

CSE 417T

Introduction to Machine Learning

Lecture 13

Instructor: Chien-Ju (CJ) Ho

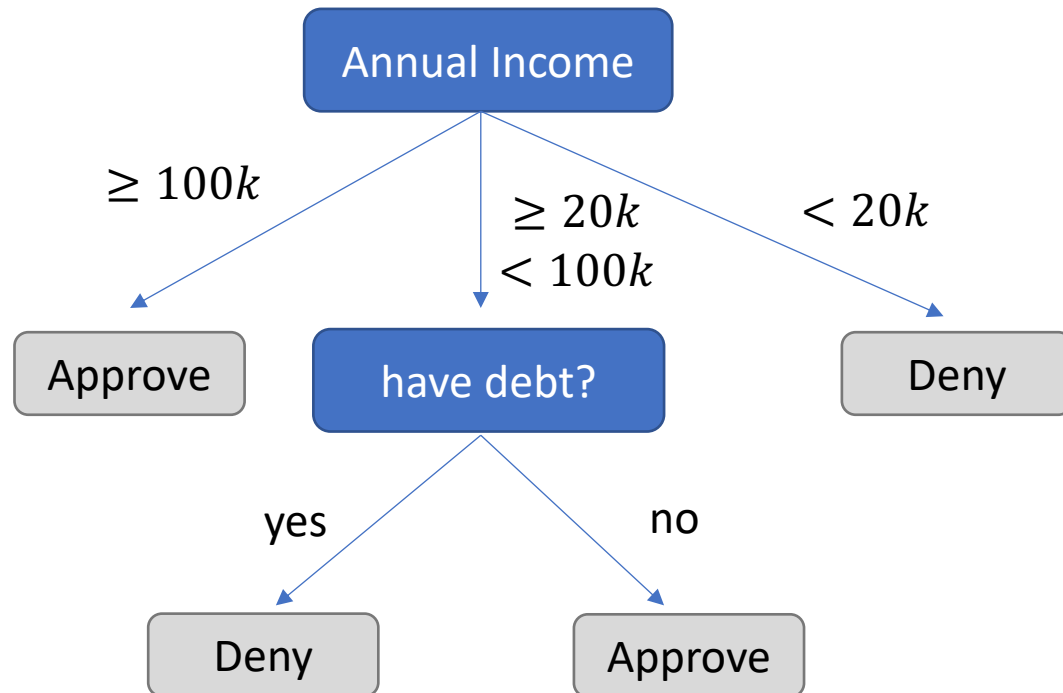
Logistics

- Homework 3: due on **Oct 19 (Wednesday)**
 - Track your own late-day usages
 - Assignments over-using late days won't be graded
- Exam 1: **October 27 (Thursday)**
 - Topics: LFD Chapters 1 to 5
 - Timed exam (75 min) during lecture time
 - Location TBD
 - Closed-book exam with 2 letter-size cheat sheets allowed (4 pages in total)
 - No format limitations (it can be typed, written, or a combination)
- October 25 (Tuesday) will be a review session

Recap

Decision Tree

Decision Tree Hypothesis



Credit Card Approval Example

- Pros
 - Easy to interpret (interpretability is getting attention and is important in many domains)
 - Can handle multi-type data (Numerical, categorical. ...)
 - Easy to implement (Bunch of if-else rules)
- Cons
 - Generally speaking, **bad generalization**
 - VC dimension is infinity
 - High variance (small change of data leads to very different hypothesis)
 - Easily overfit
- Why we care?
 - One of the classical model
 - Building block for other models (e.g., random forest)

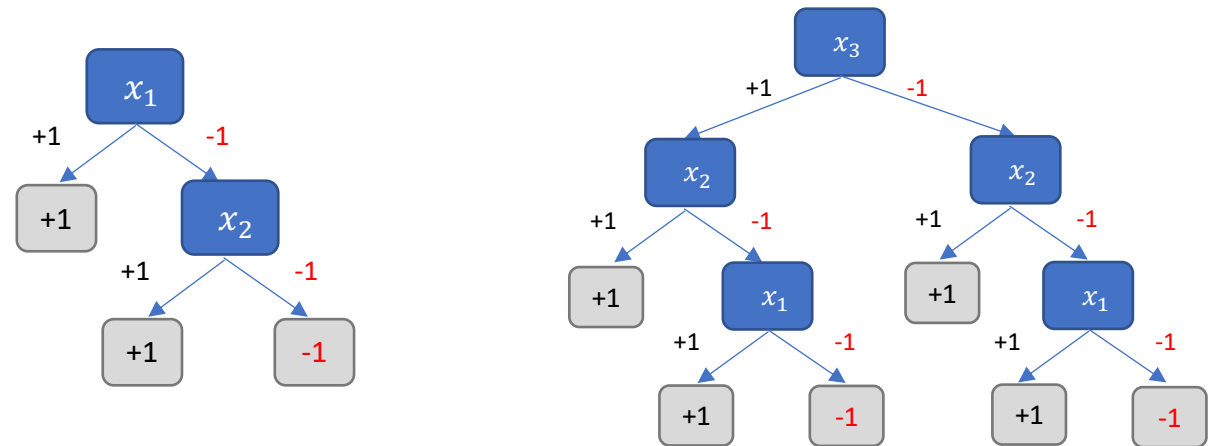
Learning Decision Tree from Data

- Given dataset D , how to learn a decision tree hypothesis?

x_1	x_2	x_3	y
+1	+1	+1	+1
+1	+1	-1	+1
+1	-1	+1	+1
+1	-1	-1	+1
-1	+1	+1	+1
-1	+1	-1	+1
-1	-1	+1	-1
-1	-1	-1	-1

- Potential approach:
 - Empirical risk minimization
 - Find $g = \operatorname{argmin}_{h \in H} E_{in}(h)$

- Multiple decision trees with zero E_{in}



How to avoid overfitting?

Learning Decision Tree from Data

- Conceptual intuition to deal with overfitting
 - Regularization: **Constrain H**
- Informally,

$$\begin{array}{ll} \text{minimize} & E_{in}(\vec{w}) \\ \text{subject to} & \text{size}(tree) \leq C \end{array}$$
- This optimization is generally computationally intractable.
- Most decision tree learning algorithms rely on **heuristics** to approximate the goal.

Greedy-Based Decision Tree Algorithm

- Greedily, recursively, choose the next feature to split
- DecisionTreeLearn(D): Input a dataset D , output a decision tree hypothesis
 - Create a root node
 - If **termination conditions** are met
 - return a single node tree with **leaf prediction** based on D
 - Else: Greedily find a feature A to split according to **split criteria**
 - For each possible value v_i of A
 - Let D_i be the dataset containing data with value v_i for feature A
 - Create a subtree DecisionTreeLearn(D_i) that being the child of root
- Most decision tree learning algorithms follow this template, but with different choices of **heuristics**

ID3: Using Information Gain as Selection Criteria

- Information gain of choosing feature A to split
 - $Gain(D, A) = H(D) - \sum_i \frac{|D_i|}{|D|} H(D_i)$ [The amount of decrease in entropy]
- ID3: Choose the split that maximize $Gain(D, A)$

Notations:

$H(D)$: Entropy of D

$|D|$ is the number of points in D

DecisionTreeLearn(D)

Create a root node r

If **termination conditions** are met

return a single node tree with **leaf prediction** based on

Else: Greedily find a feature A to split according to **split criteria**

For each possible value v_i of A

Let D_i be the dataset containing data with value v_i for feature A

Create a subtree DecisionTreeLearn(D_i) that being the child of root r

- ID3 termination conditions
 - If all labels are the same
 - If all features are the same
 - If dataset is empty
- ID3 leaf predictions
 - Most common labels (majority voting)
- ID3 split criteria
 - Information gain

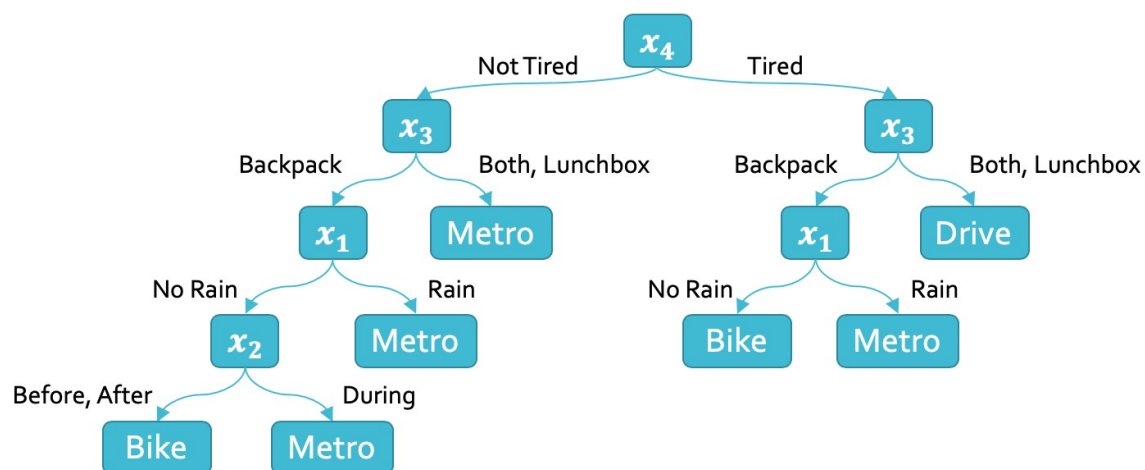
Illustration of "High Variance" of Decision Trees

x_1	x_2	x_3	x_4	y
Rain	Before	Both	Tired	Drive
Rain	During	Both	Not Tired	Metro
Rain	During	Both	Tired	Drive
Rain	After	Backpack	Not Tired	Metro
Rain	After	Backpack	Tired	Metro
Rain	After	Lunchbox	Tired	Drive
No Rain	Before	Backpack	Tired	Bike
No Rain	Before	Lunchbox	Not Tired	Metro
No Rain	Before	Lunchbox	Tired	Drive
No Rain	During	Backpack	Not Tired	Metro
No Rain	During	Both	Tired	Drive
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No Rain	After	Both	Not Tired	Metro
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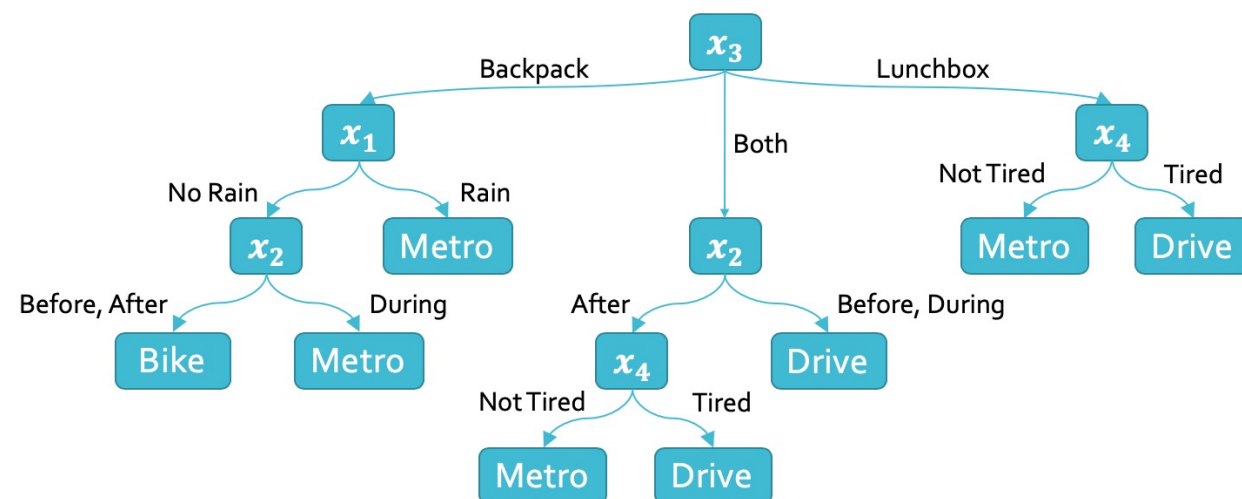
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High variance: A small deviation of data would lead to very different learned hypothesis

Decision Tree Hypothesis



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 - Easily overfit
- Why we care?
 - One of the classical model
 - **Building block for other models**

Today's Lecture

The notes are not intended to be comprehensive. They should be accompanied by lectures and/or textbook.
Let me know if you spot errors.

Ensemble Learning

Ensemble Learning

- Assume we are given a set of learned hypothesis
 - g_1, g_2, \dots, g_M
- What can we do?
 - Use validation to pick the best one
 - What if all of them are not good enough
- Can we **aggregate** them?

An Anecdote about Aggregation



- At a 1906 country fair, ~800 people participate in a contest to guess the weight of an ox.
- Reward is given to the person with the closest guess.
- The average guess is 1,197lbs.
The true answer is 1,198lbs.

How to do Aggregation

- Given a set of **weak learners** g_1, \dots, g_M , how to output a **stronger learner** that performs better?
- Uniform aggregation
 - Regression (average): $\bar{g}(\vec{x}) = \frac{1}{M} \sum_{m=1}^M g_m(\vec{x})$
 - Classification (majority vote): $\bar{g}(\vec{x}) = \text{sign} \left(\frac{1}{M} \sum_{m=1}^M g_m(\vec{x}) \right)$
- Weighted aggregation
 - Regression (average): $\bar{g}(\vec{x}) = \frac{1}{M} \sum_{m=1}^M \alpha_m g_m(\vec{x})$
 - Classification (majority vote): $\bar{g}(\vec{x}) = \text{sign} \left(\frac{1}{M} \sum_{m=1}^M \alpha_m g_m(\vec{x}) \right)$
- Stacking (won't talk about this in this course)
 - Take the prediction of g_1 to g_m as input features, train another model on top of that

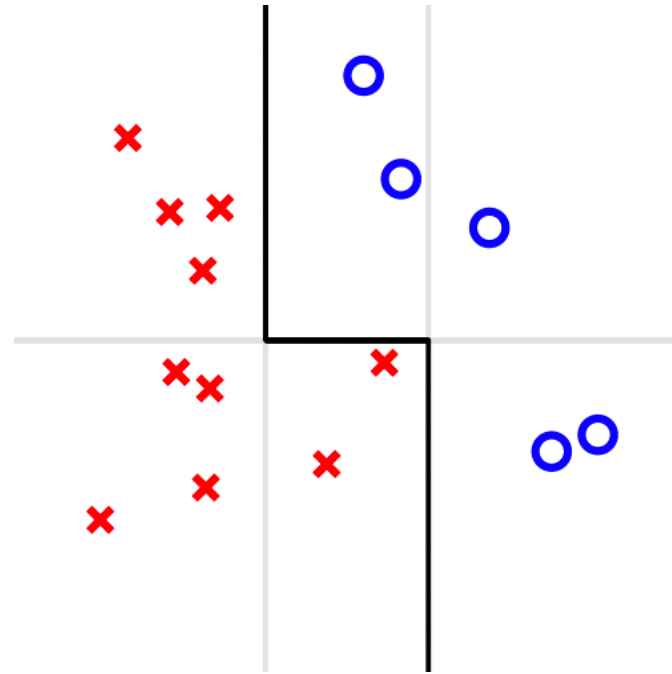
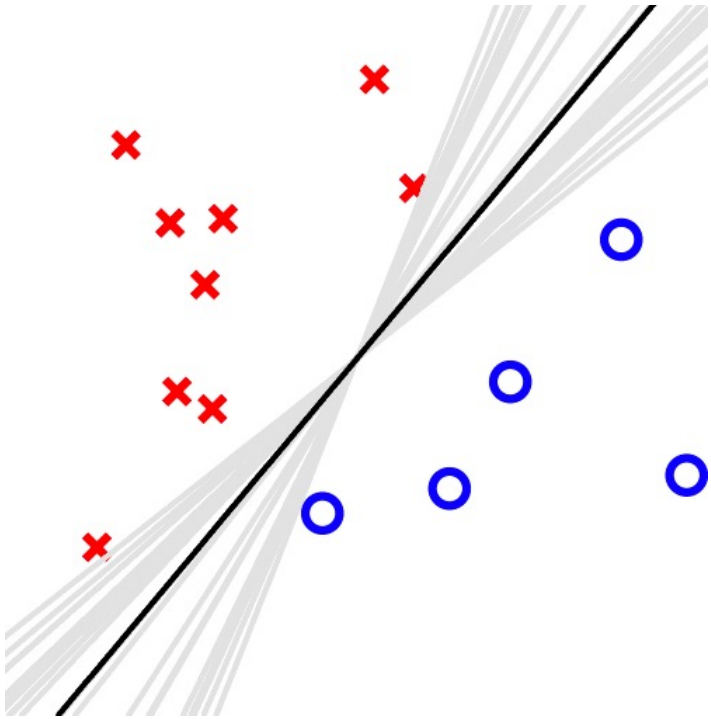
Mathematically, majority voting and average is similar with +1/-1 labels

Is Aggregation a Good Idea?

- Some illustrative examples

Is Aggregation a Good Idea?

- Some illustrative examples



Is Aggregation a Good Idea?

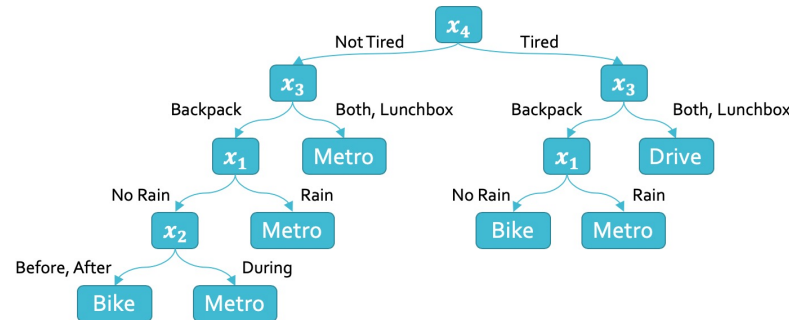
- Maybe
 - If the hypothesis is **diverse**, and “on average” they seem good
 - (If you take humans as weak learners, this is almost democracy)
- Question:
 - How do we **find** a set of hypothesis that are **diverse** and “on average” good
 - How do we **aggregate** the set of hypothesis
- Ensemble learning
 - Bagging – Random Forest (This lecture)
 - Boosting – AdaBoost (Next lecture)

Diverse Weak Learners

- One common way to construct weak learners is via **decision trees**

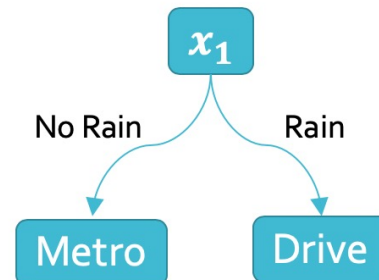
- Fully grown decision trees

- High variance
- Low bias



- Decision stump (One-depth decision trees, split on only one attribute)

- Low variance
- High bias



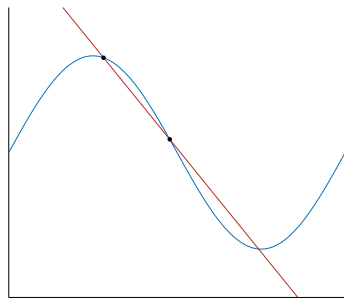
Bagging

Bootstrapped Aggregating

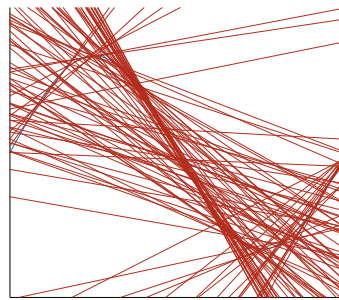
(Using randomization to construct diverse weak learners)

Review: Bias-Variance Decomposition

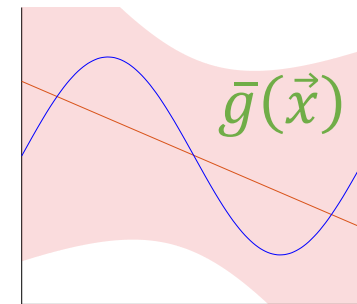
- f : sine function, $H: h(x) = ax + b, N=2$



For each dataset,
learn a hypothesis.



Draw many datasets,
learn many hypothesis



Take average.

- Observations

- The variance of each learned hypothesis is high
- The variance of “average” of them ($\bar{g}(\vec{x})$) is lower

- Can we apply similar intuitions?

- Generate a lot of **high-variance but low bias** weak learners
- Aggregate them using uniform aggregation

We only have one
dataset in practice!

Bootstrapping

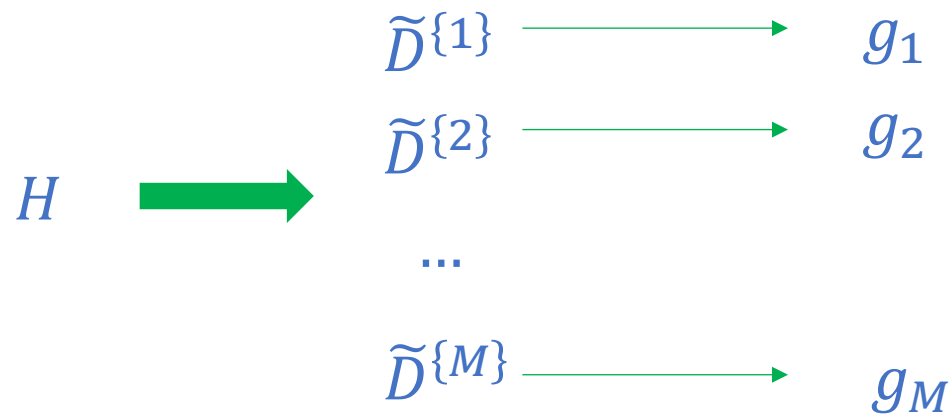
- Intuition:
 - Use the dataset D we have to approximate the data distribution
 - Sample (with replacement) from D to create bootstrapped datasets
- Bootstrapping:
 - Let $D = \{(\vec{x}_1, y_1), \dots, (\vec{x}_N, y_N)\}$ be the dataset we have
 - Repeatedly uniformly sample N points from D with replacement
 - The number of sampled points doesn't have to be N , but it's a reasonable/common choice.
 - Obtain many bootstrapped datasets
 - $\tilde{D}^{(1)} = \{(x_1, y_1), (x_1, y_1), (x_4, y_4), \dots\}$
 - \dots
 - $\tilde{D}^{(M)}$

Bagging - Bootstrapped Aggregating

- Bootstrap M datasets $\{\tilde{D}^{\{m\}}\}$ and learn a hypothesis from each of them
- Aggregate the learned hypothesis

Bagging - Bootstrapped Aggregating

- Bootstrap M datasets $\{\tilde{D}^{(m)}\}$ and learn a hypothesis from each of them



- Aggregate the learned hypothesis

$$G(\vec{x}) = \bar{g}(\vec{x}) = \text{sign} \left(\frac{1}{M} \sum_{m=1}^M g_m(\vec{x}) \right) \quad (\text{assume we are doing classification})$$

Why/When Bagging Might Be Helpful?

- What we know from statistics
 - Consider M independent random variables x_1, x_2, \dots, x_M , each with variance σ^2
 - The variance of $\frac{1}{M} \sum_{m=1}^M x_m$ is $\frac{\sigma^2}{M}$
- If we have “weak learners” that have **high variance** but **low bias**
 - Bagging helps **reduce the variance** and **maintain low bias**
 - From bias-variance decomposition, this implies a strong learner

Break and Question

Exercise:

Given a dataset D with N points.

Consider we bootstrap a dataset $\tilde{D}^{(m)}$ by sampling N points with replacement from D , what's the probability that a given point (\vec{x}_n, y_n) is not in $\tilde{D}^{(m)}$?

Out-Of-Bag (OOB) Error

Probability for a Point to be Out of Bag

- Consider we bootstrap a dataset $\tilde{D}^{(m)}$ by sampling N points from D , what's the probability that a given point (\vec{x}_n, y_n) is not in $\tilde{D}^{(m)}$.

$$\begin{aligned} & \left(1 - \frac{1}{N}\right)^N \\ &= \left(\frac{1}{1 + \frac{1}{N-1}}\right)^N \\ &\approx \frac{1}{e} \approx 0.36 \text{ when } N \rightarrow \infty \end{aligned}$$

When N is large, for each bootstrapped dataset $\tilde{D}^{(m)}$, a significant proportion of points in D is not included.

- A point that is not in $\tilde{D}^{(m)}$ is not involved in training g_m
 - Can we utilize it to **validate** the performance of g_m ?
 - Yes, but we care about the overall performance, not just the performance of g_m ...

Out-Of-Bag (OOB) Error

	$\tilde{D}^{(1)}$	$\tilde{D}^{(2)}$	$\tilde{D}^{(3)}$	$\tilde{D}^{(4)}$...
(\vec{x}_1, y_1)	Yes	Yes	No	No	...
(\vec{x}_2, y_2)	Yes	No	No	No	...
...
(\vec{x}_N, y_N)	No	Yes	Yes	Yes	...

Whether a point is in a bootstrapped dataset

- Recall that we learn g_1, \dots, g_M using $\tilde{D}^{(1)}, \dots, \tilde{D}^{(M)}$
- Which set of hypothesis can (\vec{x}_1, y_1) be used for **validation**?

Out-Of-Bag (OOB) Error

	$\tilde{D}^{(1)}$	$\tilde{D}^{(2)}$	$\tilde{D}^{(3)}$	$\tilde{D}^{(4)}$...
(\vec{x}_1, y_1)	Yes	Yes	No	No	...
(\vec{x}_2, y_2)	Yes	No	No	No	...
...
(\vec{x}_N, y_N)	No	Yes	Yes	Yes	...

Whether a point is in a bootstrapped dataset

- G_n^- : the aggregation of hypothesis that \vec{x}_n is OOB of

- $G_1^- = \text{aggregate}(g_3, g_4, \dots)$
- $G_2^- = \text{aggregate}(g_2, g_3, g_4, \dots)$
- $G_N^- = \text{aggregate}(g_1, \dots)$

Aggregate:
Majority voting for classification
Average for regression

- OOB Error

- $E_{OOB}(G) = \frac{1}{N} \sum_{n=1}^N \text{error}(G_n^-(\vec{x}_n), y_n)$

Error:
Binary error for classification
Squared error for regression

Out-Of-Bag (OOB) Error

$$E_{OOB}(G) = \frac{1}{N} \sum_{n=1}^N \text{error}(G_n^-(\vec{x}_n), y_n)$$

- Bagging provided an **intrinsic** mechanism for us to perform validation
 - We don't need to split the dataset into training and validation
- Practical issues (you might face this in HW4)
 - What if some \vec{x}_n appears in all bootstrapped datasets?
 - The probability of this happening is small when the number of bags M is large
 - Let S be the set of points that is out of bag for at least one bootstrapped dataset
 - $E_{OOB}(G) = \frac{1}{|S|} \sum_{(\vec{x}_n, y_n) \in S} \text{error}(G_n^-(\vec{x}_n), y_n)$

Random Forest

What We Have Learned

Bagging:

A method to generate and aggregate many **high-variance** weak learners into a stronger one.



Decision tree:

Various nice properties
Bad generalization
- Due to **high variance**



Random Forest:

1. Construct many random trees
2. Aggregate the random trees

Random Forest

- Construct many random trees
 - Bootstrapping datasets and learn a **max-depth tree** for each of them
 - Other randomizations (not required in HW4)
 - When choosing split features, choose from a random subset (instead of all features)
 - Randomly project features (similar to non-linear transformation) for each tree
- Aggregate the random trees
 - Classification: Majority vote $\bar{g}(\vec{x}) = \text{sign} \left(\frac{1}{M} \sum_{m=1}^M g_m(\vec{x}) \right)$
 - Regression: Average $\bar{g}(\vec{x}) = \frac{1}{M} \sum_{m=1}^M g_m(\vec{x})$

Questions?

- Note that in HW4, you will be asked to implement Bagging Decision Tree and calculate the OOB errors.
- Make sure you know the definitions/algorithm well.

Brief Discussion on Feature Importance

- Not all features are equally important
 - Some features could be **redundant** -- (birth year, age)
 - Some features might be **irrelevant** -- feature: name, label: prob of heart attack
- How do we know which features are more important?
 - Linear models:
 - The **size of the weight** is a proxy for feature importance
 - Applying L1 regularization is one way to reduce the number of features
 - Decision tree:
 - The feature **closer to the root** is probably more important
 - Random forest:
 - **Average “information gain”** of all trees is a proxy for feature importance
- See LFD e-Chap 9.2 for more discussion on feature selection

Boosting

Ensemble Learning

- Goal: Utilize a set of **weak learners** to obtain a **strong learner**
- Format of ensemble learning
 - **Construct** many **diverse** weak learners
 - **Aggregate** the weak learners

Bagging:

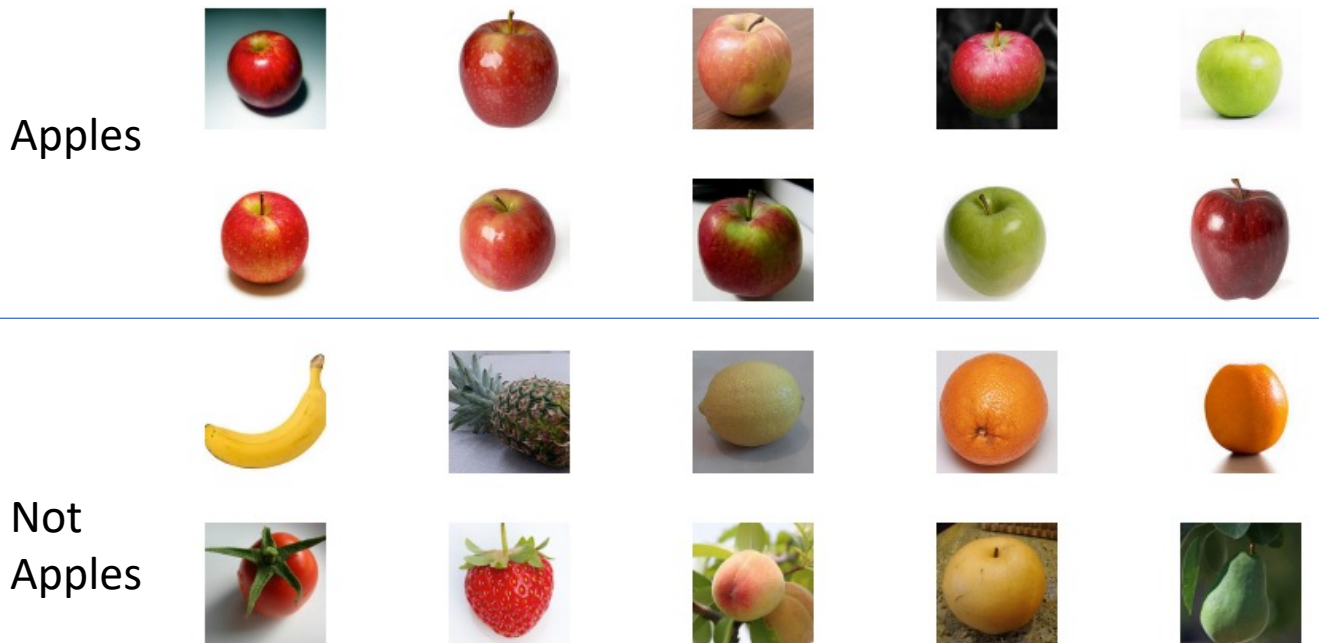
- Construct diverse weak learners
 - (**Simultaneously**) bootstrapping datasets
 - Train weak learners on them
- Aggregate the weak learners
 - **Uniform** aggregation

Boosting

- Construct diverse weak learners
 - **Adaptively** generating datasets
 - Train weak learners on them
- Aggregate the weak learners
 - **Weighted** aggregation

Informal Intuitions about Boosting

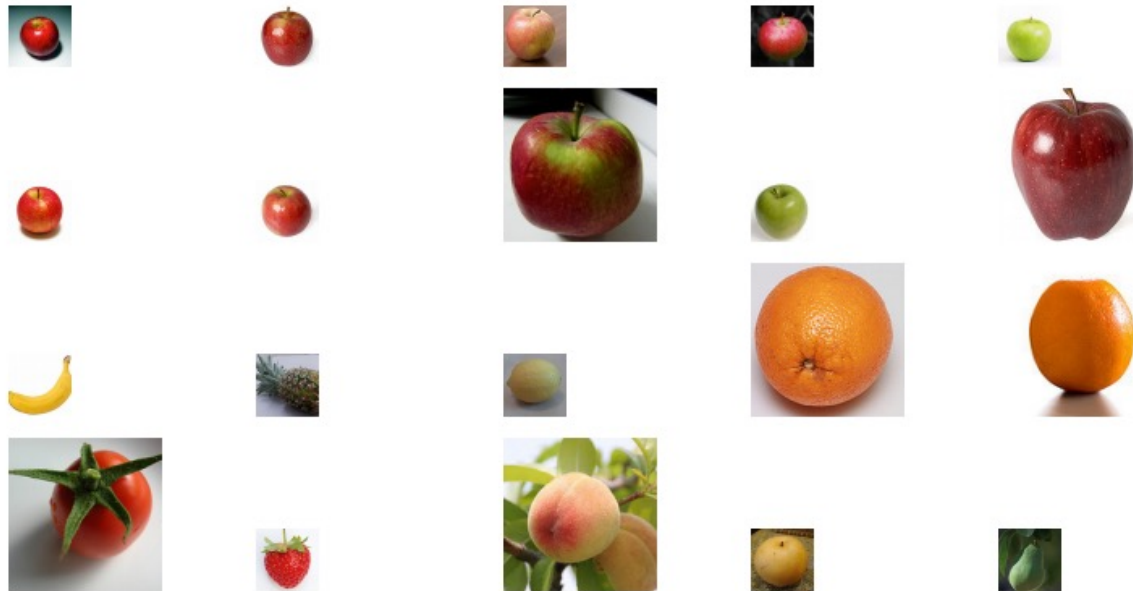
- Example : Teach a class of kids to identify apples from data



- Alice: Apples are **circular**
- Teacher:
Circular is a good feature, but using this feature might make some mistakes
Let me **highlight** the mistakes.
 - Make correct images smaller
 - Make incorrect images larger

Informal Intuitions about Boosting

- Example : Teach a class of kids to identify apples from data



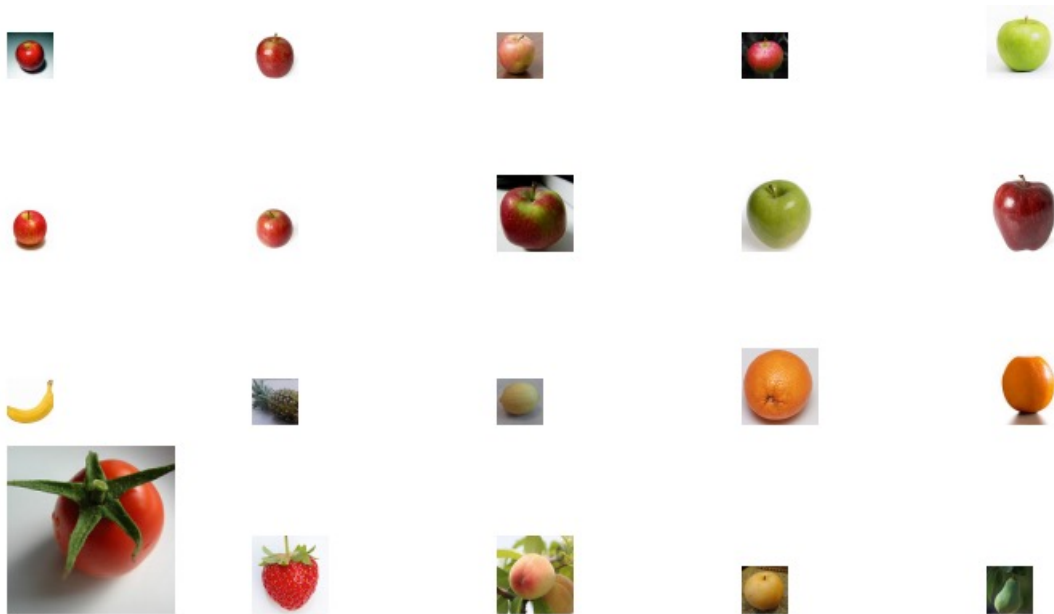
- Alice: Apples are **circular**
- Bob: Apples are **red**
- Teacher:
Yes, many apples are red but it could still make mistakes.

Let me **highlight** the mistakes.

- Make correct images smaller
- Make incorrect images larger

Informal Intuitions about Boosting

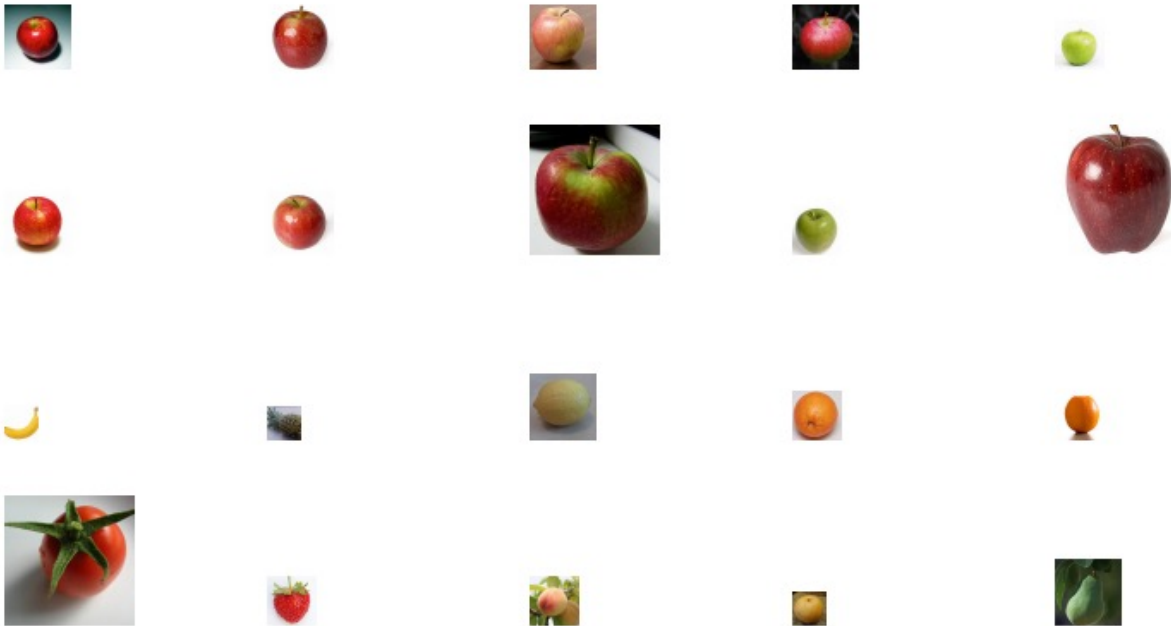
- Example : Teach a class of kids to identify apples from data



- Alice: Apples are **circular**
- Bob: Apples are **red**
- Charlie: Apples could be **green**

Informal Intuitions about Boosting

- Example : Teach a class of kids to identify apples from data



- Alice: Apples are **circular**
- Bob: Apples are **red**
- Charlie: Apples could be **green**
- David: Apples have **stems** at the top
- Class: Apples are **somewhat circular, somewhat red, possibly green, and may have stems at the top**

Informal Intuitions about Boosting

- Example : Teach a class of kids to identify apples from data



Key steps of this process:

- Learn a **simple** hypothesis for each dataset
- Iteratively update the dataset to focus on what we got wrong (i.e., create **diversity**)
- **Aggregate** the learned simple hypothesis



- Alice: Apples are **circular**
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Outline of a Boosting Algorithm

- Initialize D_1 (usually the same as the initial dataset D)
- For $t = 1$ to T
 - Learn g_t from D_t
 - Reweight the distribution and obtain D_{t+1} based on g_t and D_t
- Output **weighted**-aggregate(g_1, \dots, g_T)
 - Classification: $G(\vec{x}) = \bar{g}(\vec{x}) = \text{sign}\left(\frac{1}{T} \sum_{t=1}^T \alpha_t g_t(\vec{x})\right)$

Questions

How to learn g_t from D_t

How to reweight the distribution and obtain D_{t+1}

How to perform weighted aggregation