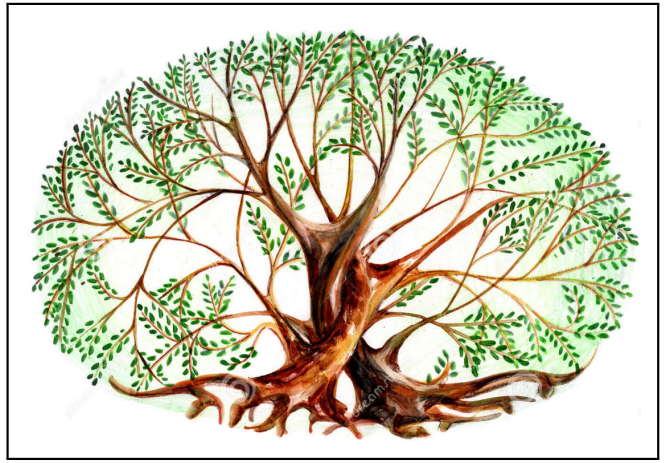

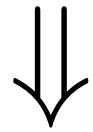

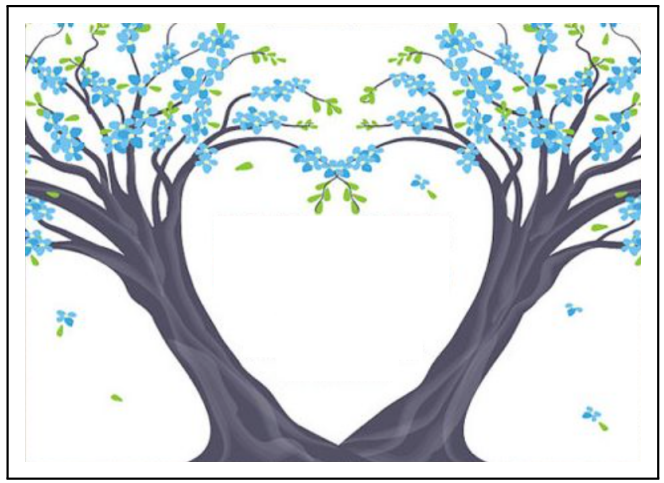

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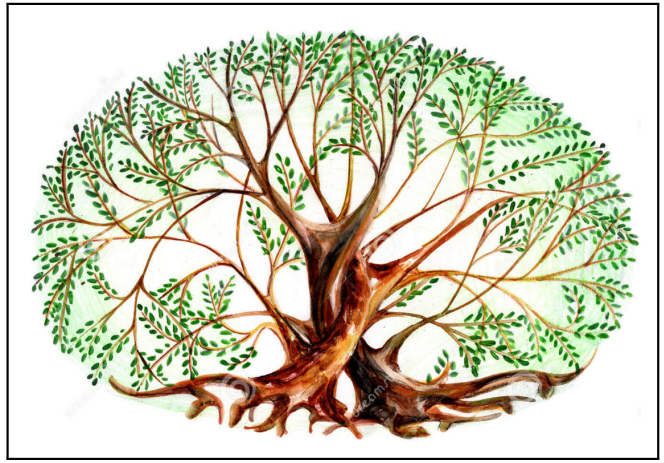
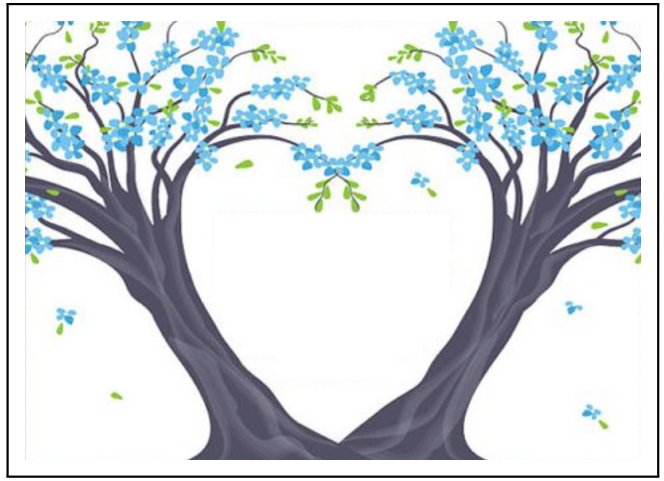
How can we make constructed tree not exactly the same?





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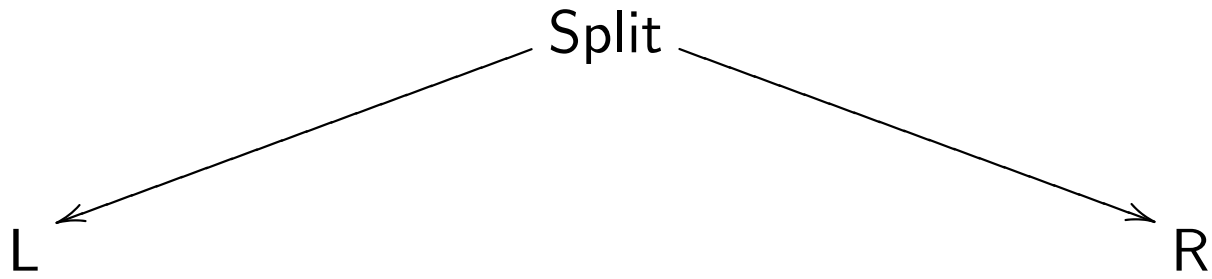

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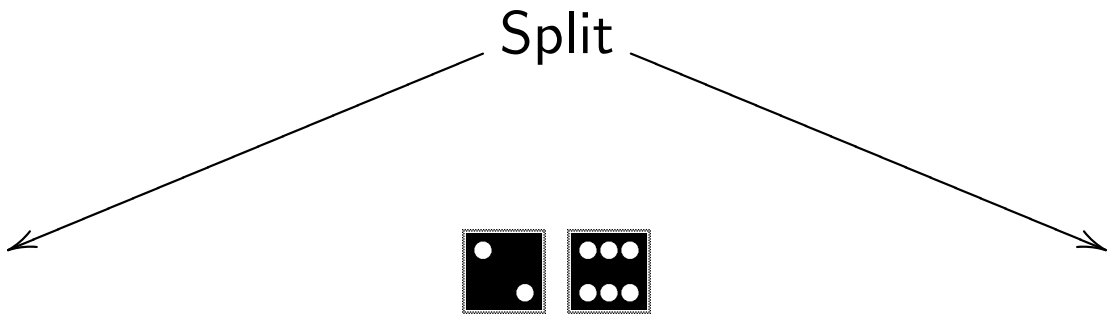

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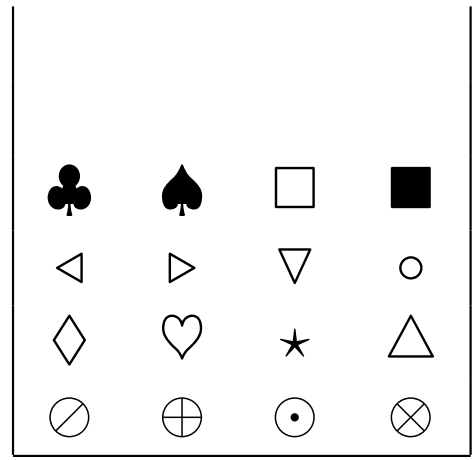

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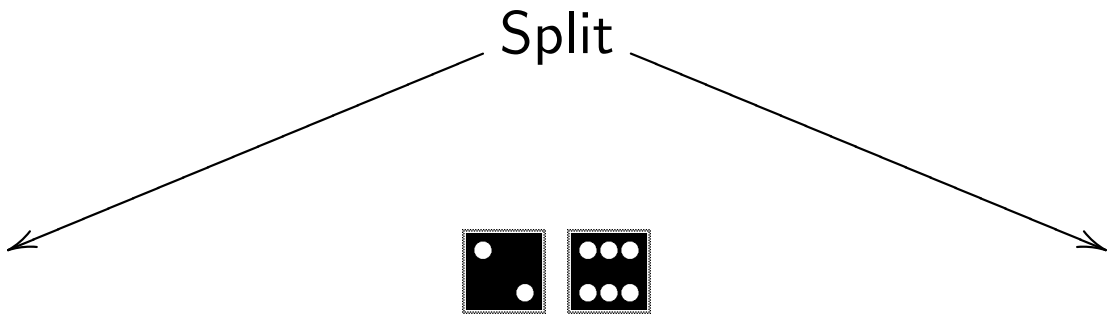

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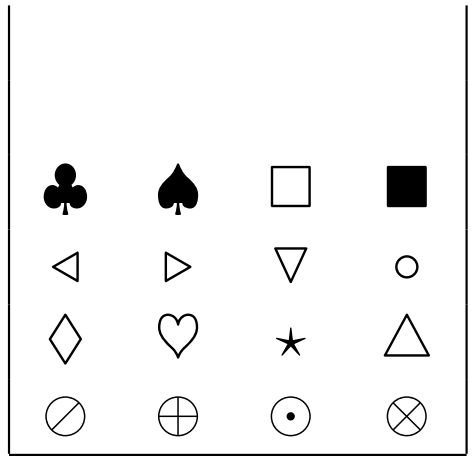

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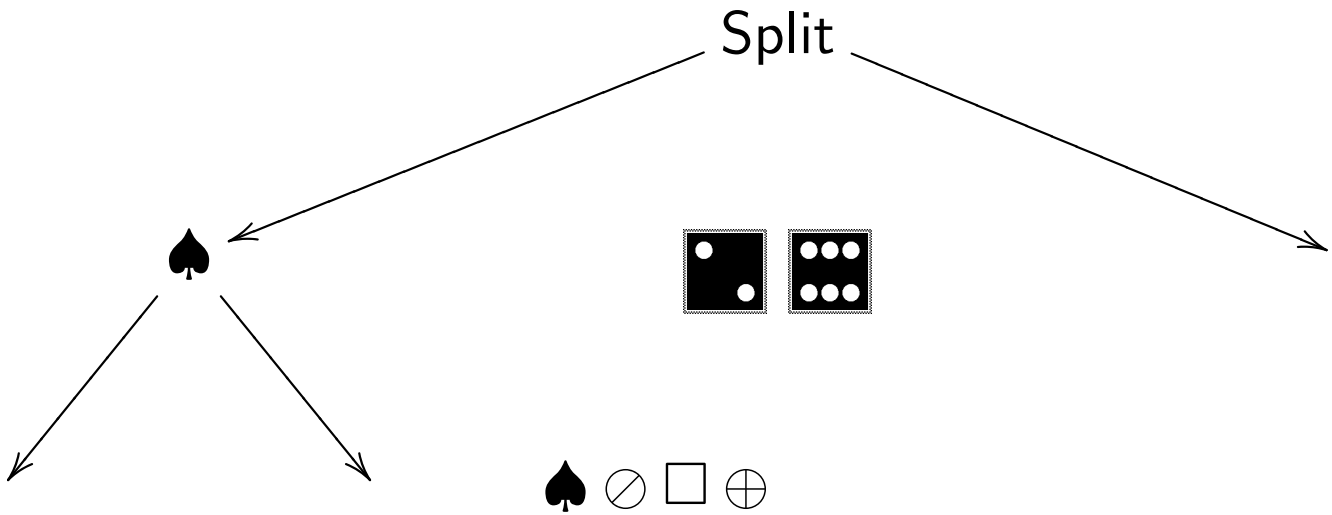

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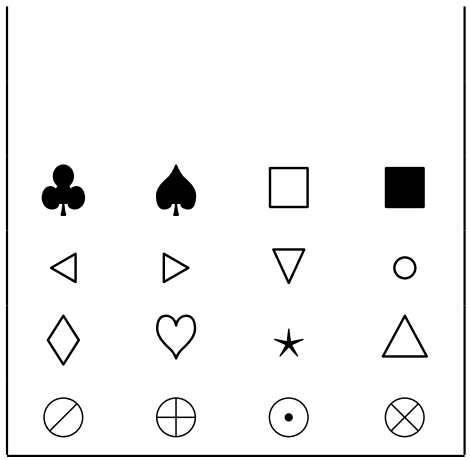

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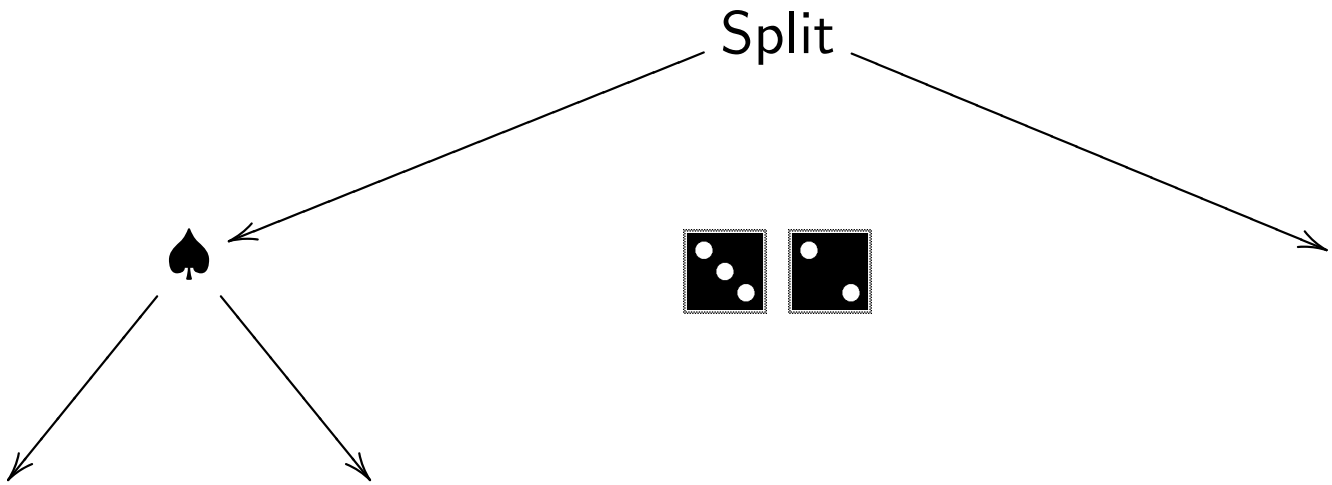

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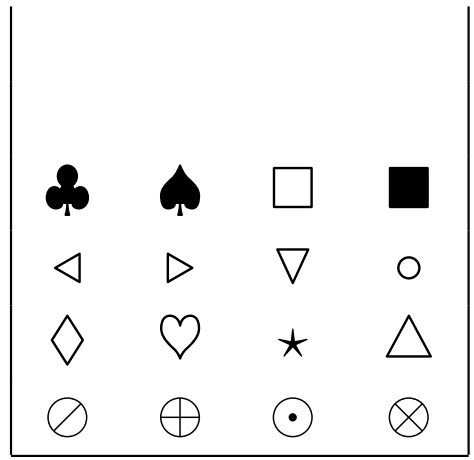

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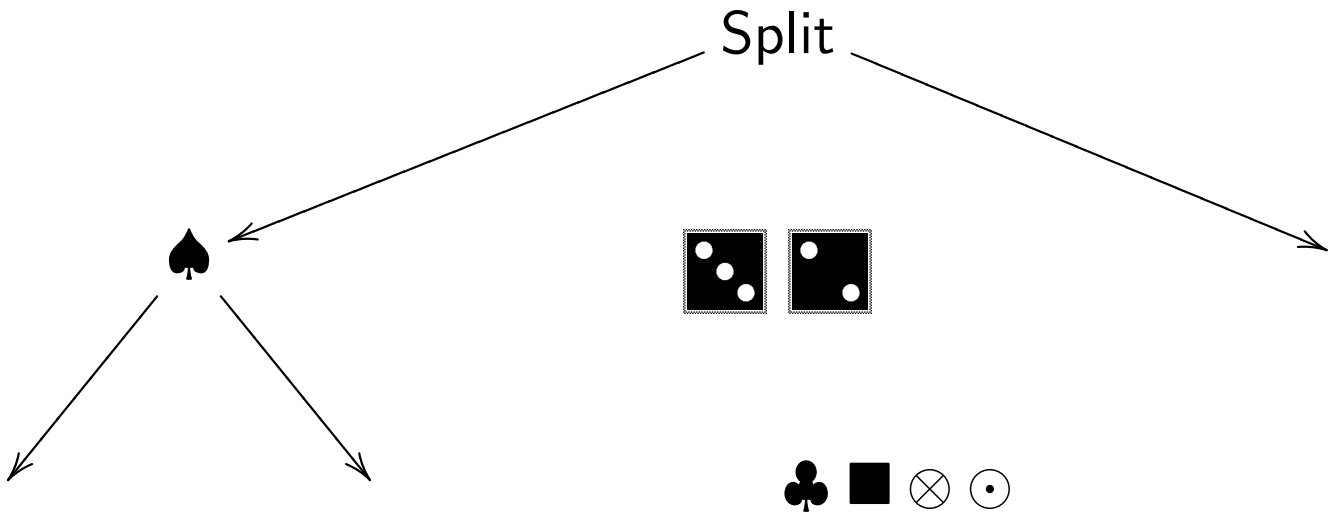

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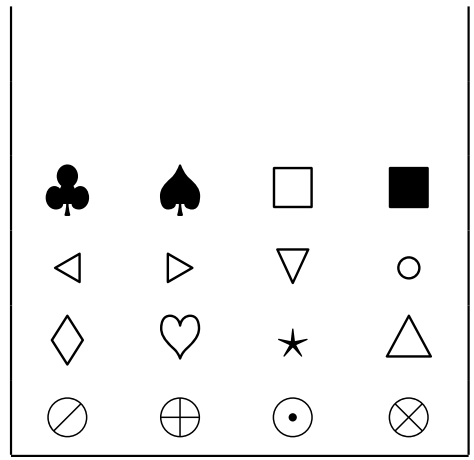

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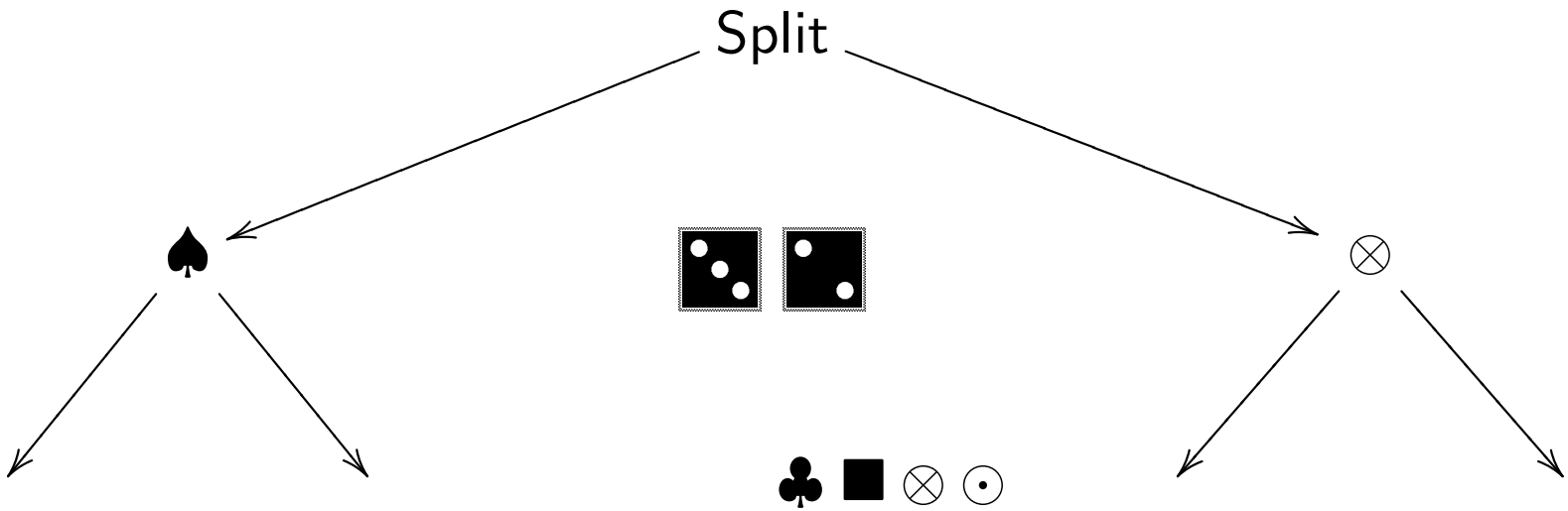

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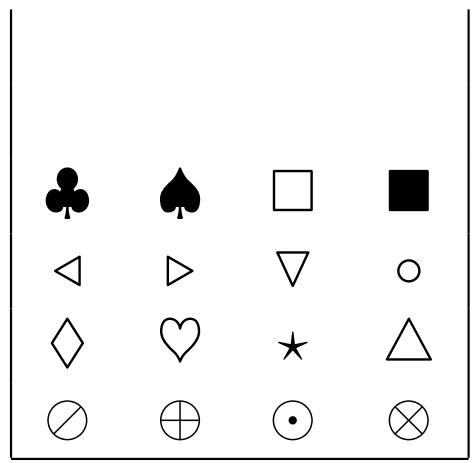

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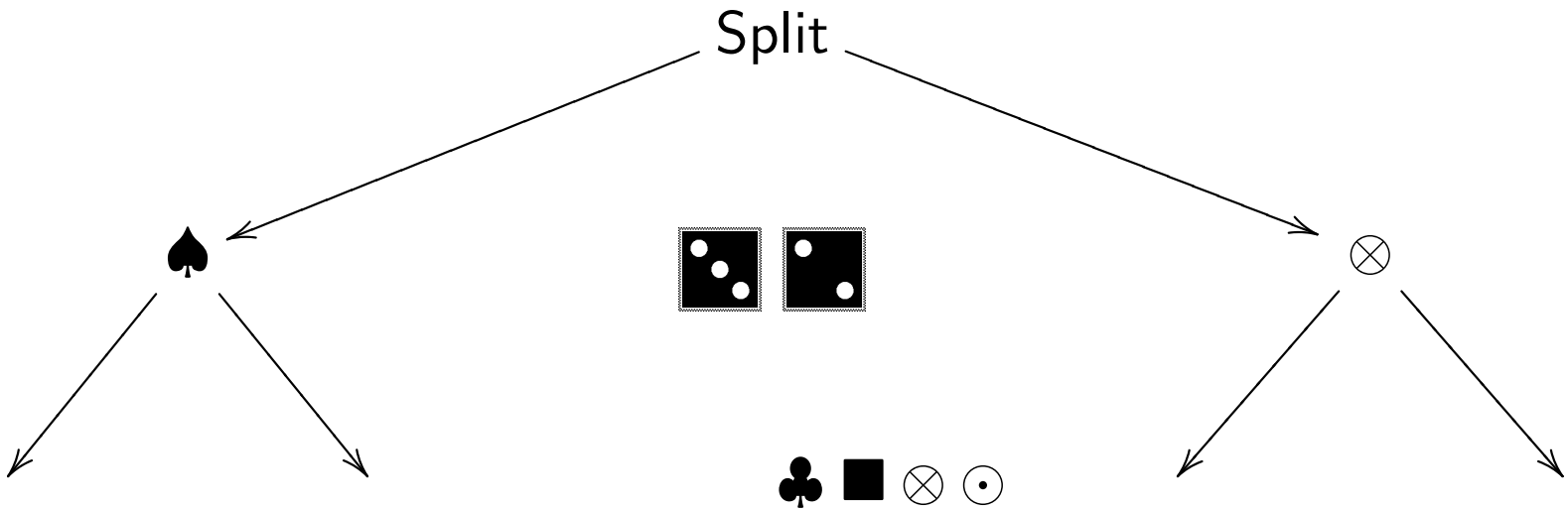

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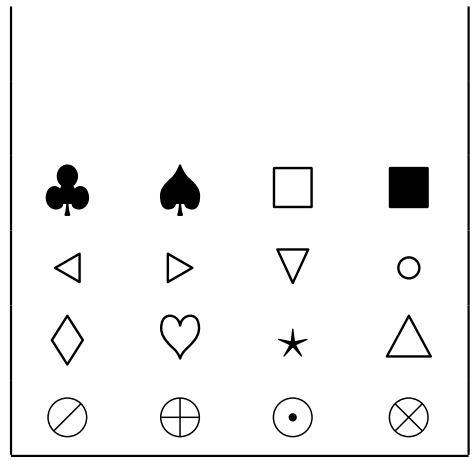

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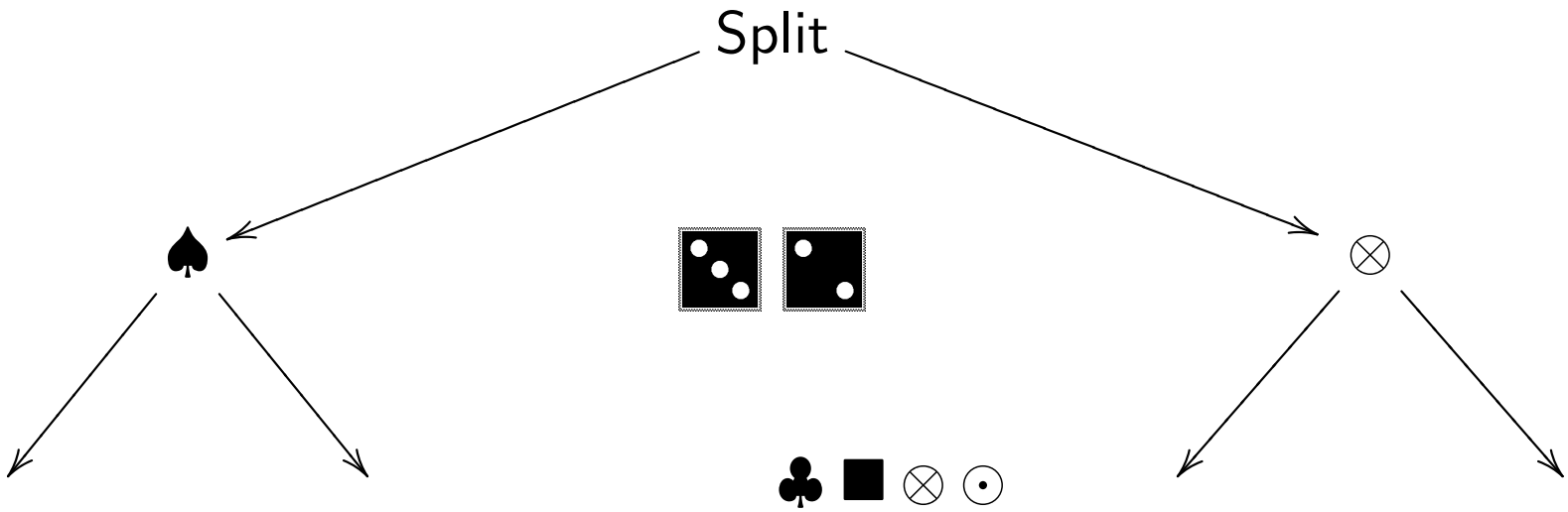

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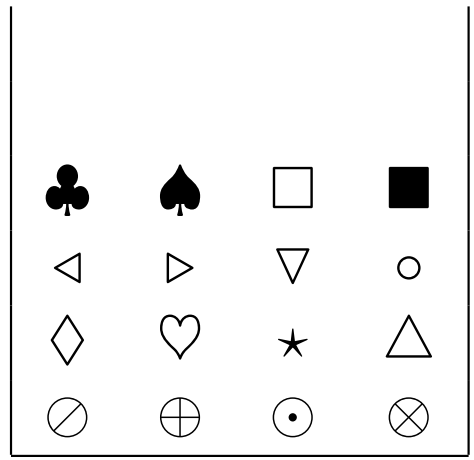

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- Number considered is a tuning parameter
- More: stronger but more correlated trees (features only randomly excluded *per split*)

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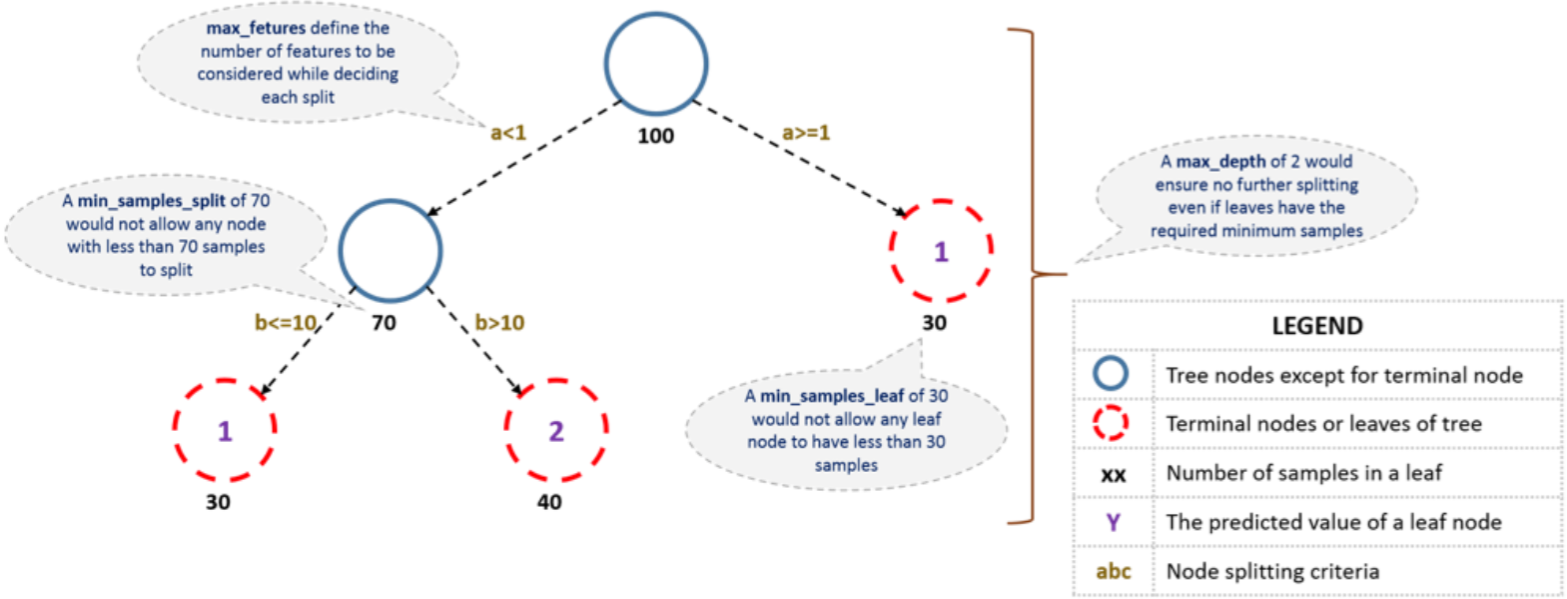

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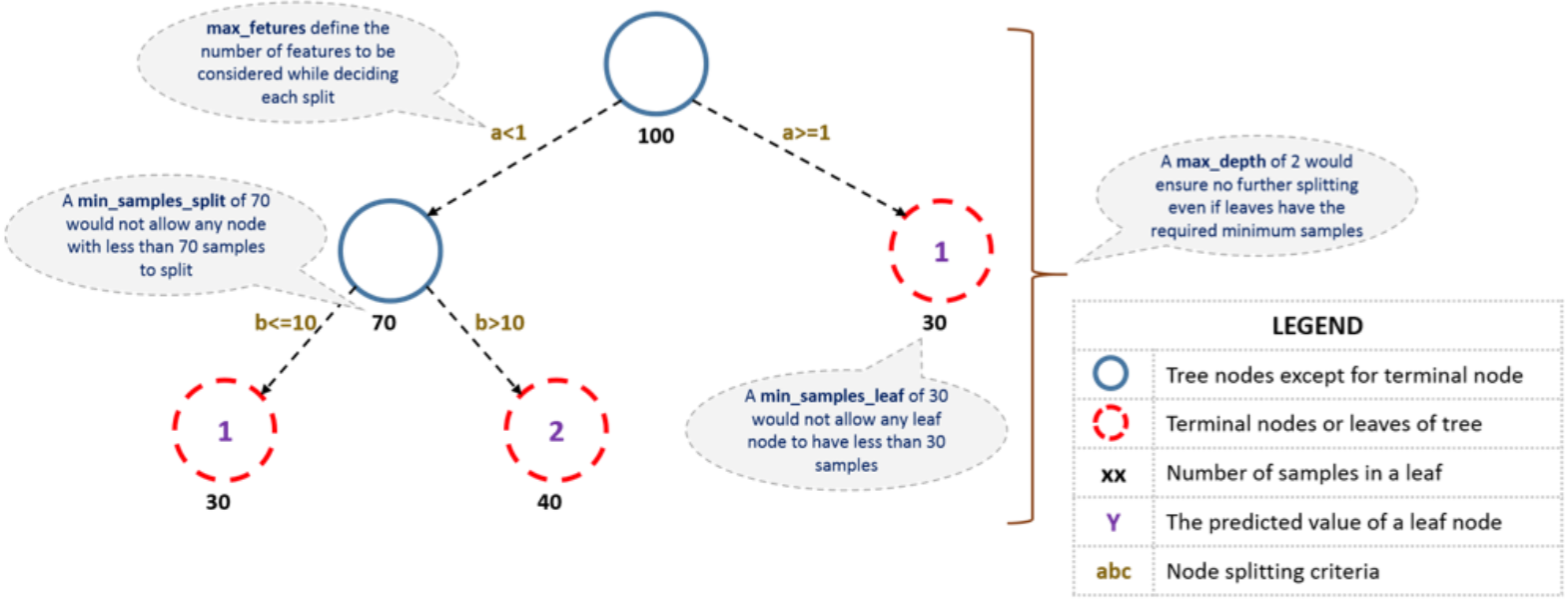

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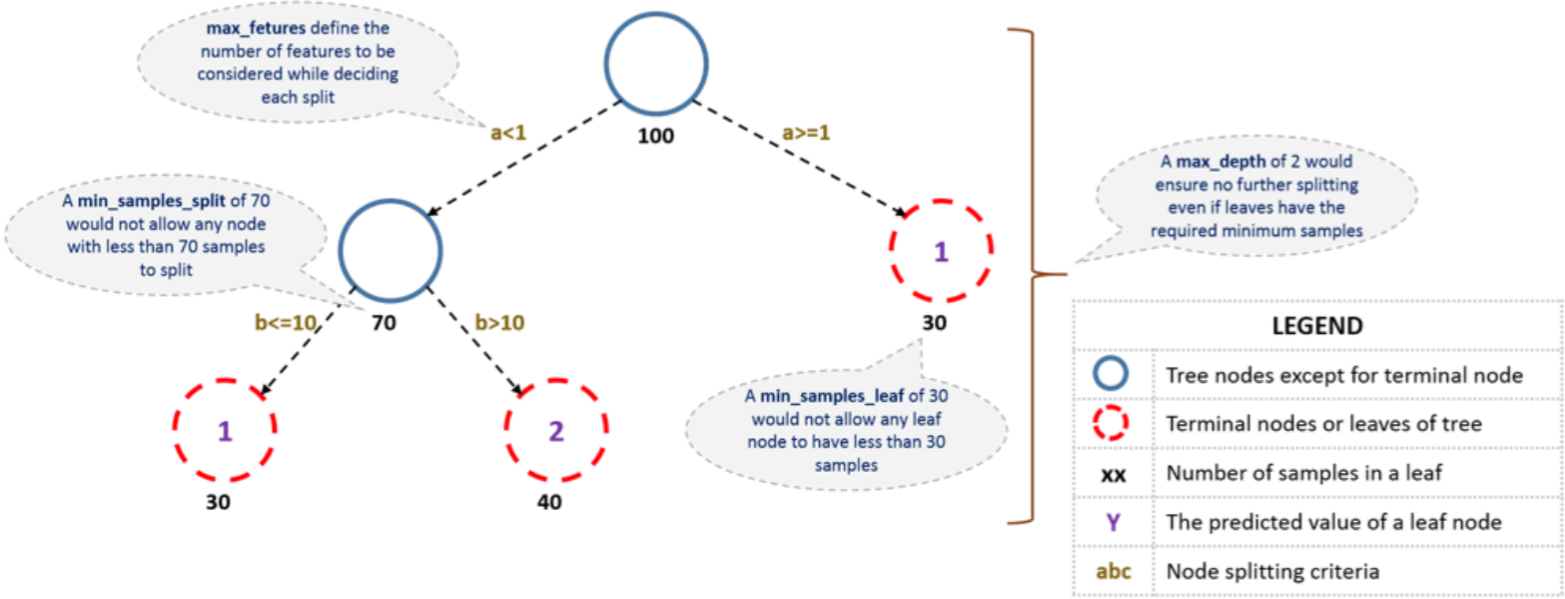

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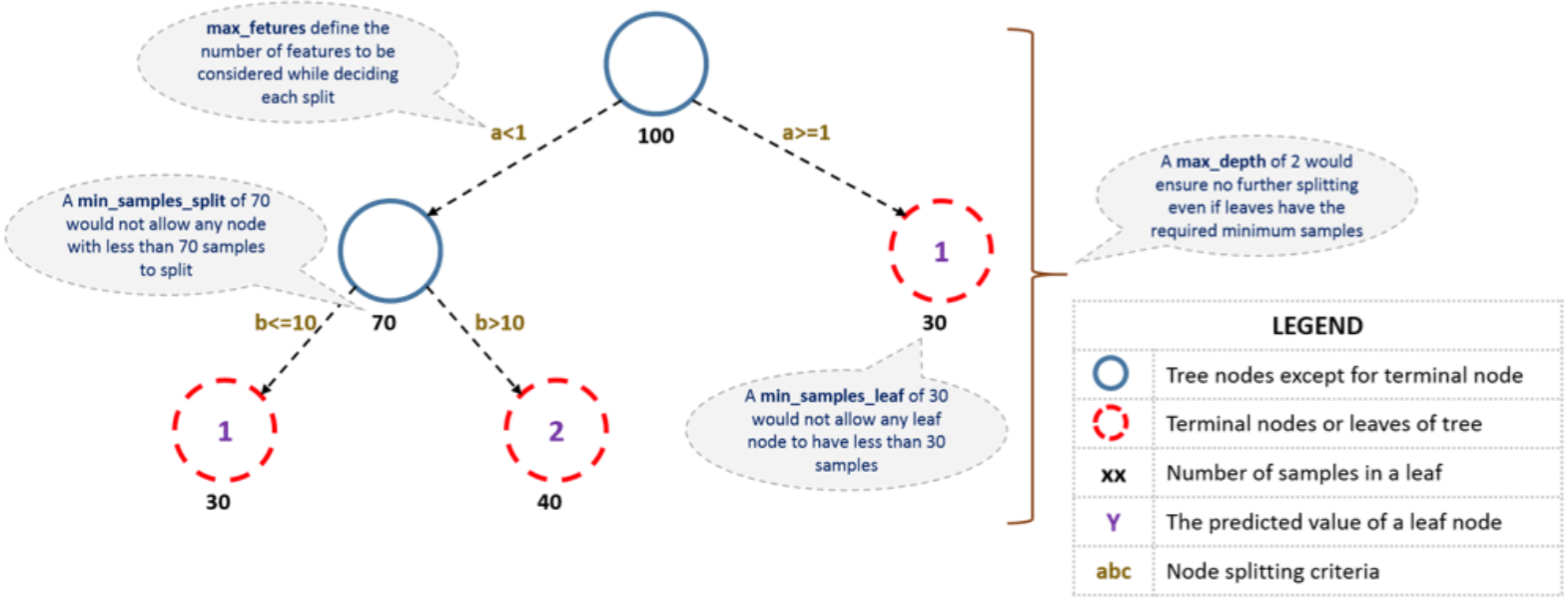

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  - Cross-validation is still needed for methodology comparisons...

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)

"You can't see the forest for the treeeeeeees!"

– M. Manson (1996)

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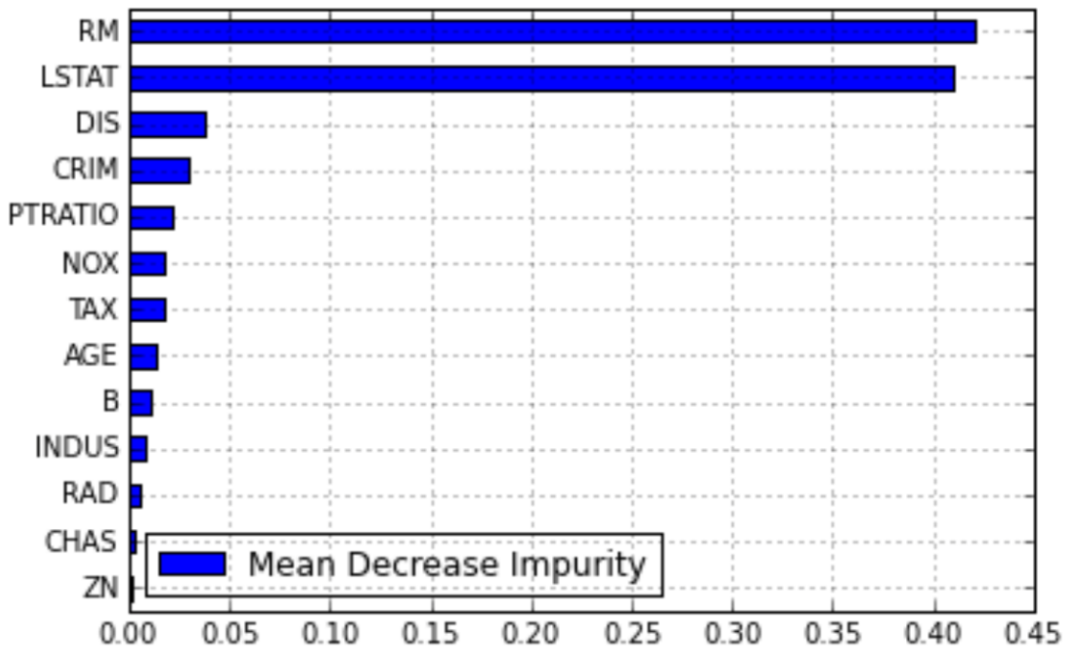

In Boston, the most relevant associations with neighborhood home values are (1) number of rooms and (2) proportion of low income households in the neighborhood

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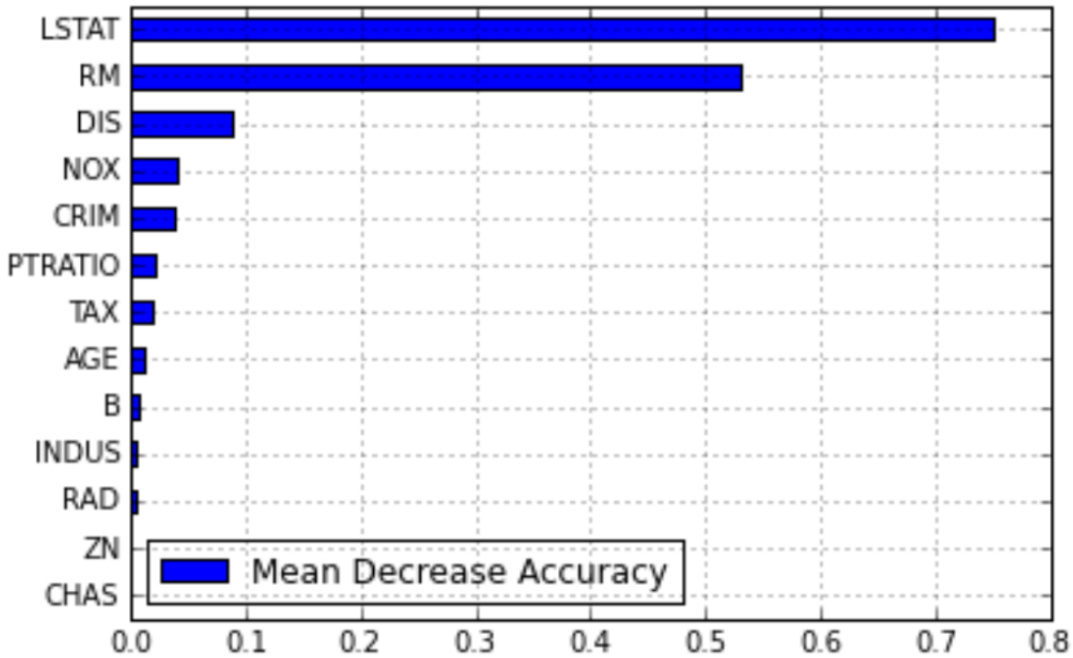

This approach suggests prediction is more sensitive to (1) low income proportion rather than (2) room number

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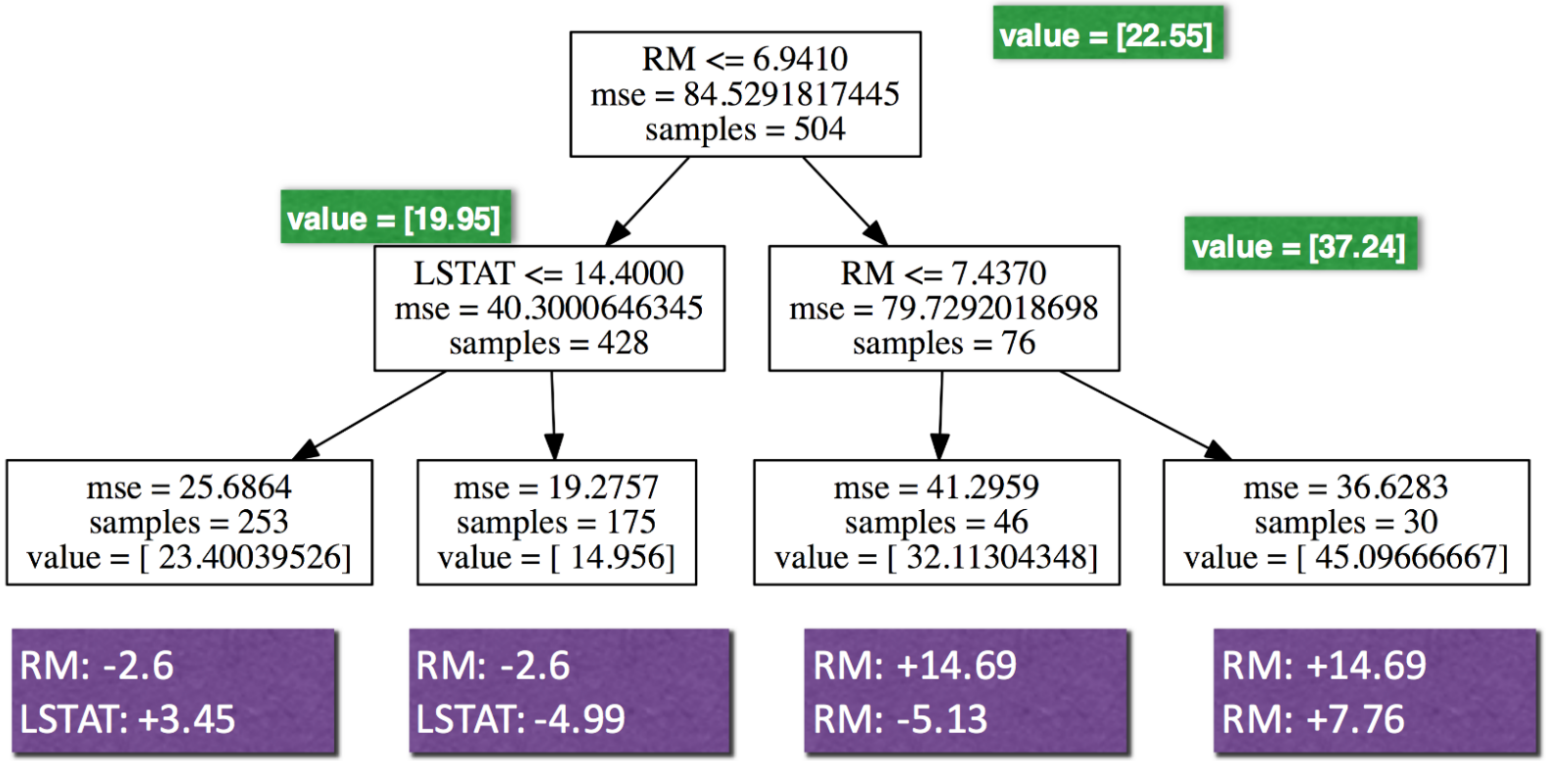

Variable Importance (v3.0)

1. Follow test samples down the tree through each split s on V
2. Record the change in prediction $\epsilon_V^{(s)}$ due to V split at s
3. Sum up all the changes $\epsilon_V^{(s)}$ due to feature V

   These values are then averaged by tree

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)

1. Calculate proportion of samples visiting feature V in each tree

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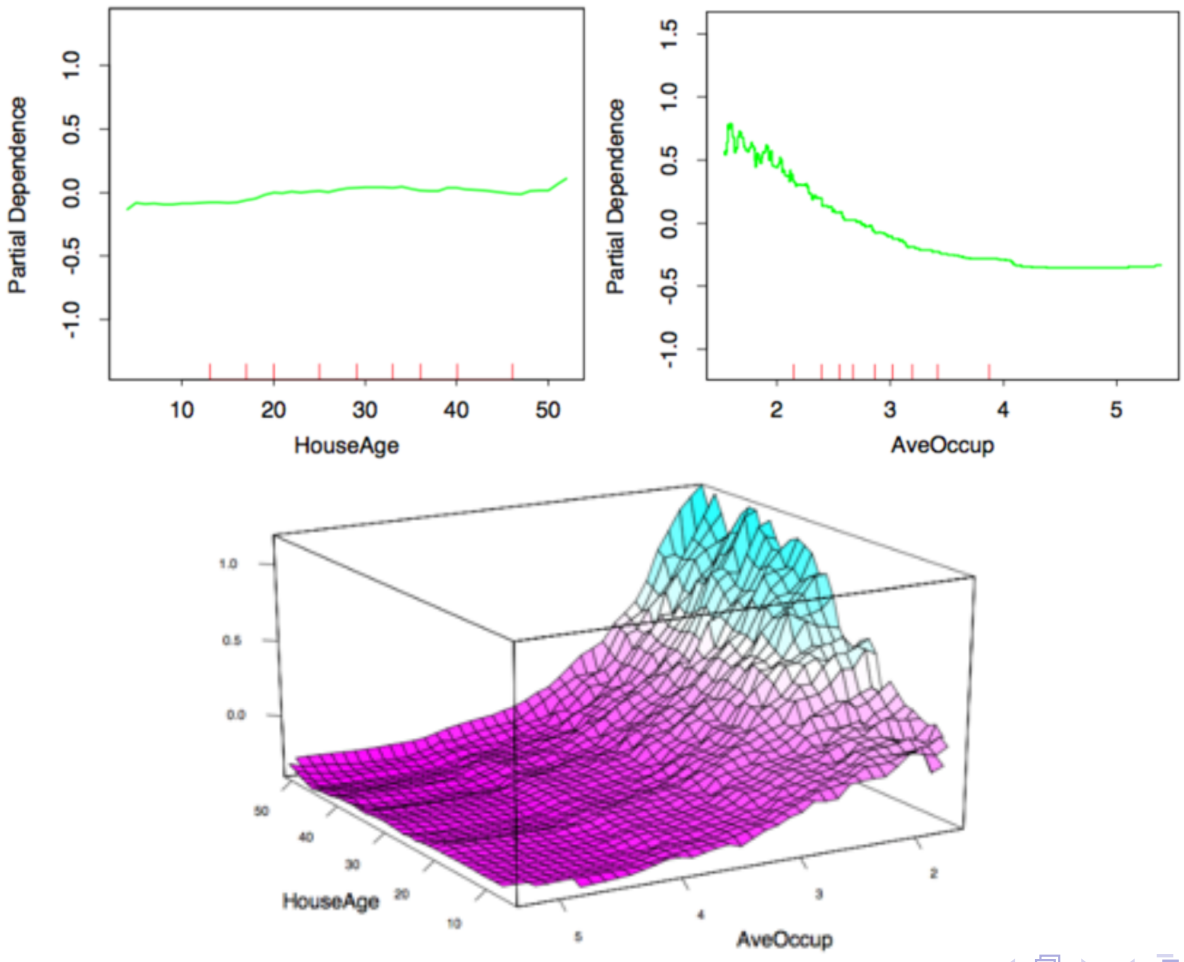
1. Calculate proportion of samples visiting feature V in each tree (conditions higher in the tree typically visited by more data)
2. Average the "proportion of samples visited" across all trees

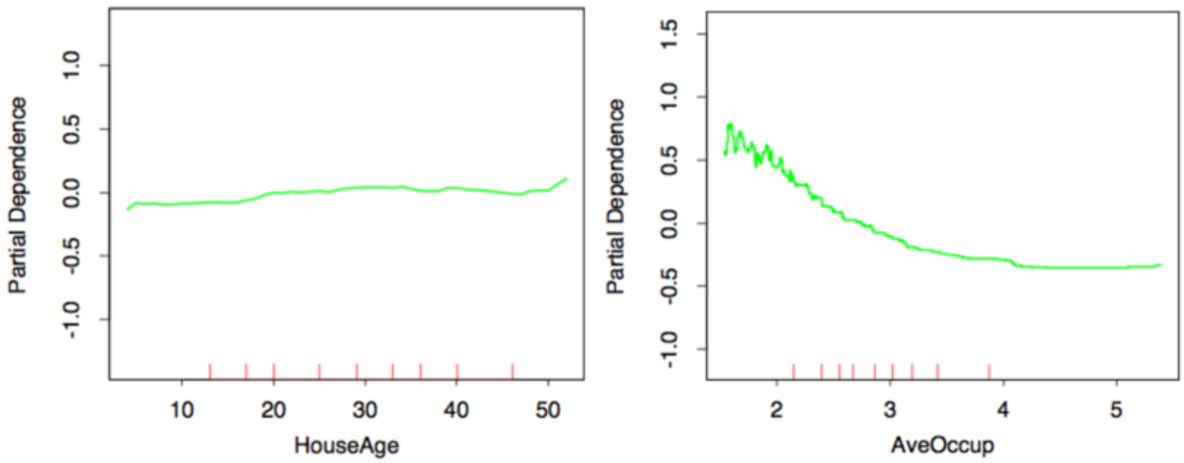
Partial Dependency Plots

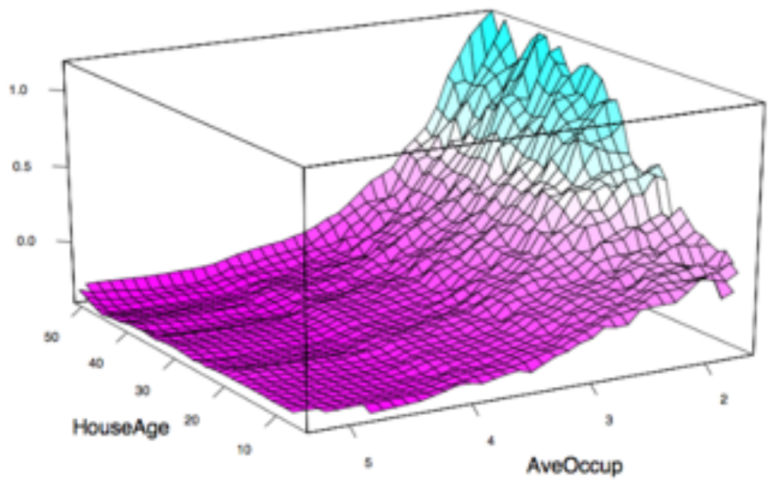
1. Set feature $V = v$ for a single values v



Partial Dependency Plots

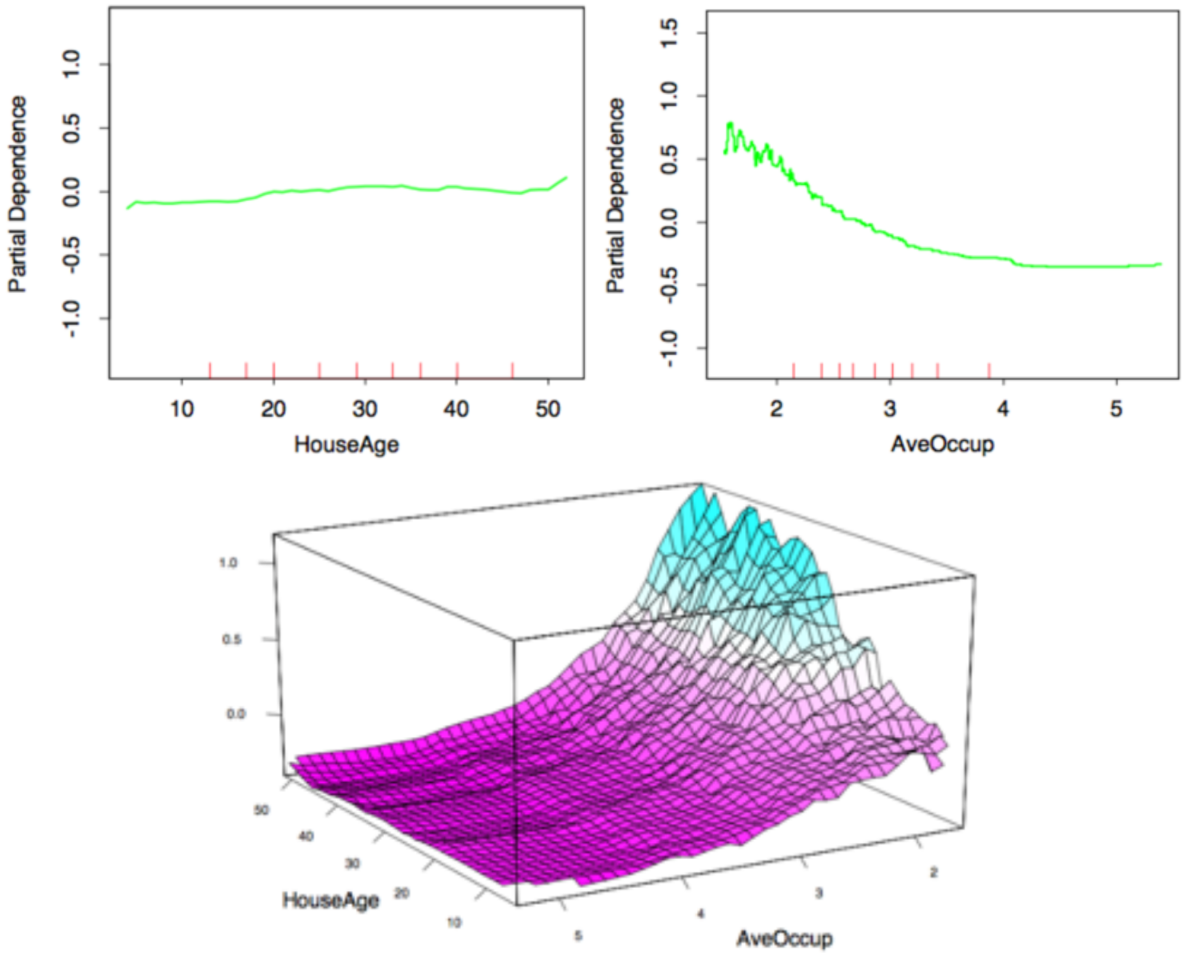
1. Set feature $V = v$ for a single values v
2. Record average predictions $\frac{1}{n}\sum_{i=1}^{n} \hat{Y}_i^{(v)}$ over "synthetic" data





Partial Dependency Plots

1. Set feature $V = v$ for a single values v
2. Record average predictions $\frac{1}{n}\sum_{i=1}^{n} \hat{Y}_i^{(v)}$ over "synthetic" data
3. Plot $\frac{1}{n}\sum_{i=1}^{n} \hat{Y}_i^{(v)}$ at v



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