CSE 417T
Introduction to Machine Learning

Lecture 13

Instructor: Chien-Ju (CJ) Ho

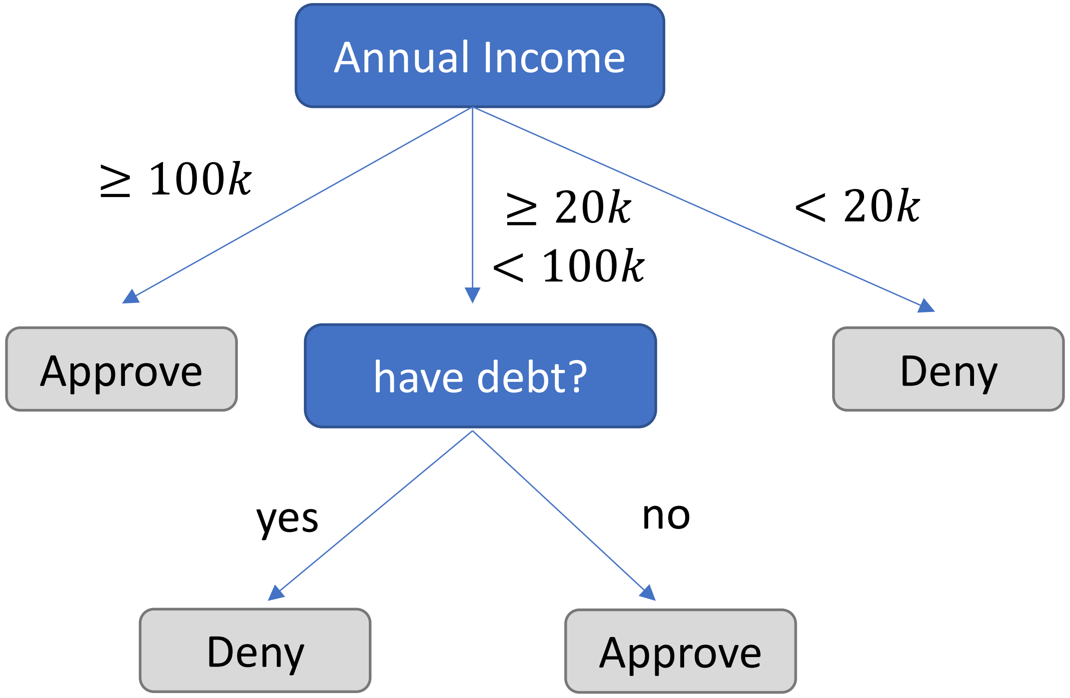
Logistics

- Homework 3: Due **Mar 5** (Sat)
  - Keep track of your own late-day usages
- Exam 1: **Mar 10 (Thursday)**
  - Topics: LFD Chapters 1 to 5
  - Covid-permitting
    - Timed exam (75 min) during lecture time in the classroom
    - 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)
  - Mar 8 (Tuesday) will be a review lecture

Recap

Decision Tree

Decision Tree Hypothesis



Credit Card Approval Example

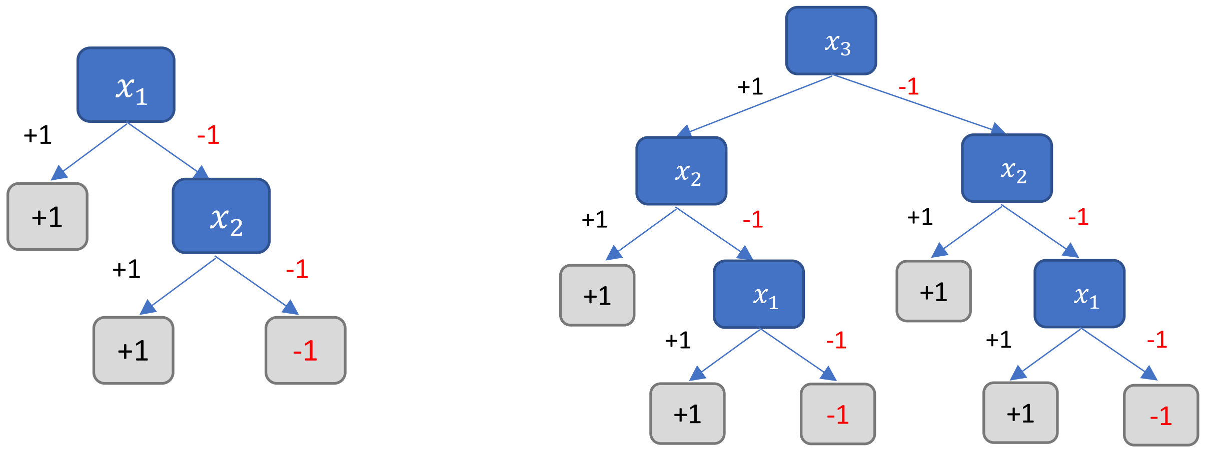
- Pros
  - Easy to interpret (interpretability is getting attention and is important in some domains)
  - Can handle multi-type data (Numerical, categorical. …)
  - Easy to implement (Bunch of if-else rules)
- Cons
  - Generally speaking, bad generalization
  - VC dimension is infinity
  - High variance (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 $g = argmin_{h \in H} E_{in}(h)$
- 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,

$$\text{minimize} \quad E_{in}(\vec{w})$$
$$\text{subject to} \quad size(tree) \leq C$$

- 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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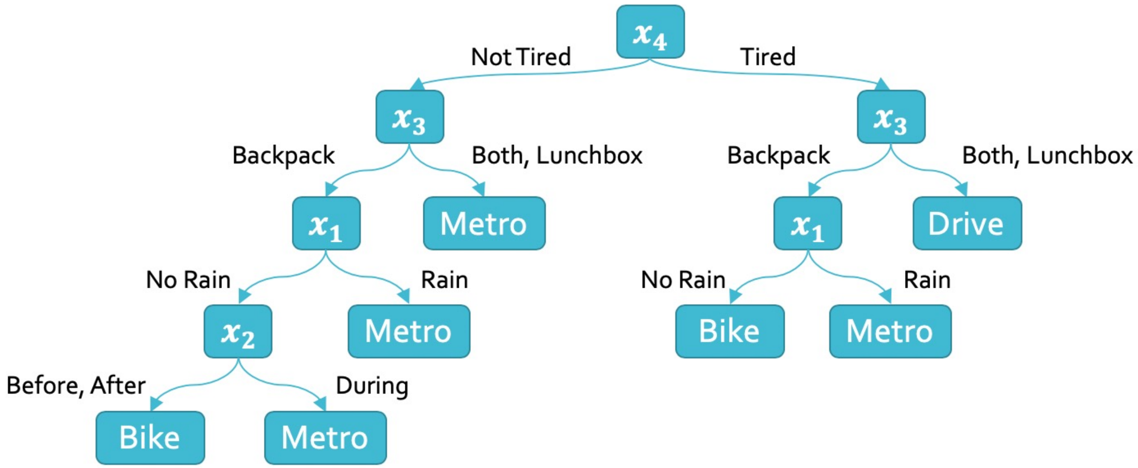

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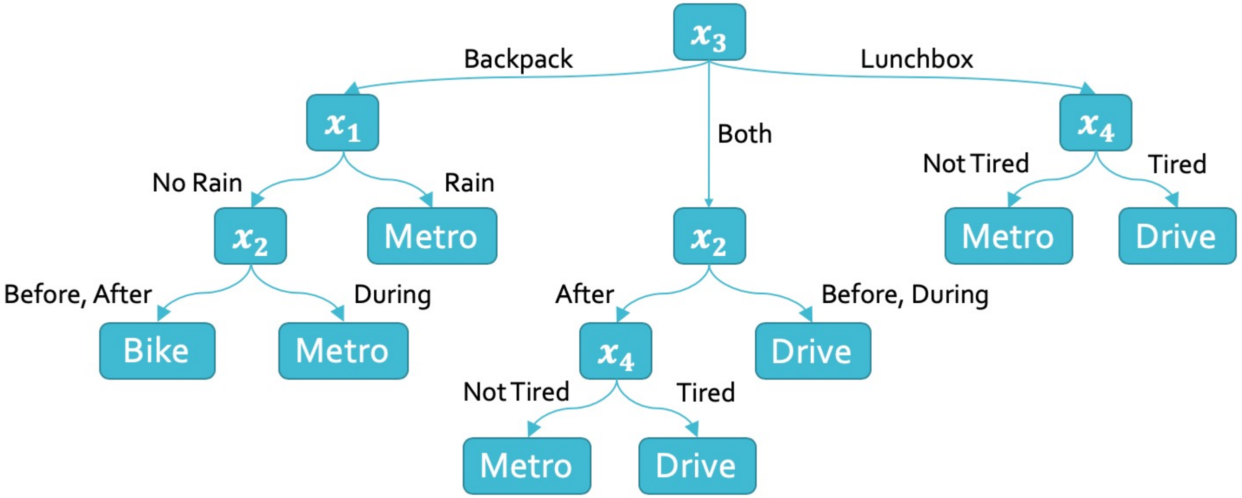
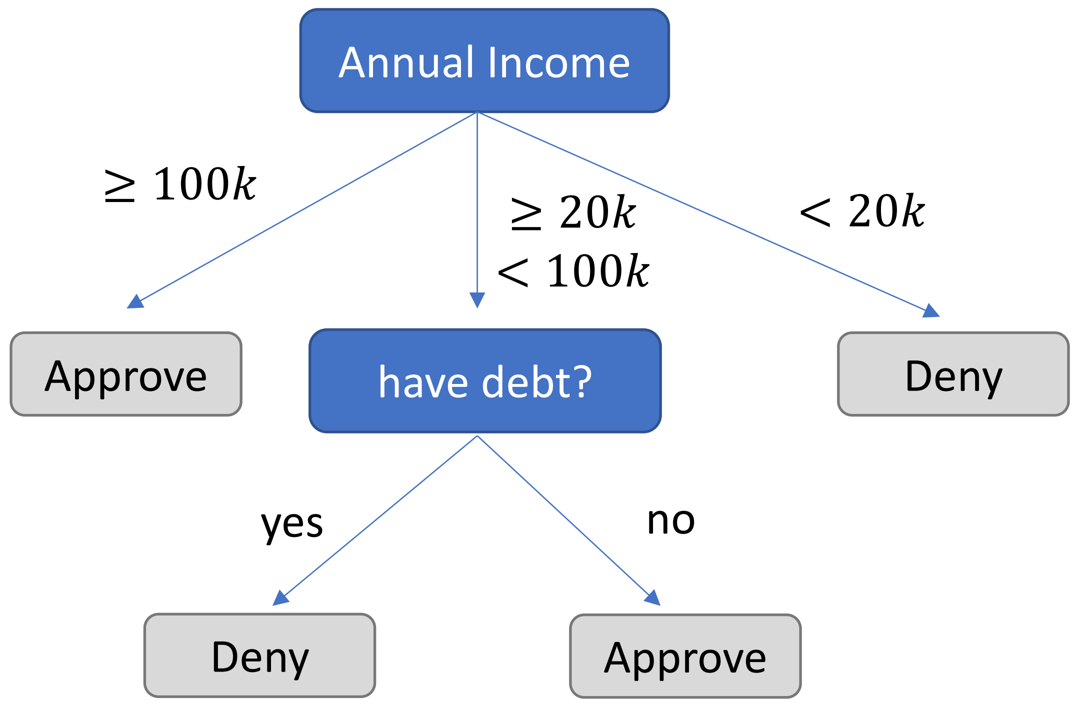


High variance: A small deviation of data would lead to very different learned hypothesis

Decision Tree Hypothesis



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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
  - $g_1, g_2, \ldots, g_M$
- What can we do?
  - Select the best one: use validation for model selection
  - What if all of them are not good enough?
- Can we aggregate them?

Aggregation

- Given a set of weak learners $g_1, \dots, g_M$, how to output a stronger learner that performs better?

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

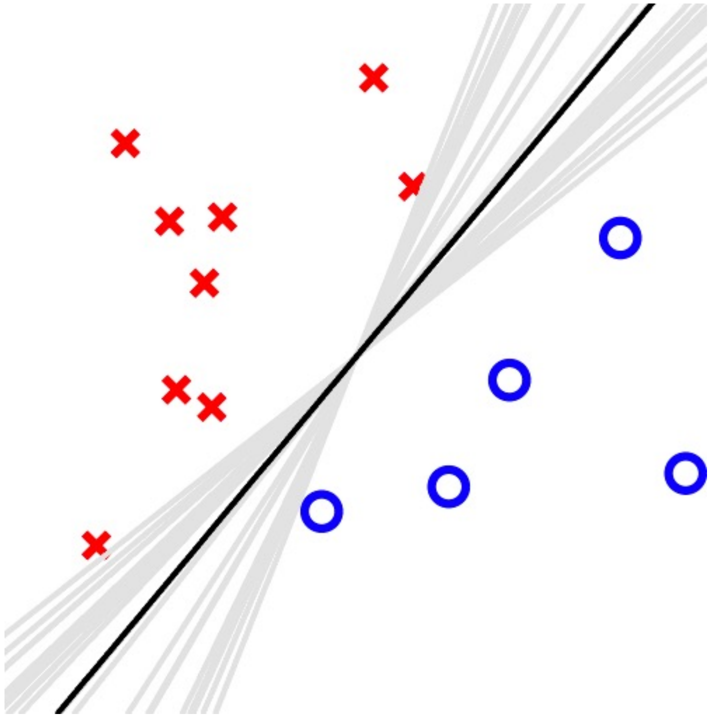
- Uniform aggregation
  - Regression (average): $\bar{g}(\vec{x}) = \frac{1}{M}\sum_{m=1}^{M} g_m(\vec{x})$
  - Classification (majority vote): $\bar{g}(\vec{x}) = sign\left(\frac{1}{M}\sum_{m=1}^{M} g_m(\vec{x})\right)$
- Weighted aggregation
  - Regression (average): $\bar{g}(\vec{x}) = \frac{1}{M}\sum_{m=1}^{M} \alpha_m g_m(\vec{x})$
  - Classification (majority vote): $\bar{g}(\vec{x}) = sign\left(\frac{1}{M}\sum_{m=1}^{M} \alpha_m g_m(\vec{x})\right)$
- 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

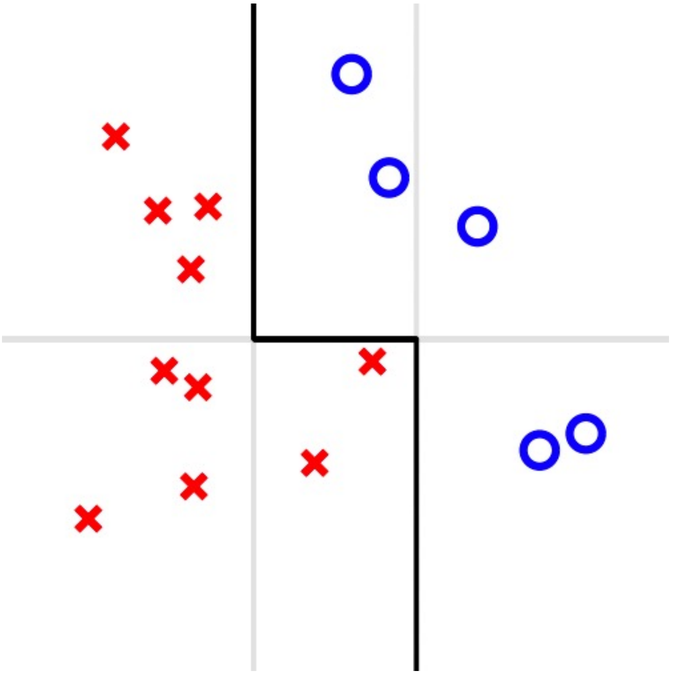
Is Aggregation a Good Idea?

- Some illustrative examples

Is Aggregation a Good Idea?

- Some illustrative examples



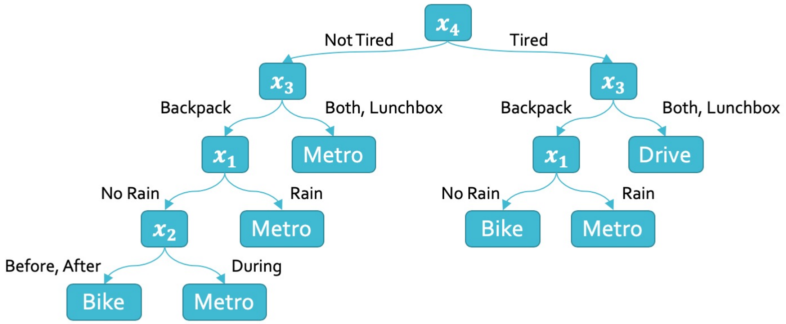


Is Aggregation a Good Idea?

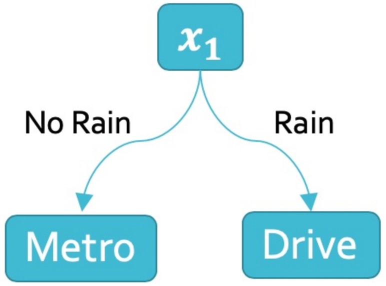
- Maybe
  - If the hypothesis is diverse, and “on average” they seem good
  - (If you take humans as weak learners, this is almost democracy)
- Question:
  - How do we find a set of hypothesis that are diverse and “on average” good
  - How do we aggregate the set of hypothesis
- Ensemble learning
  -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



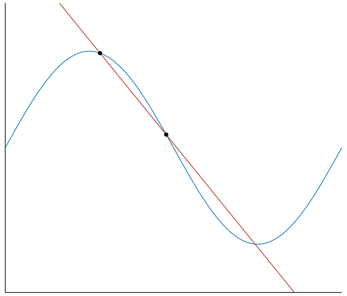
Bagging

Bootstrapped Aggregating

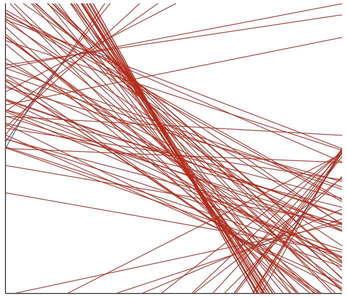
(Using randomization to construct weak learners)

Review: Bias-Variance Decomposition

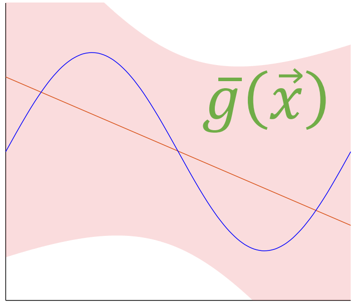
- f: sine function, $H: h(x) = ax + b$, N=2



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
    - $\widetilde{D}^{(1)} = \{(x_1, y_1), (x_1, y_1), (x_4, y_4), \dots\}$
    - …
    - $\widetilde{D}^{(M)}$

Bagging - Bootstrapped Aggregating

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

- Aggregate the learned hypothesis (assume we are doing classification)

Bagging - Bootstrapped Aggregating

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

$$H \Longrightarrow \begin{array}{ccc} \widetilde{D}^{\{1\}} & \longrightarrow & g_1 \\ \widetilde{D}^{\{2\}} & \longrightarrow & g_2 \\ \cdots & & \\ \widetilde{D}^{\{M\}} & \longrightarrow & g_M \end{array}$$

- Aggregate the learned hypothesis (assume we are doing classification)

$$G(\vec{x}) = \bar{g}(\vec{x}) = sign\left(\frac{1}{M}\sum_{m=1}^{M} g_m(\vec{x})\right)$$

Why/When Bagging Might Be Helpful?

- What we know from statistics
  - Consider M independent random variables $x_1, x_2, \dots, x_M$ with variance σ^2
  - The variance of $\frac{1}{M}\sum_{m=1}^{M} x_m$ is $\frac{\sigma^2}{M}$

- If you 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 Time

Exercise:

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

Out-Of-Bag (OOB) Error

Probability for a Point to be Out of Bag

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

$$\left(1 - \frac{1}{N}\right)^N$$
$$= \left(\frac{1}{1 + \frac{N}{N-1}}\right)^N$$
$$\approx \frac{1}{e} \approx 0.36 \text{ when } N \to \infty$$

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

- A point that is not in $\widetilde{D}^{(m)}$ 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

	$\widetilde{D}^{(1)}$	$\widetilde{D}^{(2)}$	$\widetilde{D}^{(3)}$	$\widetilde{D}^{(4)}$	…
$(\vec{x}_1, y_1)$	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 $g_1, \ldots, g_M$ using $\widetilde{D}^{(1)}, \ldots \widetilde{D}^{(\mathrm{M})}$
- 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
  - $G_1^- = \text{aggregate}(g_3, g_4, \ldots)$
  - $G_2^- = \text{aggregate}(g_2, g_3, g_4, \ldots)$
  - $G_N^- = \text{aggregate}(g_1, , \ldots)$

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 $\bar{g}(\vec{x}) = sign\left(\frac{1}{M}\sum_{m=1}^{M} g_m(\vec{x})\right)$
  - 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

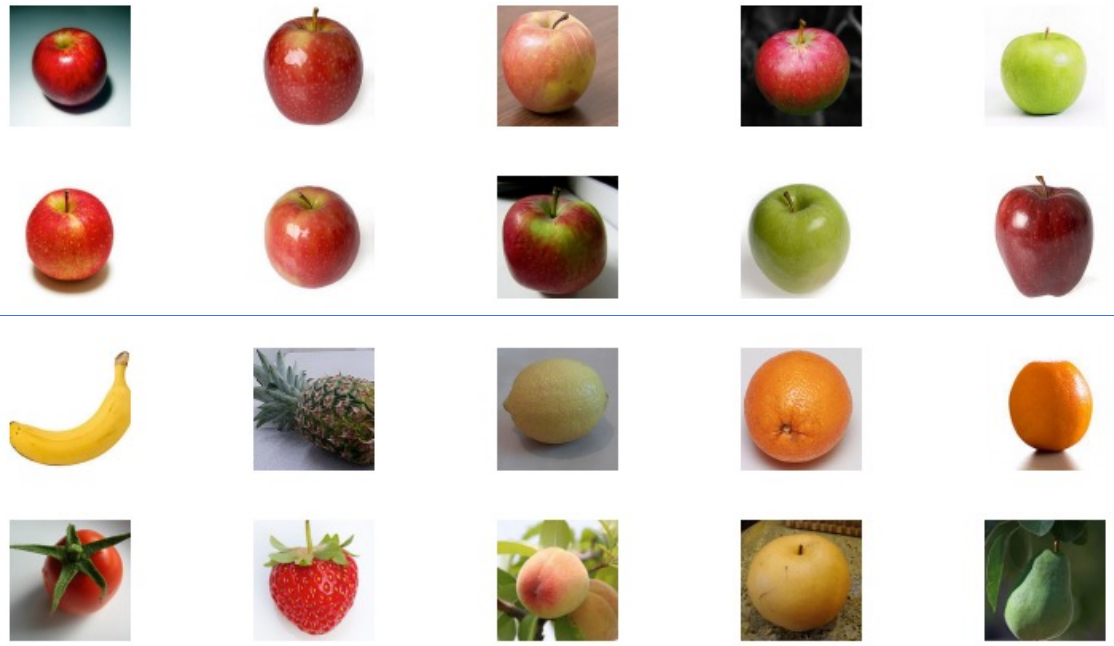
<u>Bagging:</u>
- Construct diverse weak learners
  - (Simultaneously) bootstrapping datasets
  - Train weak learners on them
- Aggregate the weak learners
  - Uniform aggregation

<u>Boosting</u>
- 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

Apples



Not Apples

- 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

Example created by Hsuan-Tien Lin

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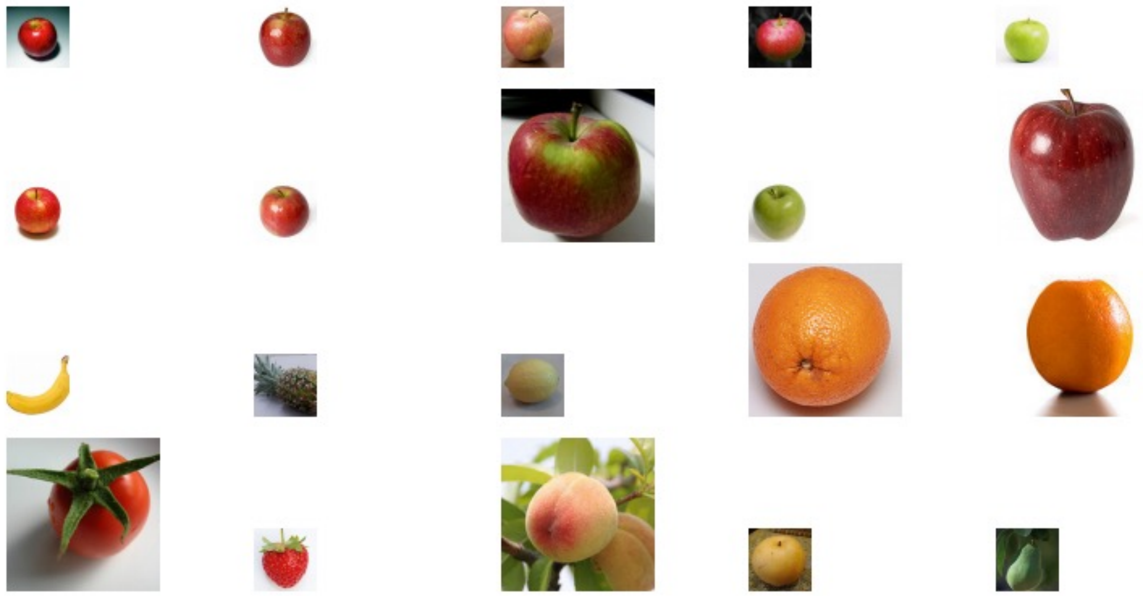

- Alice: Apples are circular
- Bob: Apples are red
- Teacher:
  Yes, many apples are red but it could still make mistakes.

  Let me highlight the mistakes.
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Example created by Hsuan-Tien Lin

Informal Intuitions about Boosting

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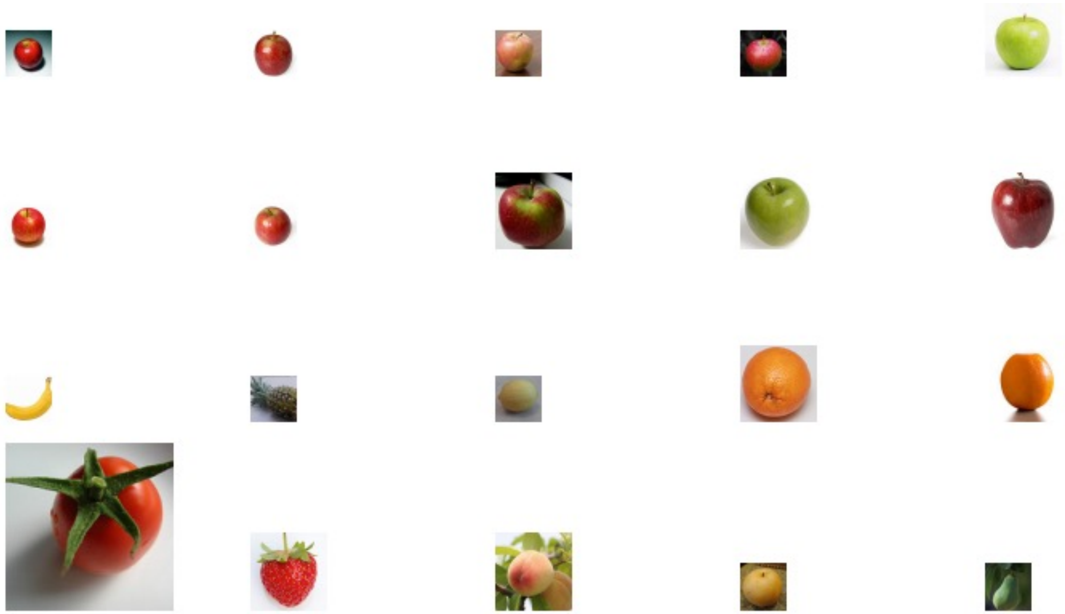
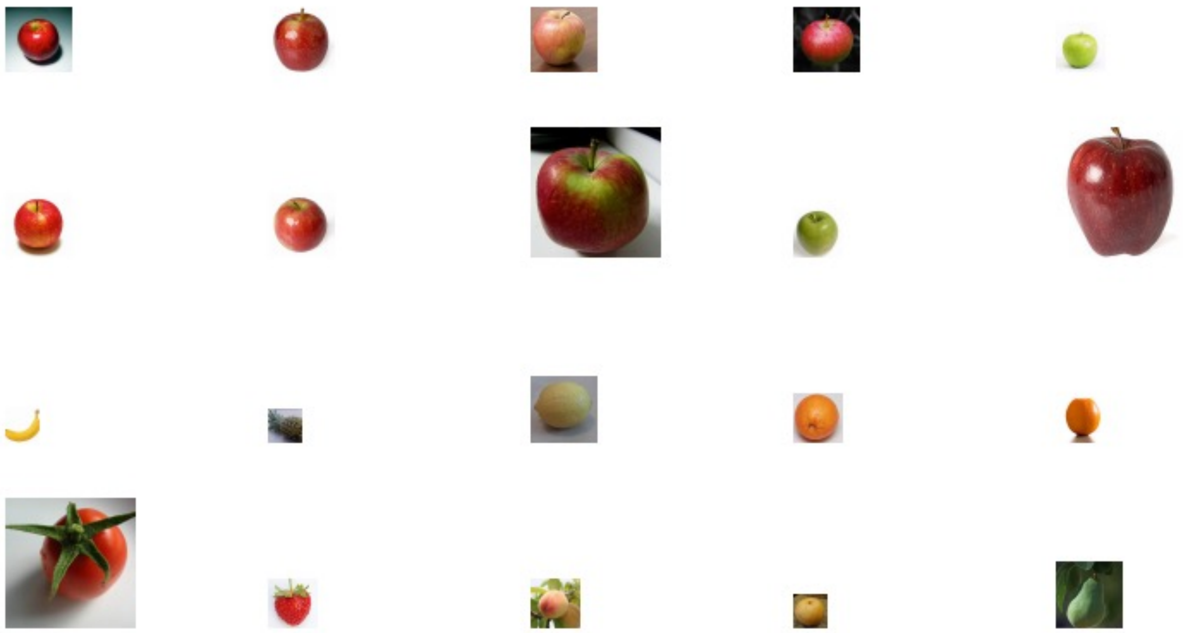


- Alice: Apples are circular
- Bob: Apples are red
- Charlie: Apples could be green

Example created by Hsuan-Tien Lin

Informal Intuitions about Boosting

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



Example created by Hsuan-Tien Lin

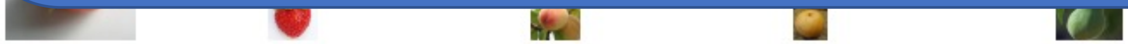
- Alice: Apples are circular
- Bob: Apples are red
- Charlie: Apples could be green
- David: Apples have stems at the top
- Class: Apples are somewhat circular, somewhat red, possibly green, and may have stems at the top

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



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Example created by Hsuan-Tien Lin

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: $G(\vec{x}) = \bar{g}(\vec{x}) = sign\left(\frac{1}{T}\sum_{t=1}^{M} \alpha_t g_t(\vec{x})\right)$

Questions

How to learn g_t from D_t
How to reweight the distribution and obtain D_{t+1}
How to perform weighted aggregation

Discussion on Re-weighted D_t (What does re-weighting mean?)

- Original Dataset $D = \{(\vec{x}_1, y_1), \dots, (\vec{x}_N, y_N)\}$
- Notation of D_t
  - $D_t(n)$ is the weight/probability of data point $(\vec{x}_n, y_n)$ in D_t
  - $\sum_{n=1}^{N} D_t(n) = 1$

- What is $E_{in}(h)$ on D_t? (Expressed as $E_{in}^{(D_t)}(h)$)
  - Re-sample dataset (noisier)
    - Re-sample the dataset from D according to distribution D_t
    - Calculate E_{in} on the re-sampled dataset as usual
  - Calculate weighted error
    - $E_{in}^{(D_t)}(h) = \sum_{n=1}^{N} D_t(n) \operatorname{error}(h(\vec{x}_n), y_n)$

When $D_t(n) = 1/N$. This reduces to standard definition of E_{in}.