Lecture 5: Decision Trees, Random Forests and the Bias-Variance Tradeoff

Machine Learning Decal

Hosted by Machine Learning at Berkeley

Agenda

Background

Decision Tree Setup

Decision Tree Algorithm and Justification

Random Forests

Boosting

The Bias-Variance Tradeoff

Questions

Background

Let's Play A Game

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- Player 1 thinks of a particular thing in a broad category e.g. People, Animals, Vegetables, etc.
- Player 2 must determine what Player 1 is thinking of.
- Player 2 can ask up to 20 **Yes or No** questions of Player 1, and he is able to correctly guess the thing, then Player 2 wins.

Let's Play The Game

Alright. I'm Player 1, and you are going to be Player 2. I'm thinking of a Person. Which of the following questions are you most likely to **ask me first?** Why?

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- "Is the person from Hawaii?"
- "Is your person male?"

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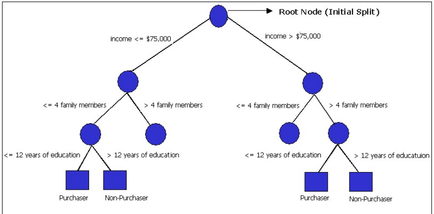
- Compared to asking the Hawaii question:
  - If from Hawaii: You have awesomely good luck. You'll likely win soon.
  - If not from Hawaii: You basically **wasted a question.**

Decision Tree Setup

Decision Tree Structure

- The **Decision Tree** is a model with a tree structure that encodes a collection of **if, then** statements in the **internal nodes**.



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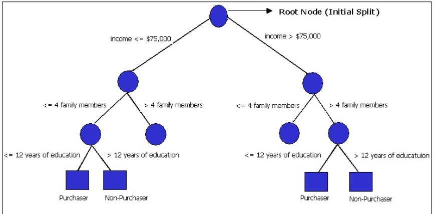

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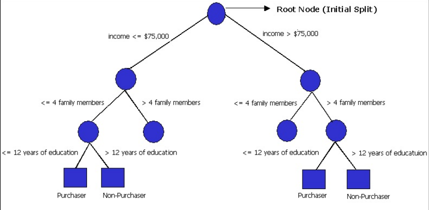
- Works naturally for continuous and categorical features!



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- We wish to "guess" $y^{(i)} \in \{0, 1\}$ for classification and $y^{(i)} \in \mathbb{R}$ for regression.

Making a Game out of Data Science

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ML@B

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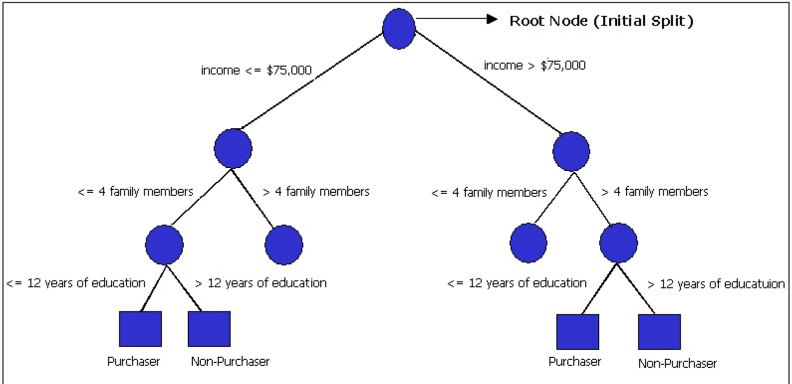
- These questions, or more formally **data splits** are what parameterize our model.

Decision Tree Example



Hypothetical Classification Tree

Somehow, we must use our training dataset to learn the **features** and **values** to choose all of the splits shown.

Decision Tree Algorithm and Justification

Decision Tree Training Algorithm

We build the decision tree with the following **recursive** algorithm.

β is the value of the feature α on which the point will be split.

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- return new *InternalNode*(α, β, GrowTree(S_l), GrowTree(S_r))

Picking Good Parameters in findSplit(S)

We have shown how to find ideal parameters θ using **gradient descent**. This works because we are **optimizing a loss function**, $J(\theta)$.

Ideal split criteria in decision trees are chosen through minimizing the amount of **entropy** in each split group.

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- $p_c = P(y_i = c) \rightarrow H(p_c) = -log_2 p_c$
- What is H(0)? H(1)? H($\frac{1}{2}$)?

What is Entropy?

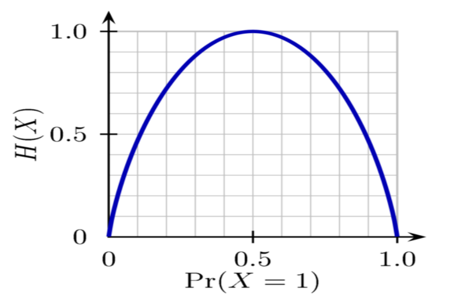
Data points belong to total of c classes, and fraction of data points in each is $[p_0...p_{c-1}] : \sum_i p_i = 1$, then **entropy (H) of the set** is:

$$H = -\sum_{i=0}^{c-1} p_i \log p_i$$

(Using log base 2) If we have two classes, what values of p_0, p_1 will maximize this function? Do you see the connection to high entropy?

Visualizing the Entropy Function

Here is a graph depicting $H(p_0)$ with $p_1 = 1 - p_0$:



To summarize: A Set S will have low entropy when $|p_0 - p_1|$ is large.

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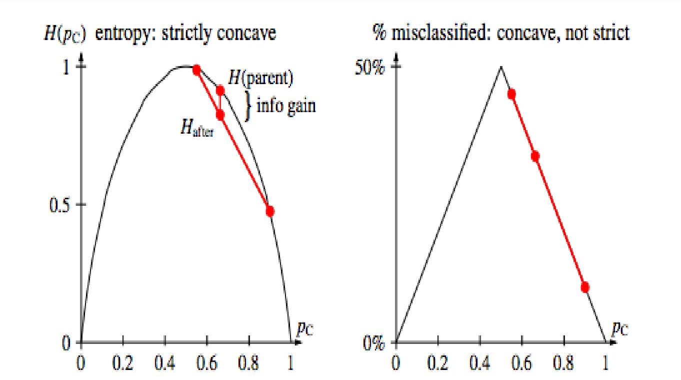
The **entropy of a split** is given as

$$H_{after} = \frac{|S_l| H_{S_l} + |S_r| H_{S_r}}{|S_l| + |S_r|}$$

Visualizing Optimal Split



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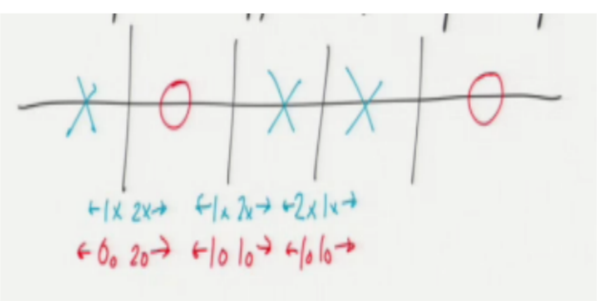
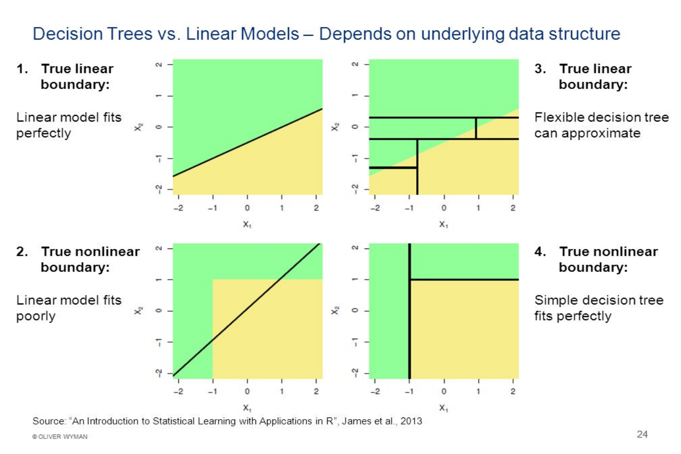
- With n data points, d features, and up to k splits on a feature: runtime is $\mathcal{O}(ndk)$

Optimized Split Selection

Sorting the points once per feature, we can evaluate entropy for that feature on each split in $\mathcal{O}(1)$ time. This gives us an overall runtime of $\mathcal{O}(nd \log n)$

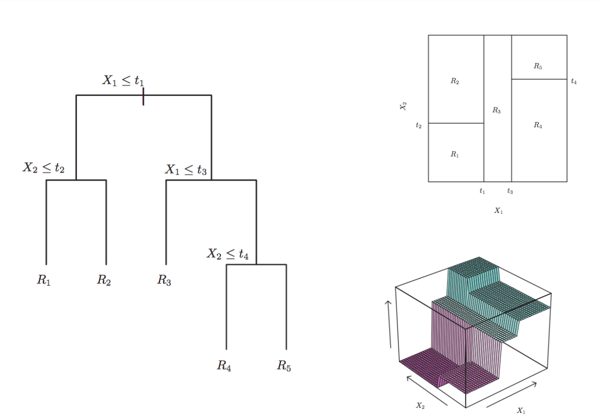


Finished tree can divide feature space into arbitrary number of *axis-aligned* regions.

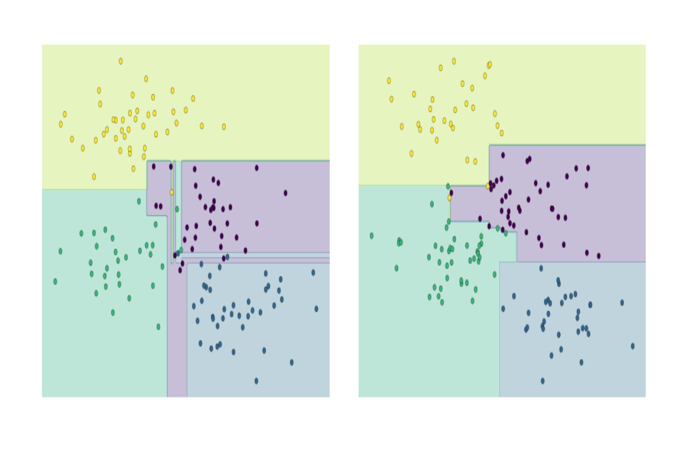


Decision Tree Decision Boundary: Regression

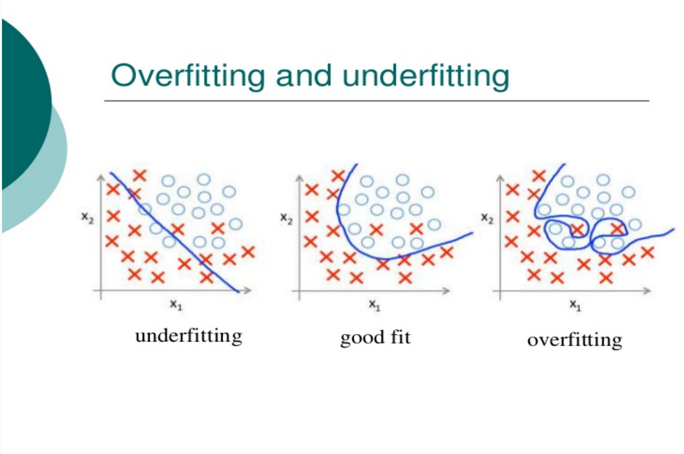
Image Credits to Professor Shewchuk



Which one would you rather have? Points are **training data.**



Overfitting vs Underfitting



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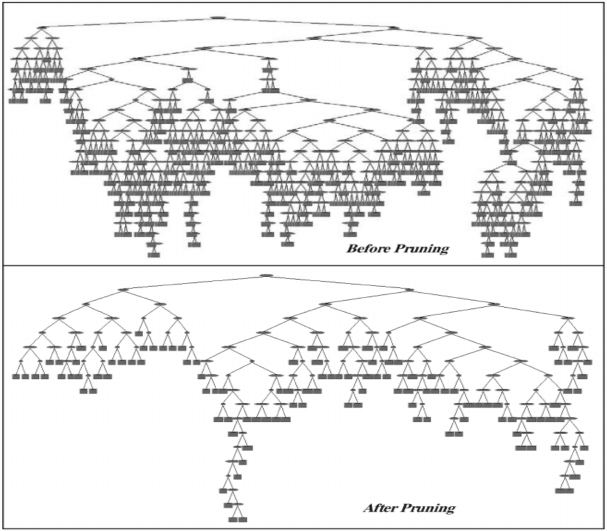
Impure leaves return majority vote (classification), average value (regression).

Neater Tree



Break: Cool Website

Let's see a cool application of Decision Trees to a somewhat-practical application: Click Me!

Random Forests

Making Decisions Trees More Powerful

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What if we made one model by **combining many decision trees?** Combine their judgments into something nuanced.

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These techniques are called **bootstrap aggregating (bagging)** and **random feature selection** respectively.

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- **Random feature selection:** Despite bagging, trees may still split on same first feature. This forces different "perspectives" on split paths.
    - *Example:* Asking "Is the person still alive?" might be better than asking if the person is male, *depending on the situation.*

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- **Random Feature Selection** $\rightarrow$ A way to address high dimensionality on optimization based strategies.
    - For random forests, $\sqrt{d}$, $\frac{d}{3}$ features are recommended for splits on classification and regression respectively.

Random Forests

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- Which all use both, bagging and random feature selection
- And work by casting majority votes (classification) or averages (regression), with values made from all of the constituent decision trees.

More About Random Forests

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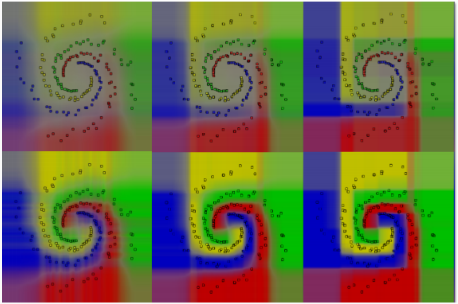
Despite this, random forests are less likely to overfit.

Random Forest Decision Boundaries



Top row: depth = 4, Bottom row: depth = 12.

Left: 1 random feature per split, Middle: 5 features, Right: 50 features

Boosting

Overview of Boosting

Instead of taking the majority vote of **many strong decision trees**, **sequentially generate weak decision trees** where each tree focuses accurately classifying the data points the last tree got wrong.

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- Train a new weak decision tree on the re-weighted datasets and repeat

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- Base model is a low variance (high bias) decision tree
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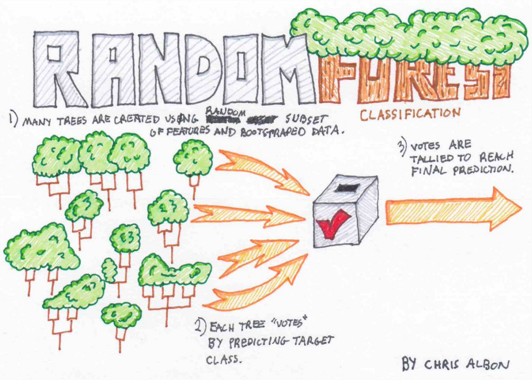
- Can strengthen weak learners

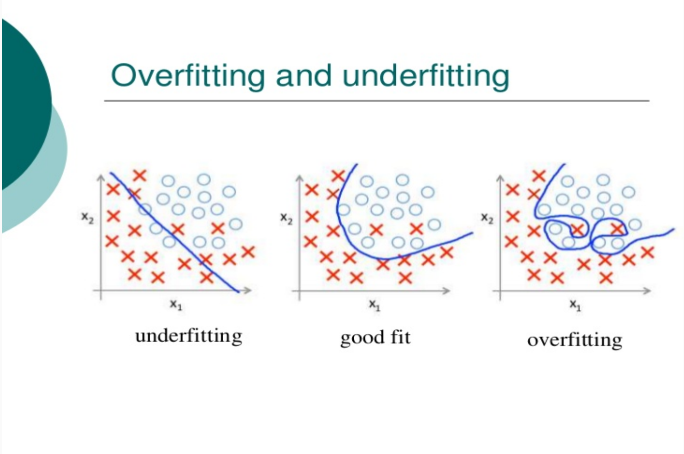
Break: Sklearn's Random Forest Class

Let's check out how our favorite data science model library presents Random Forests: Click Me!



The Bias-Variance Tradeoff

A Common Theme



Setup

We start by assuming our data comes from a true function f but also has random noise ϵ added afterward. We have a hypothesis h which is always imperfect for 2 reasons:

- **Bias:** h is unable to fit f perfectly because it lacks capacity or complexity. (Fitting a line to a parabola).

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Now, suppose we have an arbitrary point z, and a generated data point $\gamma = f(z) + \epsilon$.

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Let's analyze the Expectation of Loss when we use Mean-Squared Error as a cost function:

$$
\begin{aligned}
R(h) &= \mathbb{E}[(h(z) - \gamma)^2] \\
&= \mathbb{E}[h(z)^2] + \mathbb{E}[\gamma^2] - 2\mathbb{E}[\gamma h(z)]
\end{aligned}
$$

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$$\begin{aligned}
&= Var[h(z)] + \mathbb{E}[h(z)]^2 + Var[\gamma] + \mathbb{E}[\gamma]^2 - 2\mathbb{E}[\gamma]\mathbb{E}[h(z)] \\
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&= (\mathbb{E}[h(z)] - f(z))^2 + Var[h(z)] + Var[\epsilon]
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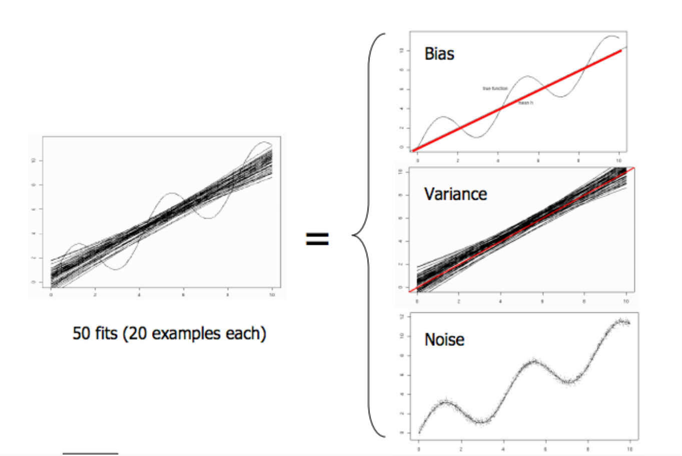
Because we are able to break down the risk of any hypothesis like so, this process is called the **Bias-Variance Decomposition**.

Visualizing Each of the Quantities



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- Assuming h has sufficient modeling capacity, bias $\rightarrow 0$ as $n \rightarrow \infty$

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Knowing the Effects of Each (Contd.)

- **Adding features:** higher quality feature $\rightarrow$ higher drop in bias.
- *Variance always increases.* $\rightarrow$ only add feature if bias drop outweighs variance gain

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  - Because of the properties of Variance, Random Forests have **lower variance** than decision trees.

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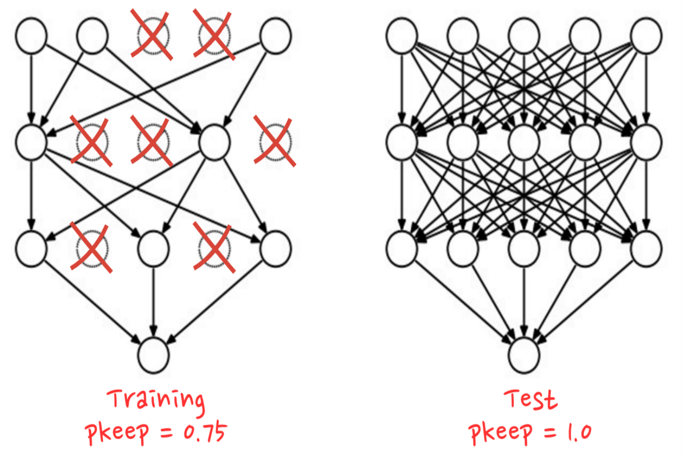
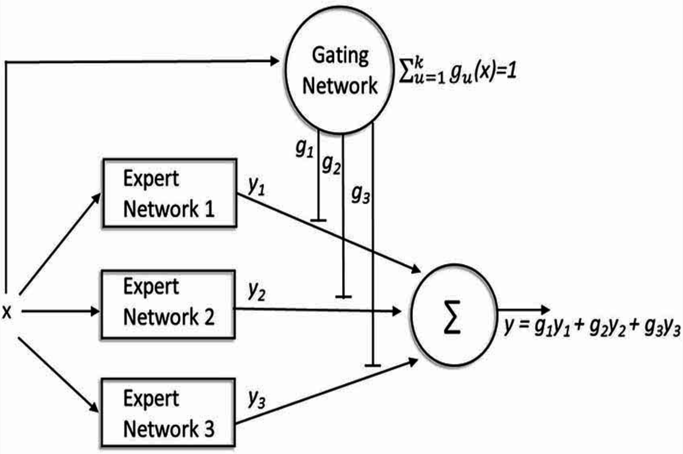
- The main consideration simply becomes training costs
- Prior to deep learning revival in 2010's, random forests and ensembled SVM's were state-of-the-art for data science classification, prediction.
- Even now, one can ensemble deep learning models e.g. dropout, mixture of experts

Bonus: Dropout



Bonus: Mixture of Experts



Questions

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