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

Data Science Decal

Hosted by Machine Learning at Berkeley

Agenda

Background

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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 your person male?

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    - If not from Hawaii: You basically **wasted a question.**

Decision Tree Setup

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- A query data point's features are used to channel the point to a **leaf node**, where it is assigned a label (classification) or value (regression).
- Works naturally for continuous and categorical features!

Making a Game out of Data Science

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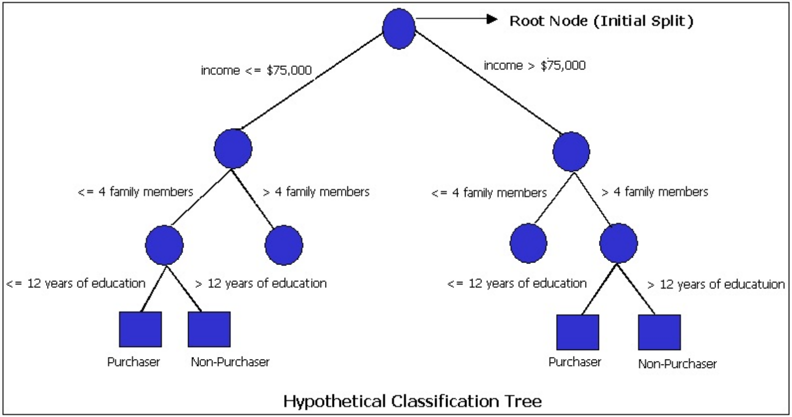
- These questions, or more formally **data splits** are what parameterize our model.

Decision Tree Example



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

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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

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?

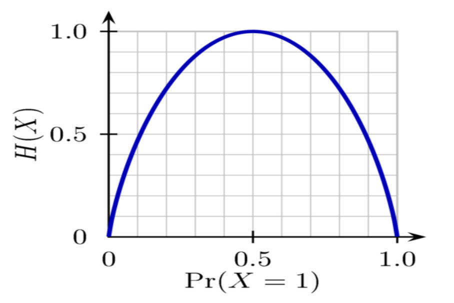
Data points belong to total of c classes, and fraction of data points in each is $[p_0 ... p_{c-1}] : \sum_i p_i = 1$, then **entropy (H) of the set** is:

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

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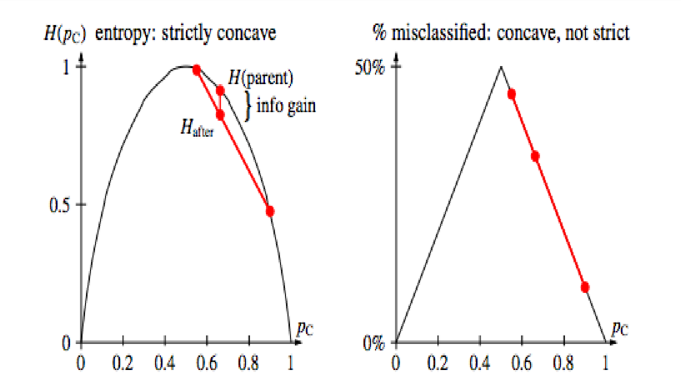
The **entropy of a split** is given as

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

Visualizing Optimal Split



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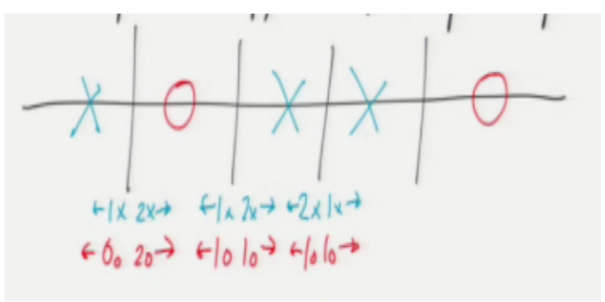
- With n data points, d features, and up to k splits on a feature: runtime is $\mathcal{O}(ndk)$

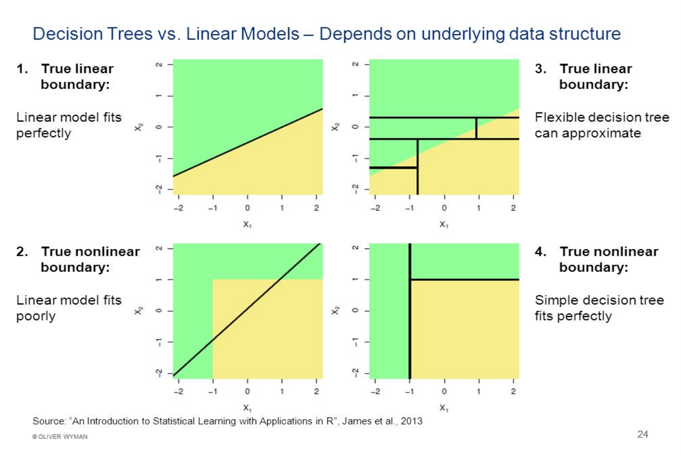
Optimized Split Selection

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 $\mathcal{O}(nd \log n)$



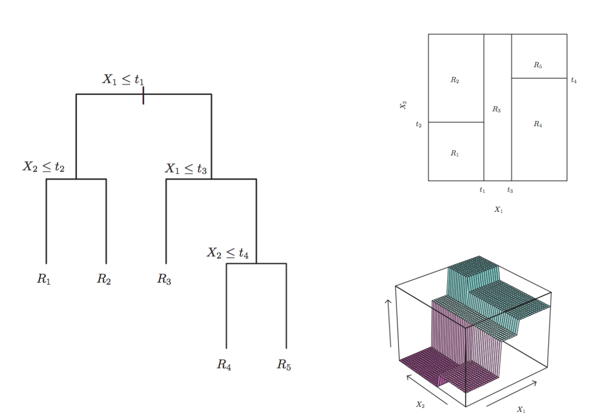
Decision Tree Decision Boundary: Classification

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



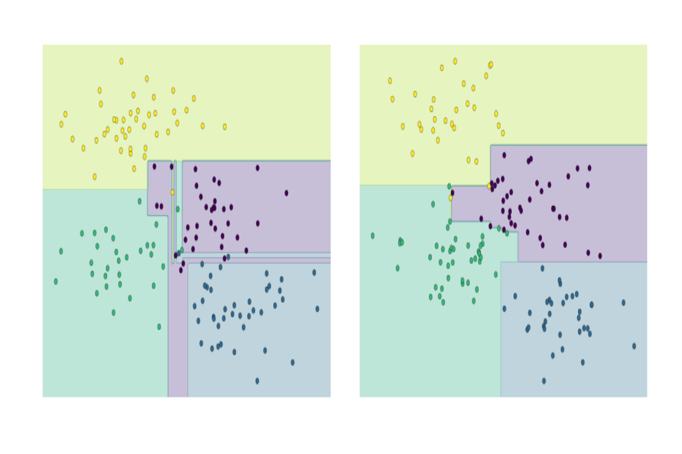
Decision Tree Decision Boundary: Regression

Image Credits to Professor Shewchuk



Decision Tree Warning

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



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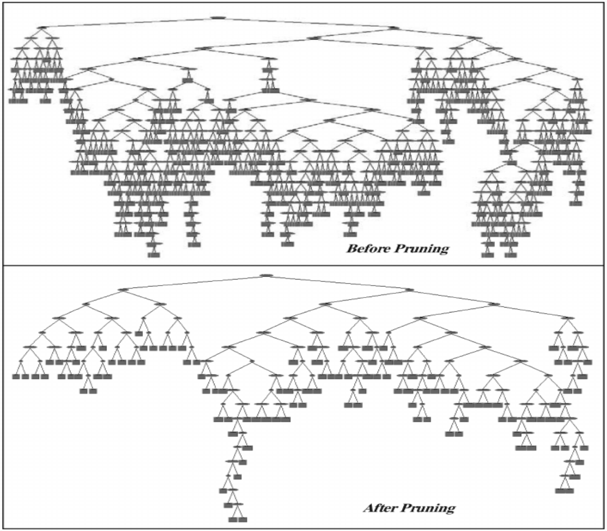
Impure leaves return majority vote (classification), average value (regression).

Neater Tree



Break: Cool Website

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

Random Forests

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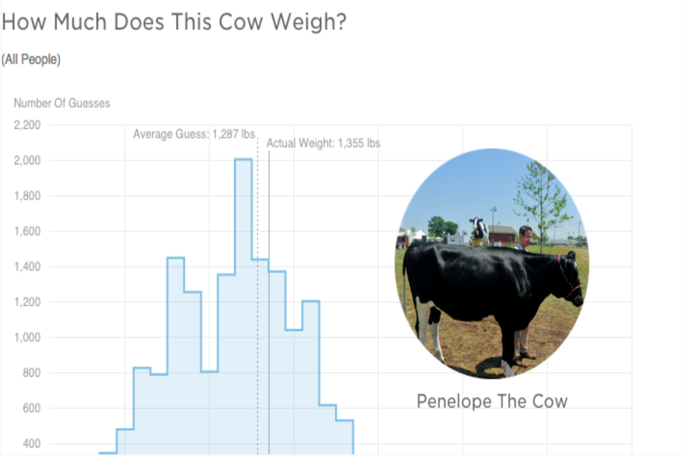
These techniques are called **bootstrap aggregating (bagging)** and **random feature selection** respectively.

Side Note: Guessing Cow Weight



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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.*

Widely Applicable Strategies

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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

ML@B

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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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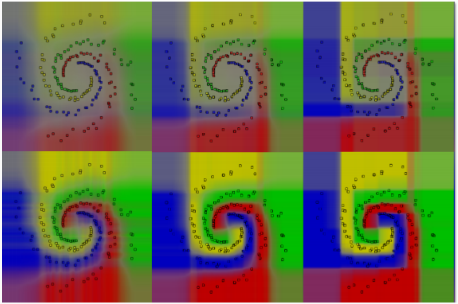
Despite this, random forests are less likely to overfit.

Random Forest Decision Boundaries

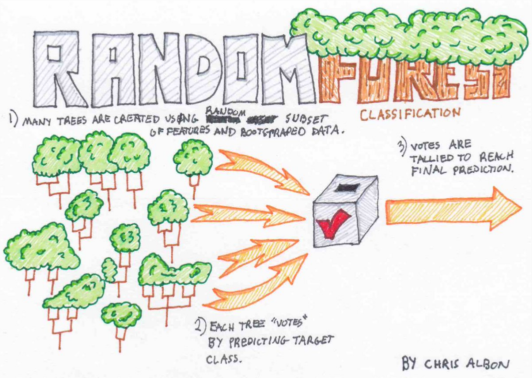


Top row: depth = 4, Bottom row: depth = 12.

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

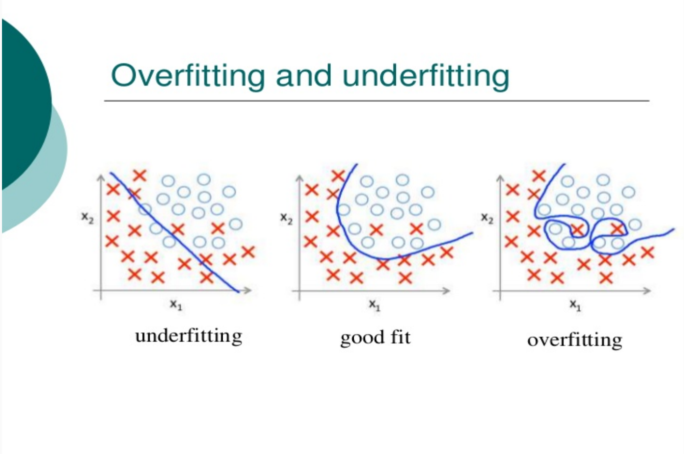
Break: Sklearn's Random Forest Class

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:

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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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$$= Var[h(z)] + \mathbb{E}[h(z)]^2 + Var[\gamma] + \mathbb{E}[\gamma]^2 - 2\mathbb{E}[\gamma]\mathbb{E}[h(z)]$$
$$= (\mathbb{E}[h(z)] - \mathbb{E}[\gamma])^2 + Var[h(z)] + Var[\gamma]$$
$$= (\mathbb{E}[h(z)] - f(z))^2 + Var[h(z)] + Var[\epsilon]$$

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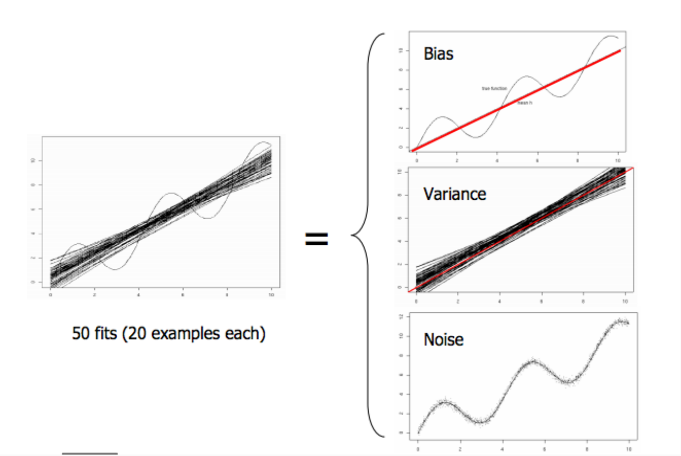
From the last slide, we see three important quantities:

- $(\mathbb{E}[h(z)] - f(z))^2$ is the squared **bias**. It is how much the model expects to differ from the real data distribution function.
- $Var[h(z)]$ is the **variance**. The risk is explicitly composed partly by the variance of our model.
- $Var[\epsilon]$ is the **irreducible error**. The noise put into the data is entirely out of our control.

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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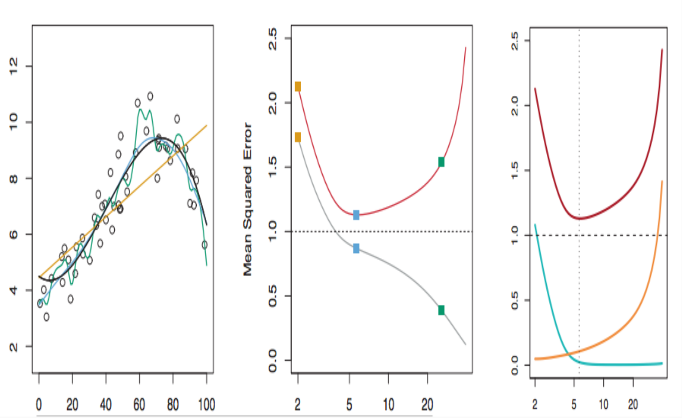
- While f is unknowable, we can pick f, synthesize data and test models for strengths and weaknesses.



Mean Squared Error

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

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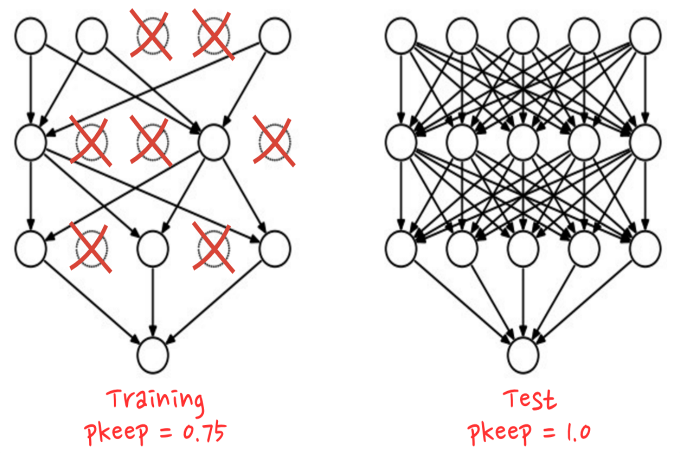
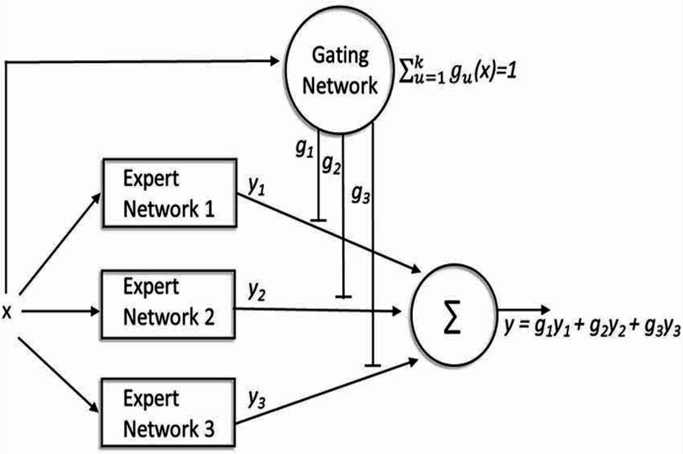
- The main consideration simply becomes training costs
- Prior to deep learning revival in 2010's, random forests and ensembled SVM's were state-of-the-art for data science classification, prediction.
- Even now, can ensemble deep learning models e.g. dropout, mixture of experts

Bonus: Dropout



Bonus: Mixture of Experts



Questions

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