10-601 Introduction to Machine Learning

Machine Learning Department
School of Computer Science
Carnegie Mellon University

# Overfitting

# +

# k-Nearest Neighbors

Matt Gormley & Henry Chai
Lecture 4
Sep. 13, 2021

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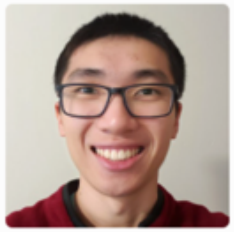
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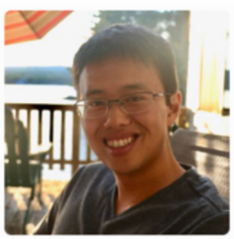
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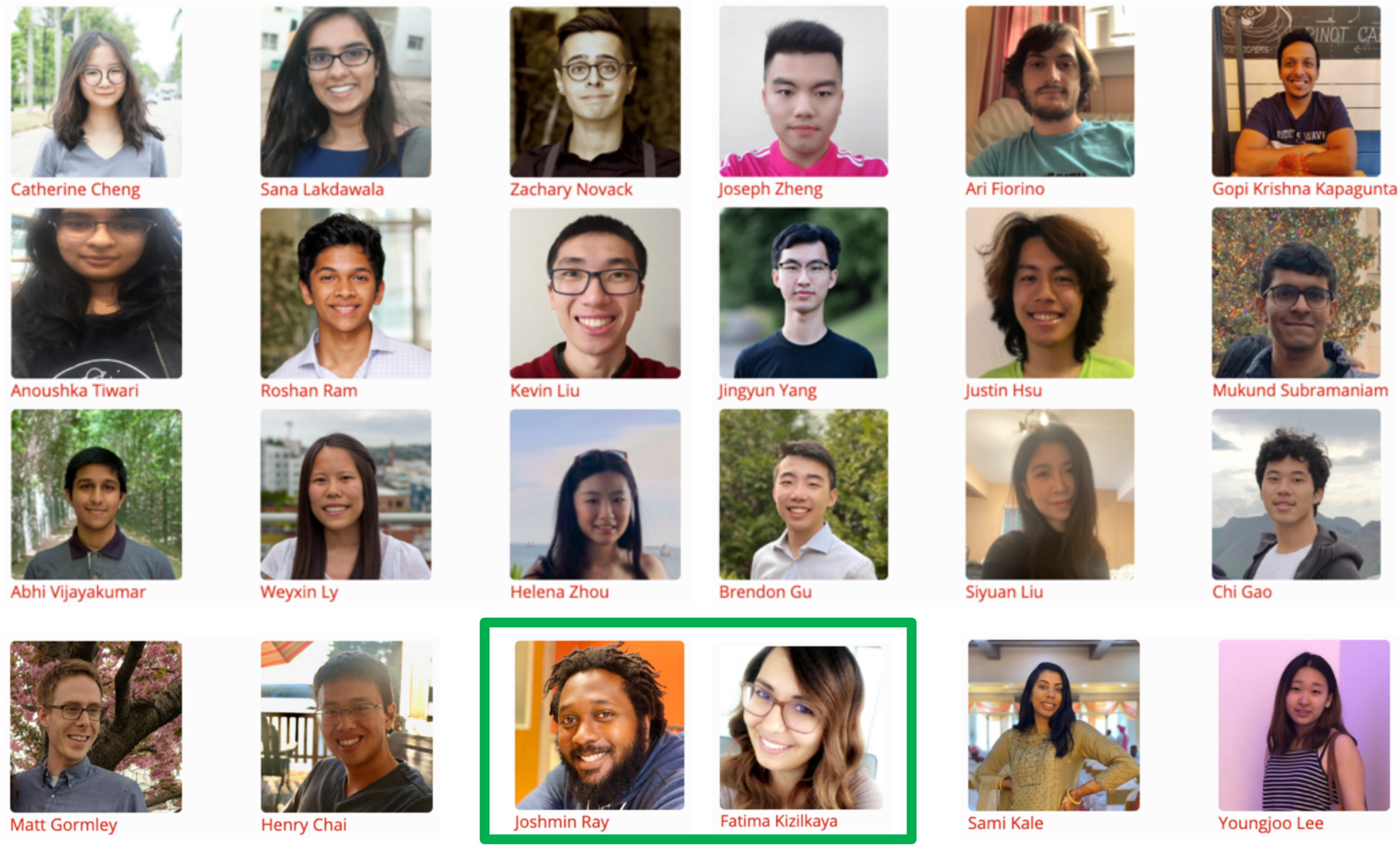


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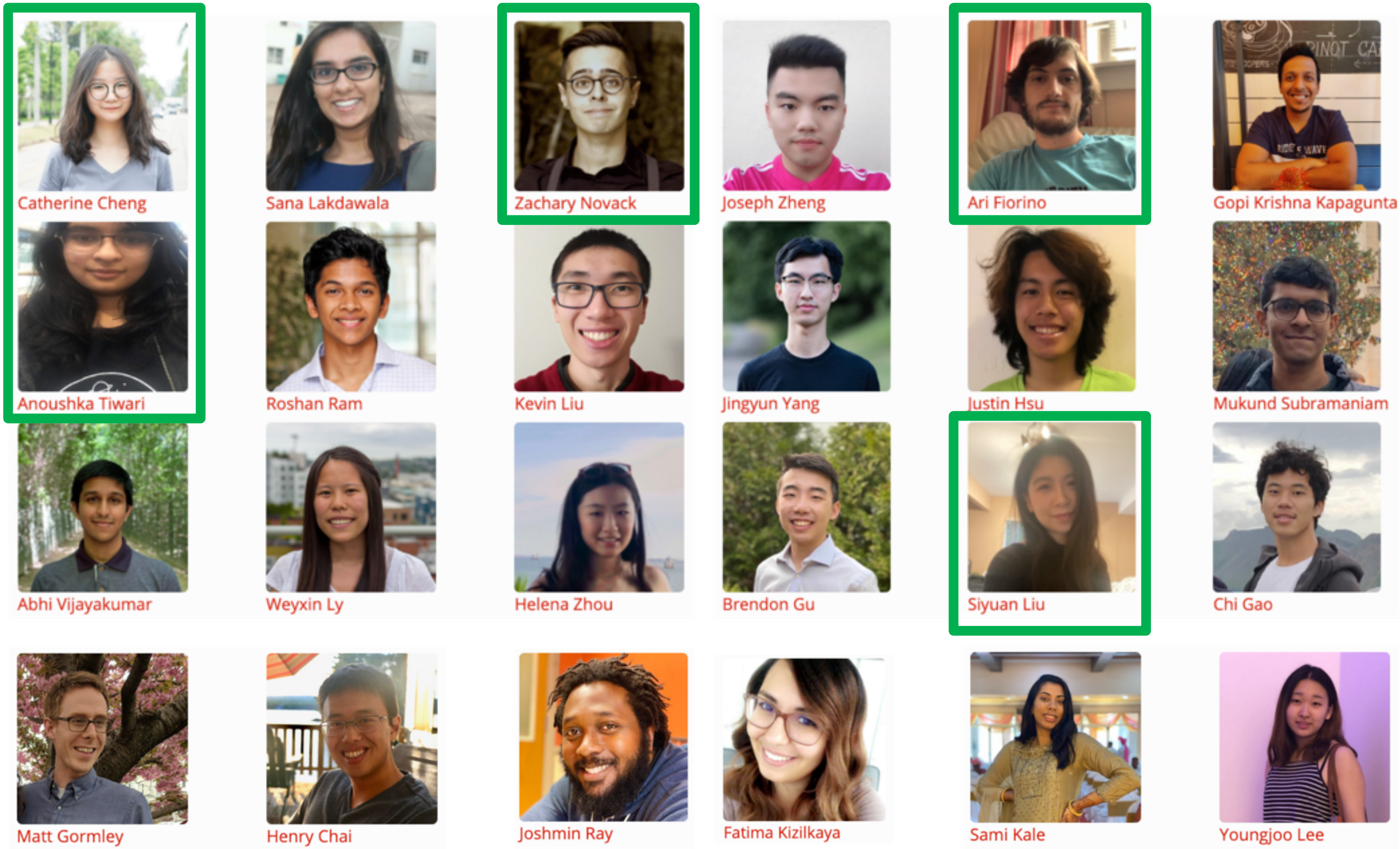


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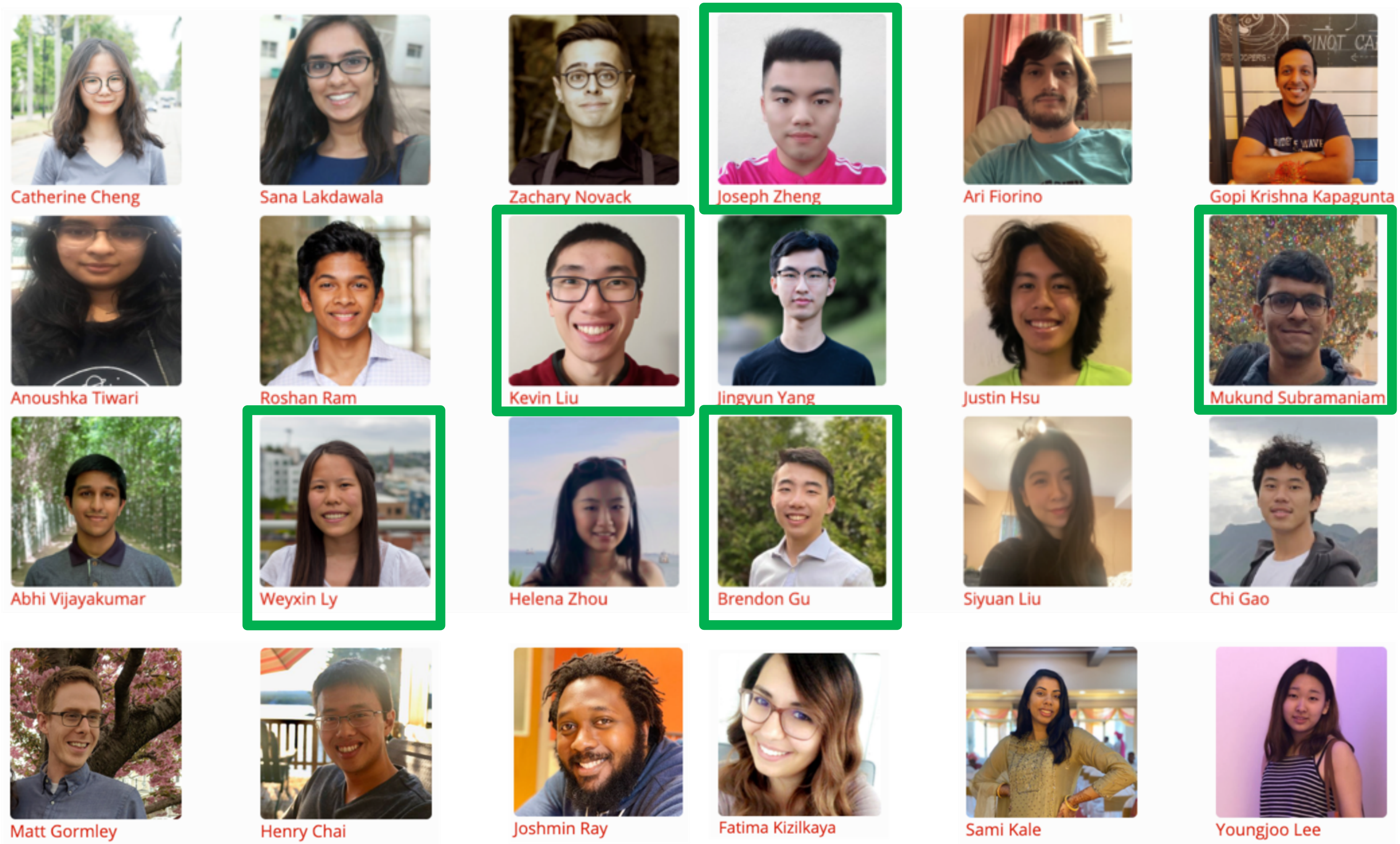


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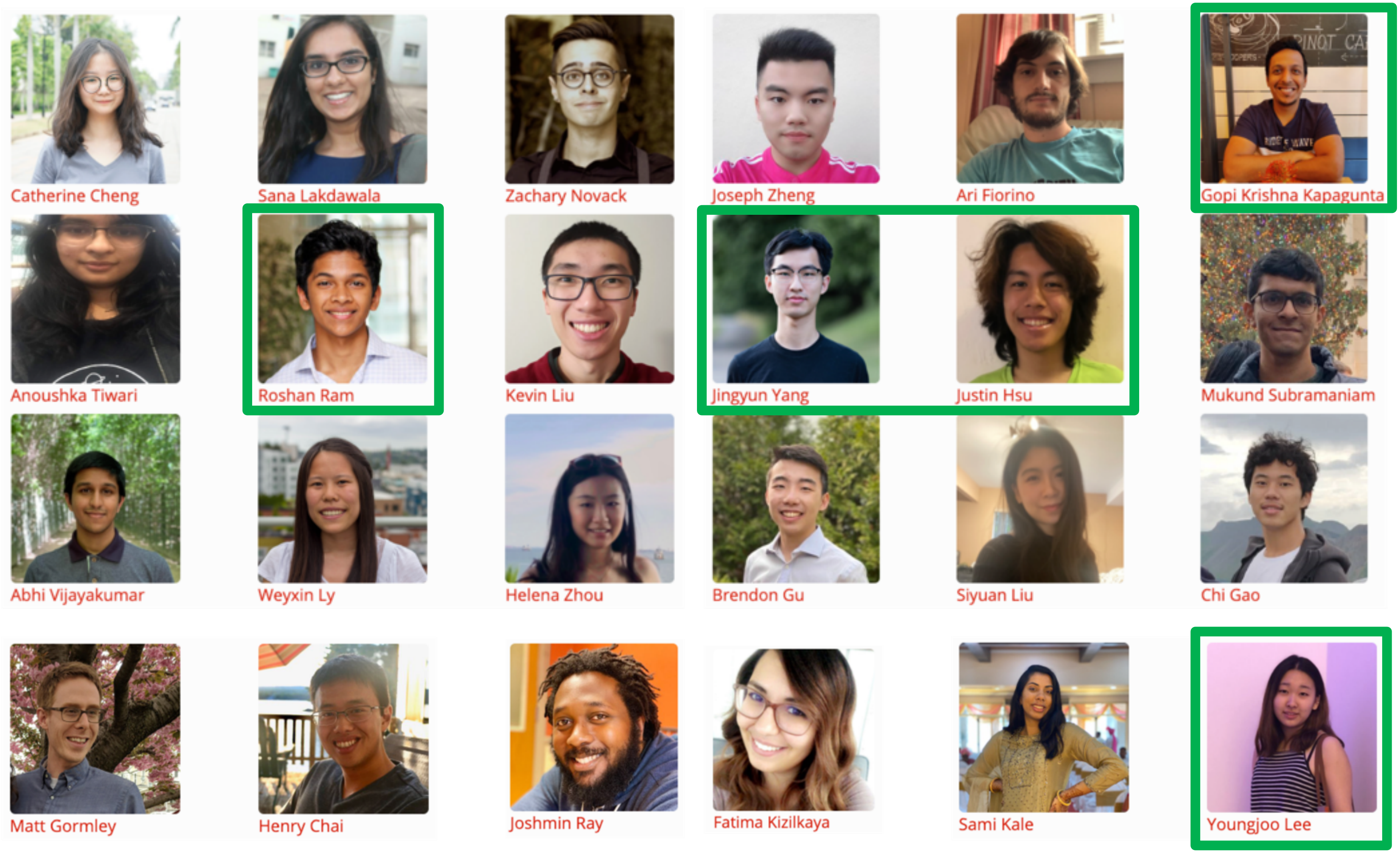


Team C

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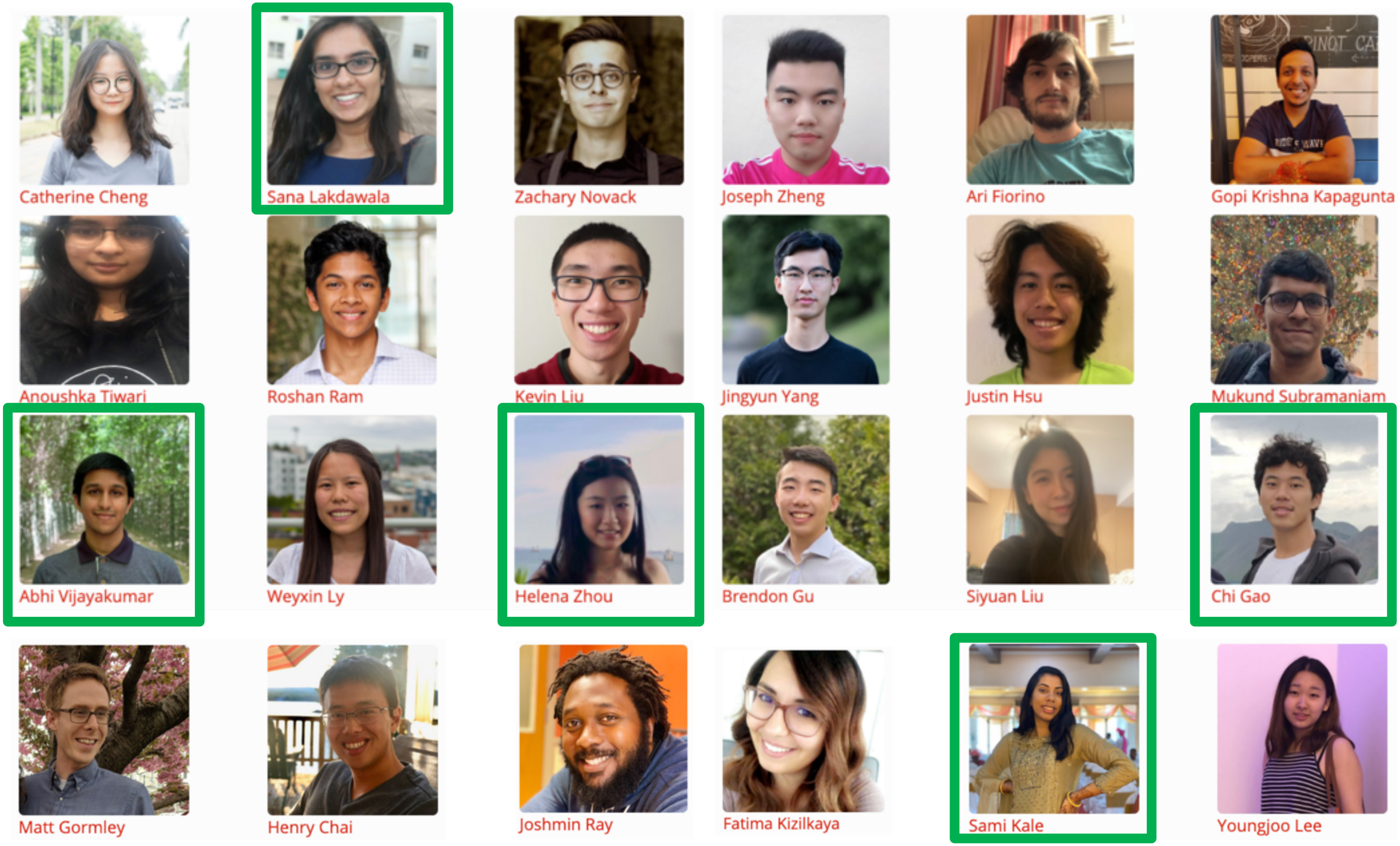



Team D

# Q&A

**Q:** When and how do we decide to stop growing trees? What if the set of values an attribute could take was really large or even infinite?

**A:** We'll address this question for discrete attributes today. If an attribute is real-valued, there's a clever trick that only considers O(L) splits where L = # of values the attribute takes in the training set. Can you guess what it does?

# Reminders

- Homework 2: Decision Trees
  - Out: Wed, Sep. 8
  - Due: Mon, Sep. 20 at 11:59pm
- Required Readings:
  - 10601 Notation Crib Sheet
  - Command Line and File I/O Tutorial (check out our Google Colab template!)

# EMPIRICAL COMPARISON OF SPLITTING CRITERIA

# Experiments: Splitting Criteria

Bluntine & Niblett (1992) compared 4 criteria (random, Gini, mutual information, Marshall) on 12 datasets

**Medical Diagnosis Datasets: (4 of 12)**

- **hypo**: data set of 3772 examples records expert opinion on possible hypo- thyroid conditions from 29 real and discrete attributes of the patient such as sex, age, taking of relevant drugs, and hormone readings taken from drug samples.
- **breast:** The classes are reoccurrence or non-reoccurrence of breast cancer sometime after an operation. There are nine attributes giving details about the original cancer nodes, position on the breast, and age, with multi-valued discrete and real values.
- **tumor:** examples of the location of a primary tumor
- **lymph**: from the lymphography domain in oncology. The classes are normal, metastases, malignant, and fibrosis, and there are nineteen attributes giving details about the lymphatics and lymph nodes

*Table 1.* Properties of the data sets

| Data Set | Classes | Attr.s | Training Set | Test Set |
|---|---|---|---|---|
| hypo | 4 | 29 | 1000 | 2772 |
| breast | 2 | 9 | 200 | 86 |
| tumor | 22 | 18 | 237 | 102 |
| lymph | 4 | 18 | 103 | 45 |
| LED | 10 | 7 | 200 | 1800 |
| mush | 2 | 22 | 200 | 7924 |
| votes | 2 | 17 | 200 | 235 |
| votesl | 2 | 16 | 200 | 235 |
| iris | 3 | 4 | 100 | 50 |
| glass | 7 | 9 | 100 | 114 |
| xd6 | 2 | 10 | 200 | 400 |
| pole | 2 | 4 | 200 | 1647 |

Table from Bluntine & Niblett (1992)

# Experiments: Splitting Criteria

*Table 3.* Error for different splitting rules (pruned trees).

| Data Set | Splitting Rule | | | |
|---|---|---|---|---|
| | GINI | Info. Gain | Marsh. | Random |
| hypo | 1.01 ± 0.29 | 0.95 ± 0.22 | 1.27 ± 0.47 | 7.44 ± 0.53 |
| breast | 28.66 ± 3.87 | 28.49 ± 4.28 | 27.15 ± 4.22 | 29.65 ± 4.97 |
| tumor | 60.88 ± 5.44 | 62.70 ± 3.89 | 61.62 ± 3.98 | 67.94 ± 5.68 |
| lymph | 24.44 ± 6.92 | 24.00 ± 6.87 | 24.33 ± 5.51 | 32.33 ± 11.25 |
| LED | 33.77 ± 3.06 | 32.89 ± 2.59 | 33.15 ± 4.02 | 38.18 ± 4.57 |
| mush | 1.44 ± 0.47 | 1.44 ± 0.47 | 7.31 ± 2.25 | 8.77 ± 4.65 |
| votes | 4.47 ± 0.95 | 4.57 ± 0.87 | 11.77 ± 3.95 | 12.40 ± 4.56 |
| votes1 | 12.79 ± 1.48 | 13.04 ± 1.65 | 15.13 ± 2.89 | 15.62 ± 2.73 |
| iris | 5.00 ± 3.08 | 4.90 ± 3.08 | 5.50 ± 2.59 | 14.20 ± 6.77 |
| glass | 39.56 ± 6.20 | 50.57 ± 6.73 | 40.53 ± 6.41 | 53.20 ± 5.01 |
| xd6 | 22.14 ± 3.23 | 22.17 ± 3.36 | 22.06 ± 3.37 | 31.86 ± 3.62 |
| pole | 15.43 ± 1.51 | 15.47 ± 0.88 | 15.01 ± 1.15 | 26.38 ± 6.92 |

Key Takeaway: GINI gain and Mutual Information are statistically indistinguishable!

Info. Gain is another name for *mutual information*

Table from Bluntine & Niblett (1992)

# Experiments: Splitting Criteria

*Table 4.* Difference and significance of error for GINI splitting rule versus others.

| | Splitting Rule | | |
|---|---|---|---|
| Data Set | Info. Gain | Marsh. | Random |
| hypo | −0.06 (0.82) | 0.26 (0.99) | 6.43 (1.00) |
| breast | −0.17 (0.23) | −1.51 (0.94) | 0.99 (0.72) |
| tumor | 1.81 (0.84) | 0.74 (0.39) | 7.06 (0.99) |
| lymph | −0.44 (0.83) | [illegible]0.11 (0.05) | 7.89 (0.99) |
| LED | 0.12 (0.17) | [illegible]8 | [illegible] |
| mush | 0.00 (0.00) | 5.86 [illegible] | [illegible] |
| votes | [illegible] | [illegible]30 | [illegible] |
| votes[illegible] | [illegible] | [illegible]34 | [illegible] |
| iris | [illegible] | [illegible]50 | [illegible] |
| glass | [illegible] | [illegible]96 | [illegible] |
| xd6 | [illegible] | [illegible]07 | [illegible] |
| pole | [illegible] | [illegible]43 | [illegible] |

Key Takeaway: GINI gain and Mutual Information are statistically indistinguishable!

Results are of the form A.AA (B.BB) where:

1. A.AA is the **average difference in errors** between the two methods
2. B.BB is the **significance** of the difference according to a two-tailed **paired t-test**

Table from Bluntine & Niblett (1992)

# INDUCTIVE BIAS (FOR DECISION TREES)

# Decision Tree Learning Example

## Dataset:

Output Y, Attributes A, B, C

1/4 1/4

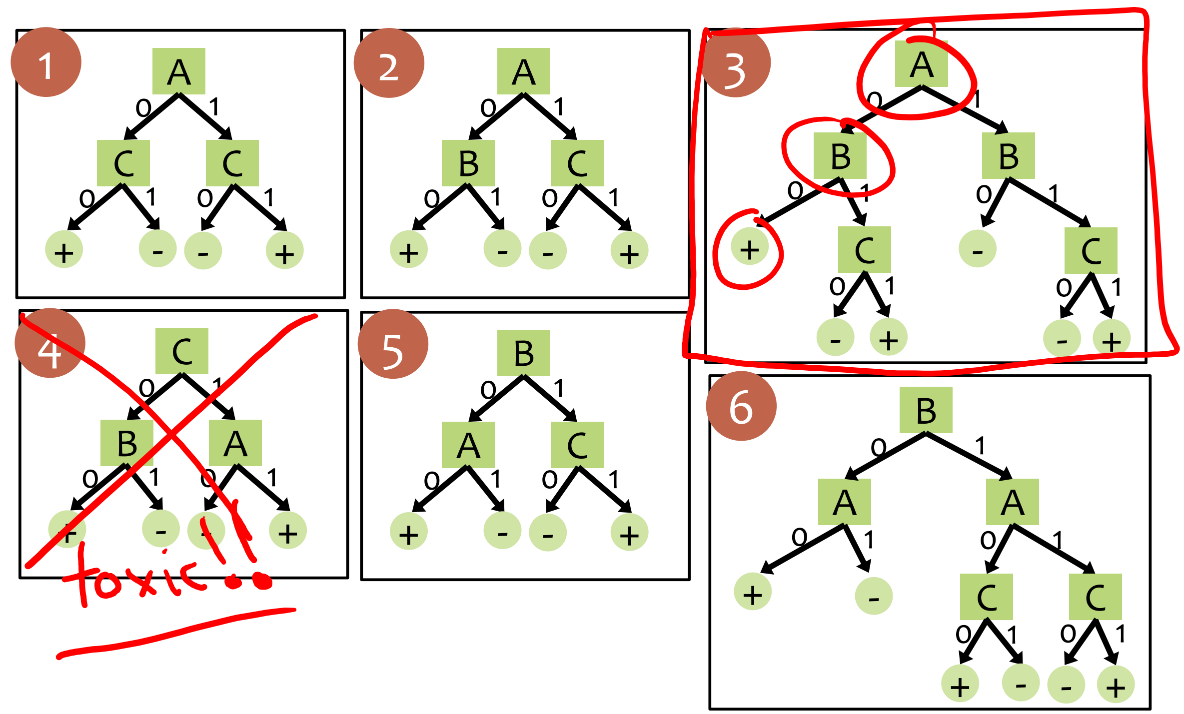
| Y | A | B | C |
|---|---|---|---|
| + | 0 | 0 | 0 |
| + | 0 | 0 | 1 |
| - | 0 | 1 | 0 |
| + | 0 | 1 | 1 |
| - | 1 | 0 | 0 |
| - | 1 | 0 | 1 |
| - | 1 | 1 | 0 |
| + | 1 | 1 | 1 |

2/8 4/8 2/8

## In-Class Exercise

Which of the following trees would be **learned by the the decision tree learning algorithm** using "error rate" as the splitting criterion?

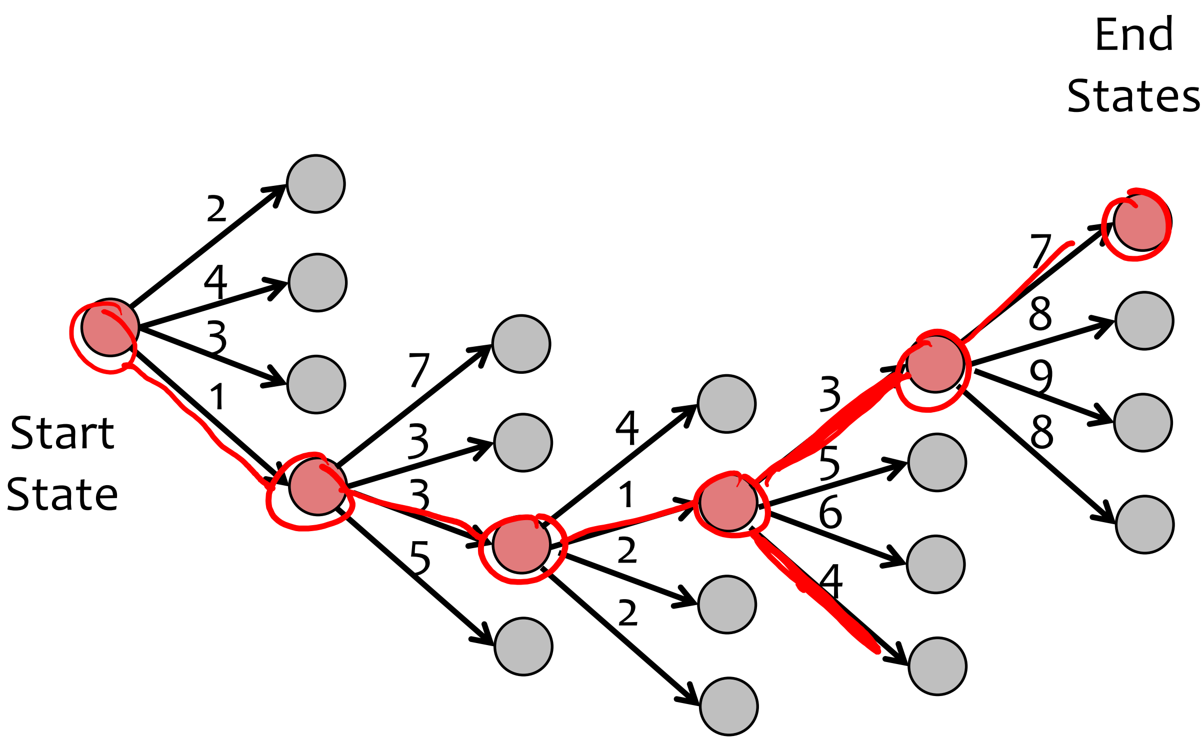
(Assume ties are broken alphabetically.)



# Question 1

- 1
- 2
- 3
- 4
- 5
- 6

# Background: Greedy Search



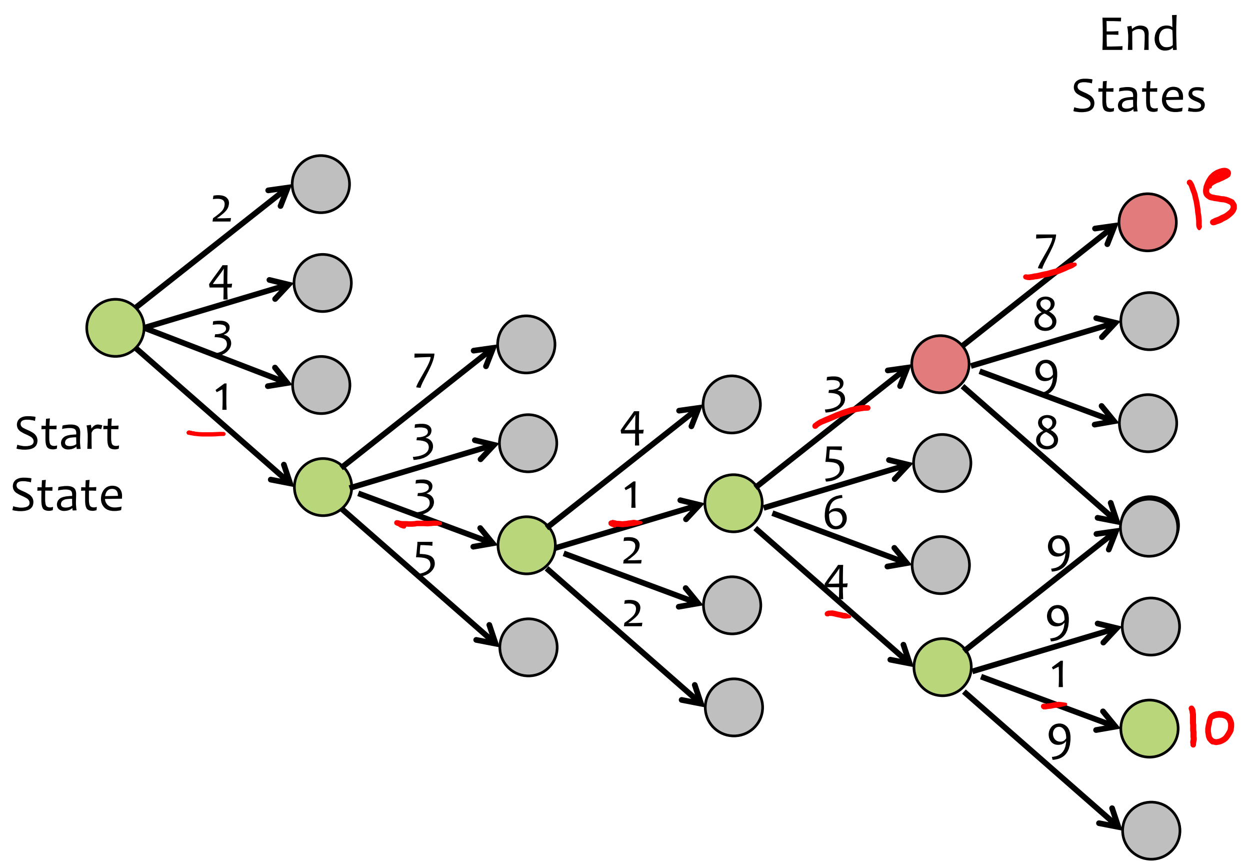

**Goal:**

- Search space consists of nodes and weighted edges
- Goal is to find the lowest (total) weight path from root to a leaf

**Greedy Search:**

- At each node, selects the edge with lowest (immediate) weight
- **Heuristic** method of search (i.e. does *not* necessarily find the best path)
- Computation time: **linear** in max path length

# Background: Greedy Search

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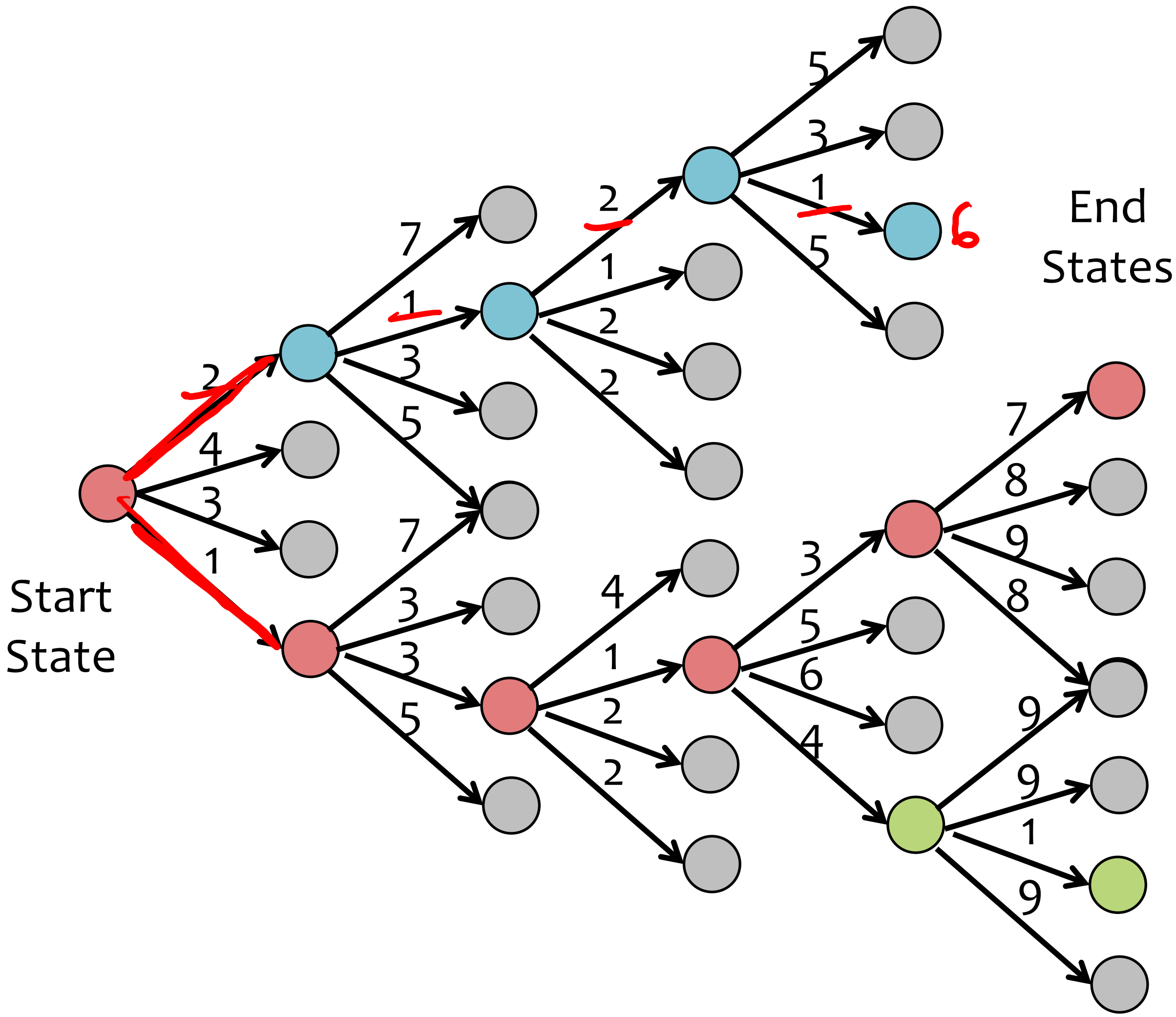


**Goal:**

- Search space consists of nodes and weighted edges
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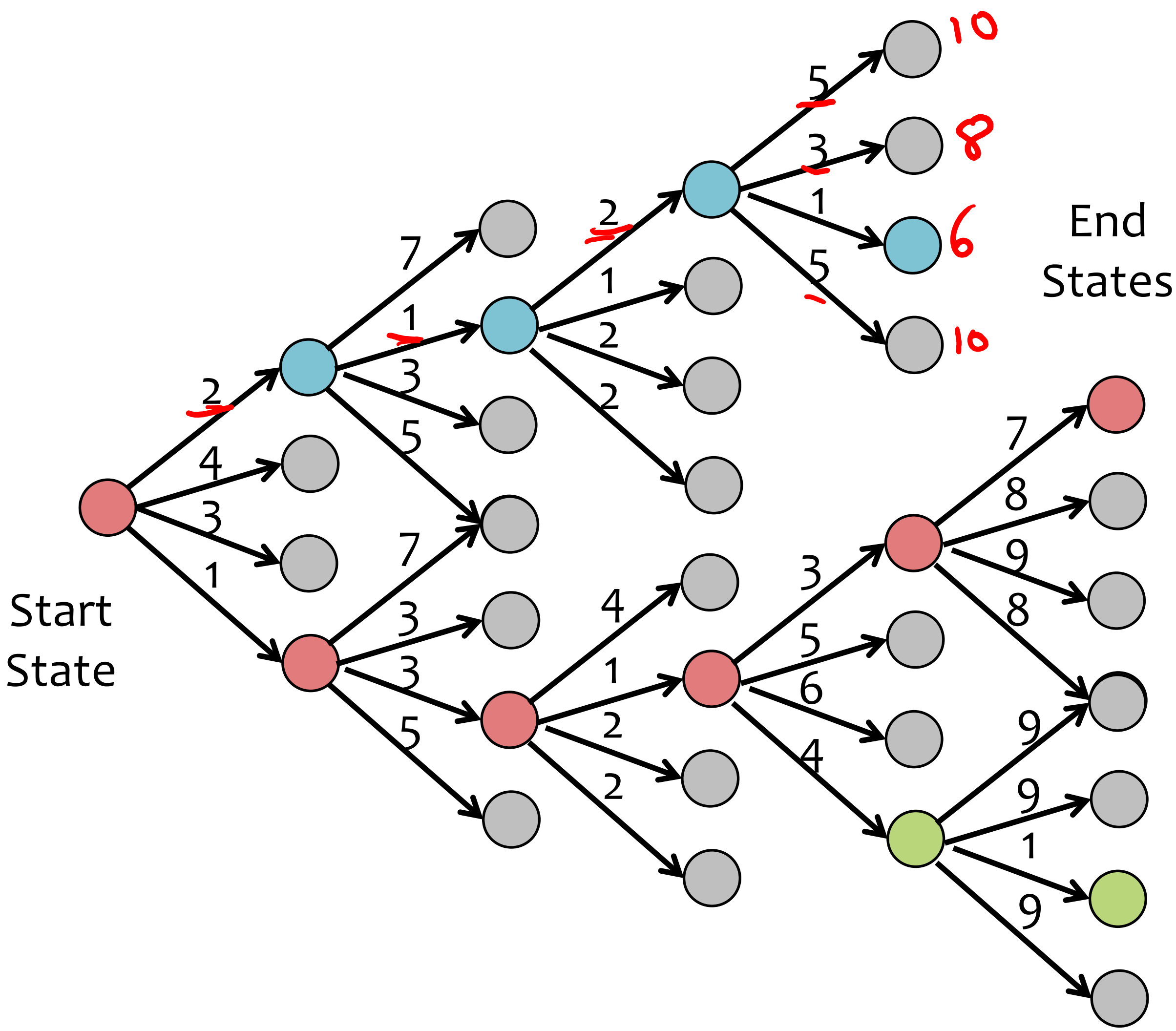
**Greedy Search:**

- At each node, selects the edge with lowest (immediate) weight
- **Heuristic** method of search (i.e. does *not* necessarily find the best path)
- Computation time: **linear** in max path length

# Background: Global Search




**Goal:**

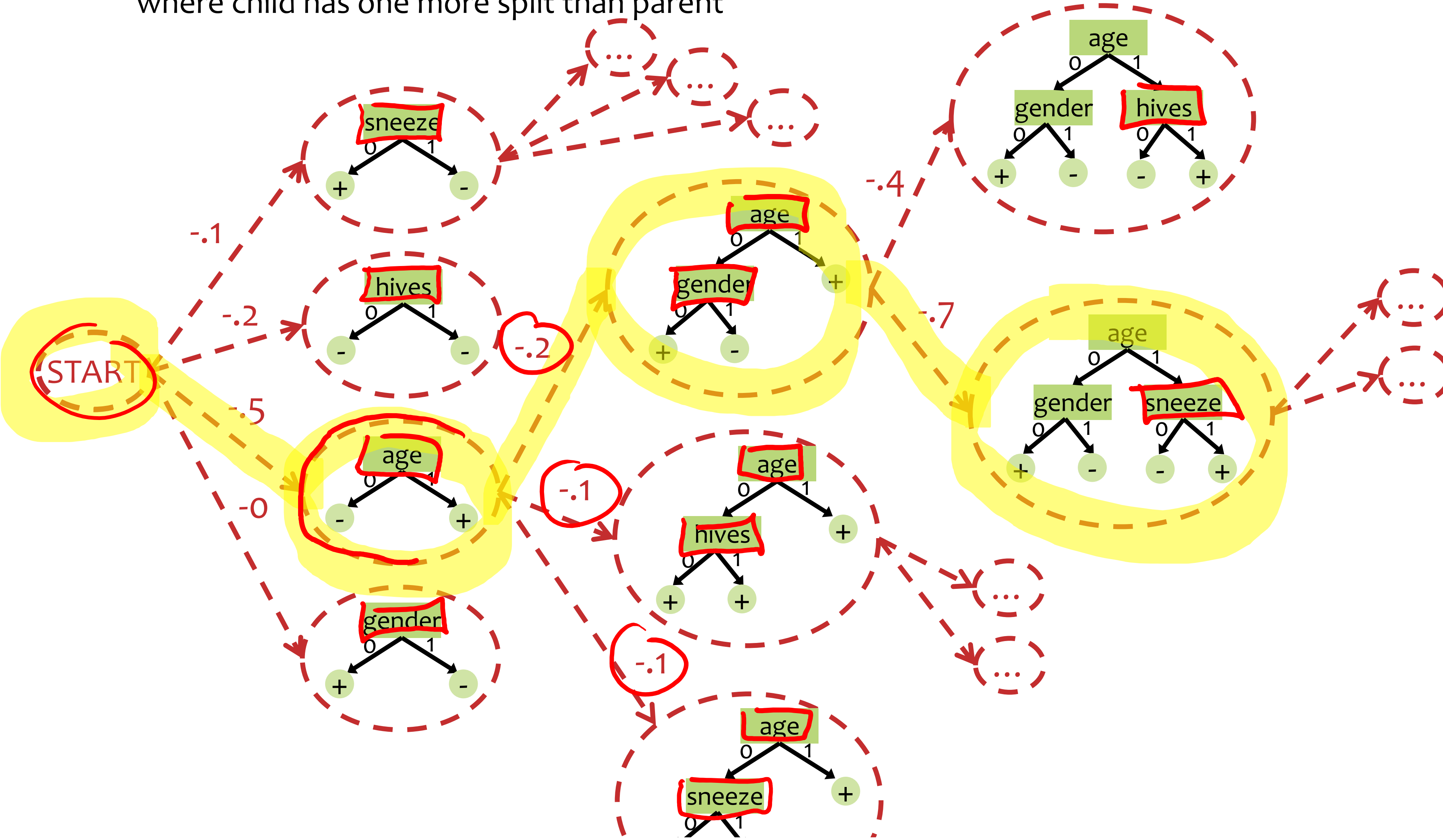
- Search space consists of nodes and weighted edges
- Goal is to find the lowest (total) weight path from root to a leaf

**Global Search:**

- Compute the weight of the path to **every** leaf
- **Exact** method of search (i.e. gauranteed to find the best path)
- Computation time: **exponential** in max path length

# Decision Tree Learning as Search

1. **search space:** all possible decision trees
2. **node:** single decision tree
3. **edge:** connects one full tree to another, where child has one more split than parent
4. **edge weight:** (negative) splitting criterion
5. **DT learning:** greedy search, maximizing our splitting criterion at each step



# Big Question:

How is it that your ML algorithm can generalize to unseen examples?

# DT: Remarks

ID3 = Decision Tree Learning with Mutual Information as the splitting criterion

**Question:** Which tree does ID3 find?

**Definition:**

We say that the **inductive bias** of a machine learning algorithm is the principal by which it generalizes to unseen examples

**Inductive Bias of ID3:**

Smallest tree that matches the data with high mutual information attributes near the top

**Occam's Razor:** (restated for ML)

Prefer the simplest hypothesis that explains the data

# Decision Tree Learning Example

## Dataset:

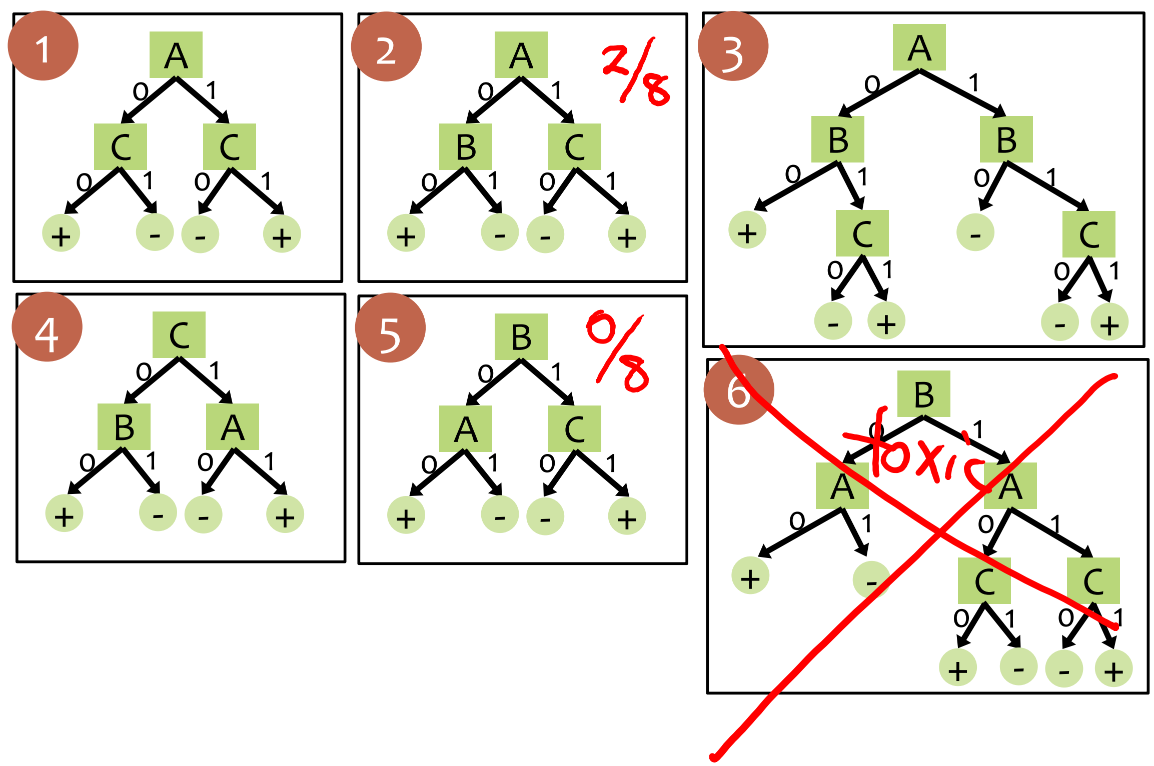
Output Y, Attributes A, B, C

| Y | A | B | C |
|---|---|---|---|
| + | 0 | 0 | 0 |
| + | 0 | 0 | 1 |
| - | 0 | 1 | 0 |
| + | 0 | 1 | 1 |
| - | 1 | 0 | 0 |
| - | 1 | 0 | 1 |
| - | 1 | 1 | 0 |
| + | 1 | 1 | 1 |

## In-Class Exercise

Suppose you had an algorithm that found **the tree with lowest training error that was as small as possible (i.e. exhaustive global search)**, which tree would it return?

(Assume ties are broken by choosing the smallest.)



When poll is active, respond at **pollev.com/10301601polls**

# Question 2

1

2

3

4

5

6

Start the presentation to see live content. For screen share software, share the entire screen. Get help at **pollev.com/app**

# OVERFITTING
# (FOR DECISION TREES)

# Decision Tree Generalization

**Question:**

*Which of the following would generalize best to unseen examples?*

A. Small tree with low training accuracy

B. Large tree with low training accuracy

C. Small tree with high training accuracy

D. Large tree with high training accuracy

**Answer:**

# Question 3

A

B

C

D

# Overfitting and Underfitting

**Underfitting**

- The model…
  - is too simple
  - is unable captures the trends in the data
  - exhibits too much bias
- *Example*: majority-vote classifier (i.e. depth-zero decision tree)
- *Example*: a toddler (that has **not** attended medical school) attempting to carry out medical diagnosis

**Overfitting**

- The model…
  - is too complex
  - is fitting the noise in the data or fitting "outliers"
  - does not have enough bias
- *Example*: our "memorizer" algorithm responding to an irrelevant attribute
- *Example*: medical student who simply memorizes patient case studies, but does not understand how to apply knowledge to new patients

# Overfitting

- Given a hypothesis *h*, its…

  …error rate over all training data: $error(h, D_{train})$

  …error rate over all test data: $error(h, D_{test})$

  …true error over all data: $error_{true}(h)$

- We say h overfits the training data if…

$$error_{true}(h) > error(h, D_{train})$$

- Amount of overfitting =

$$error_{true}(h) - error(h, D_{train})$$

In practice, $error_{true}(h)$ is **unknown**

Slide adapted from Tom Mitchell

# Overfitting in Decision Tree Learning

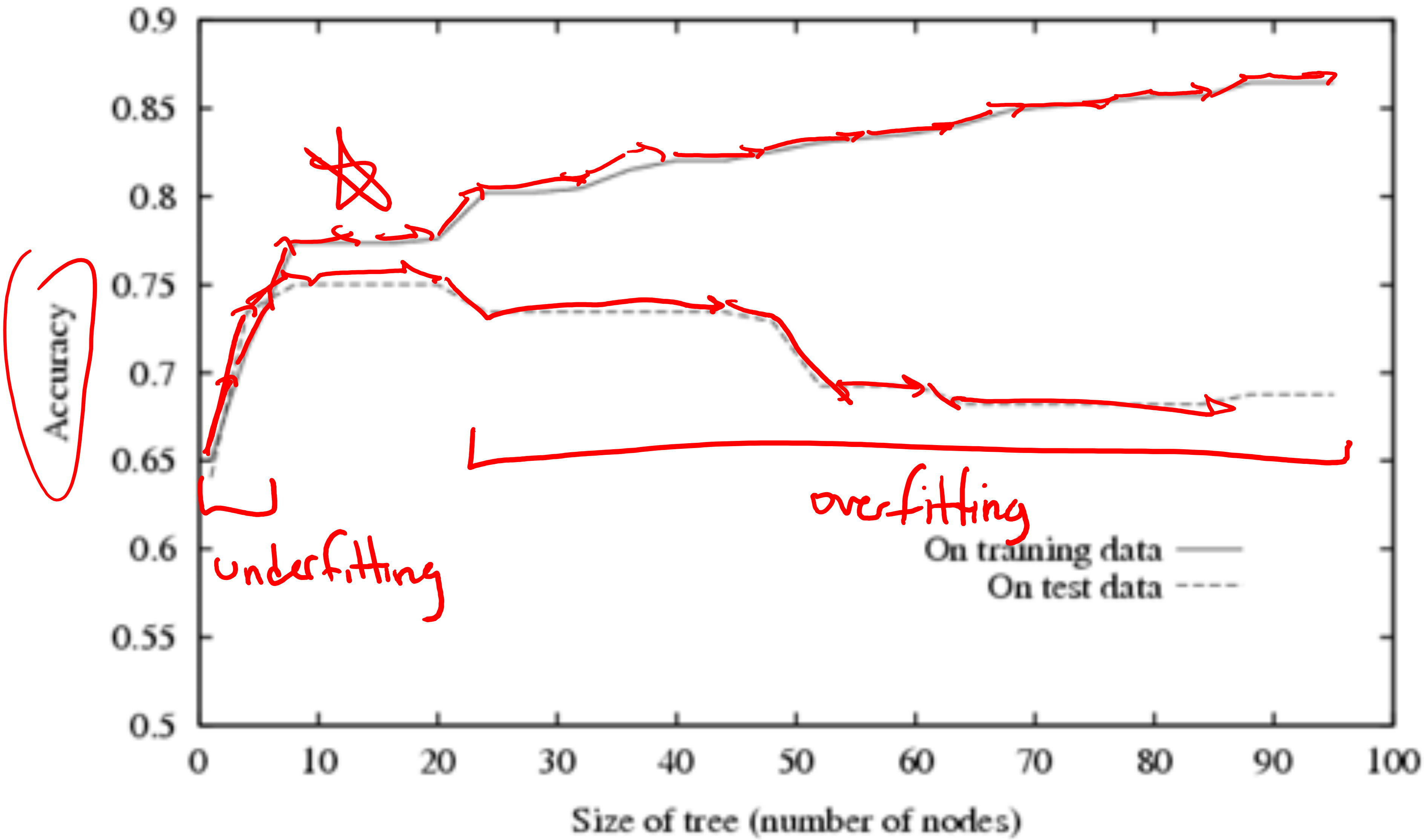



Figure from Tom Mitchell

# How to Avoid Overfitting?

For Decision Trees…

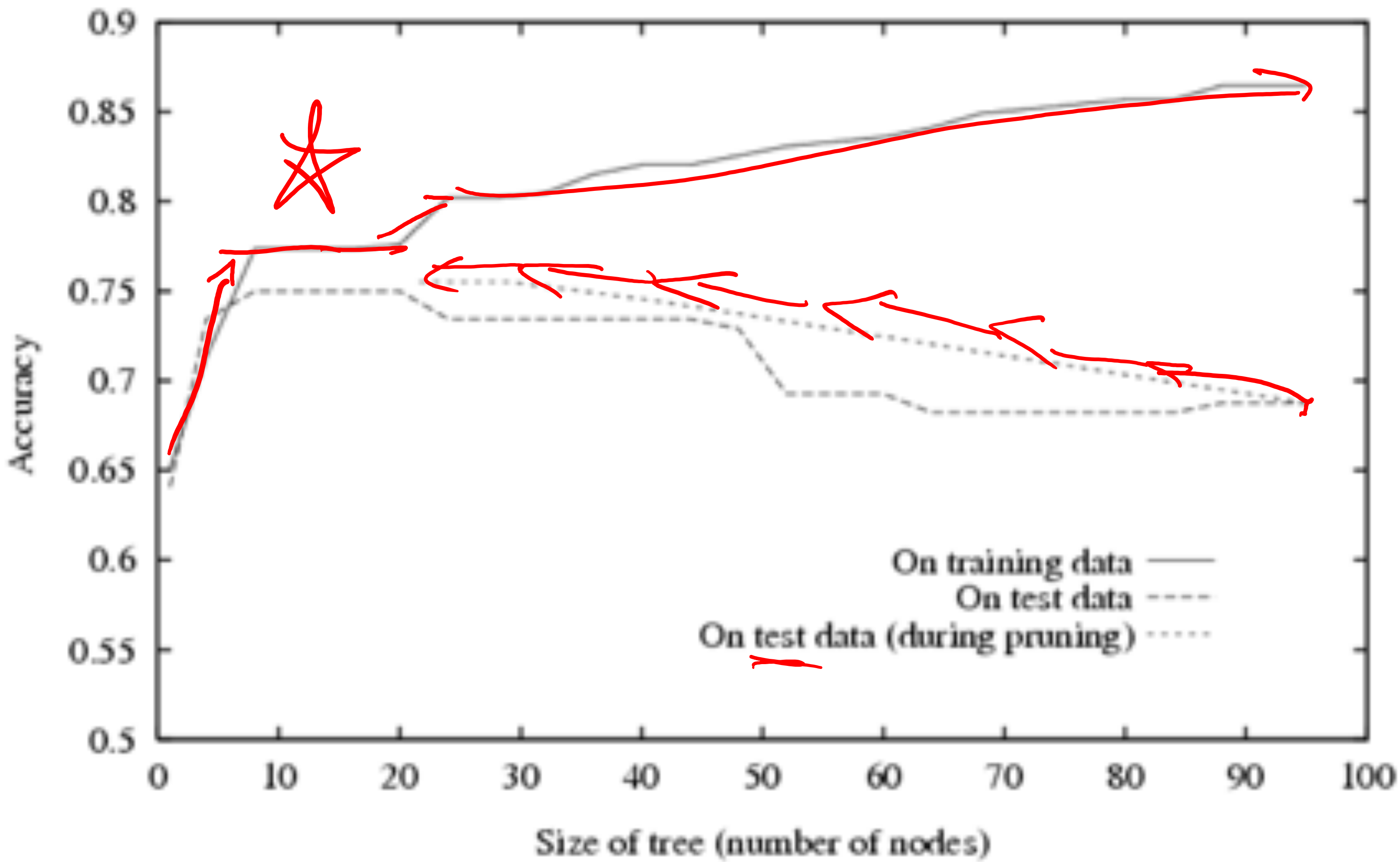
1. Do not grow tree beyond some **maximum depth**
2. Do not split if splitting criterion (e.g. mutual information) is **below some threshold**
3. Stop growing when the split is **not statistically significant**
4. Grow the entire tree, then **prune**

# Pruning

*Whiteboard*

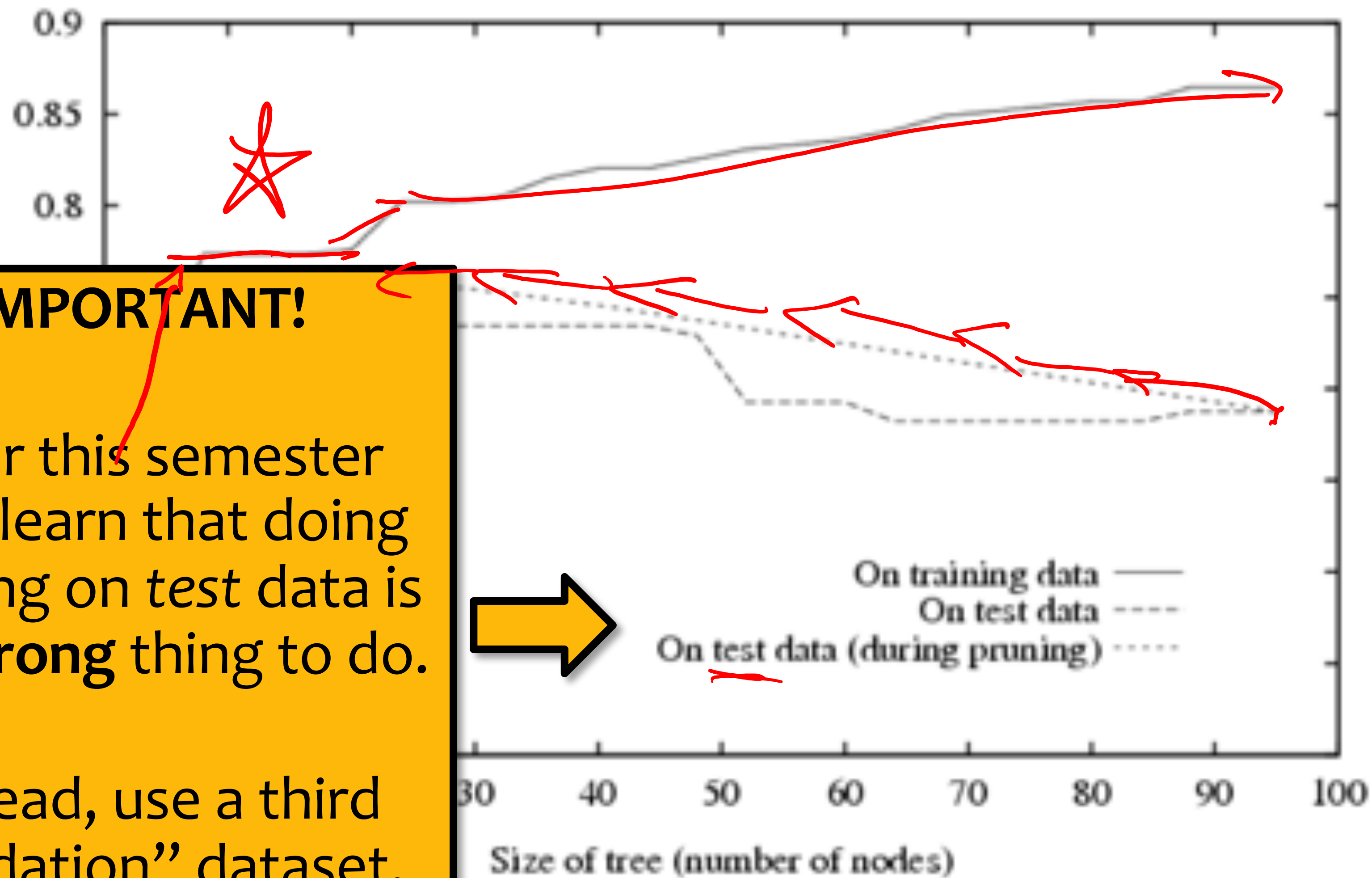
- Reduced-Error Pruning

# Effect of Reduced-Error Pruning




Slide from Tom Mitchell

# Effect of Reduced-Error Pruning




**IMPORTANT!**

Later this semester we'll learn that doing pruning on *test* data is the **wrong** thing to do.

Instead, use a third "validation" dataset.

# Decision Trees (DTs) in the Wild

- DTs are one of the most popular classification methods for practical applications
  - Reason #1: The learned representation is **easy to explain** a non-ML person
  - Reason #2: They are **efficient** in both computation and memory
- DTs can be applied to a wide variety of problems including **classification**, **regression**, **density estimation,** etc.
- **Applications of DTs** include…
  - medicine, molecular biology, text classification, manufacturing, astronomy, agriculture, and many others
- **Decision Forests** learn many DTs from random subsets of features; the result is a very powerful example of an **ensemble method** (discussed later in the course)

# DT Learning Objectives

*You should be able to…*

1. Implement Decision Tree training and prediction
2. Use effective splitting criteria for Decision Trees and be able to define entropy, conditional entropy, and mutual information / information gain
3. Explain the difference between memorization and generalization [CIML]
4. Describe the inductive bias of a decision tree
5. Formalize a learning problem by identifying the input space, output space, hypothesis space, and target function
6. Explain the difference between true error and training error
7. Judge whether a decision tree is "underfitting" or "overfitting"
8. Implement a pruning or early stopping method to combat overfitting in Decision Tree learning

# REAL VALUED ATTRIBUTES

# Fisher Iris Dataset

Fisher (1936) used 150 measurements of flowers from 3 different species: Iris setosa (0), Iris virginica (1), Iris versicolor (2) collected by Anderson (1936)

| Species | Sepal Length | Sepal Width | Petal Length | Petal Width |
|---|---|---|---|---|
| 0 | 4.3 | 3.0 | 1.1 | 0.1 |
| 0 | 4.9 | 3.6 | 1.4 | 0.1 |
| 0 | 5.3 | 3.7 | 1.5 | 0.2 |
| 1 | 4.9 | 2.4 | 3.3 | 1.0 |
| 1 | 5.7 | 2.8 | 4.1 | 1.3 |
| 1 | 6.3 | 3.3 | 4.7 | 1.6 |
| 1 | 6.7 | 3.0 | 5.0 | 1.7 |

Full dataset: https://en.wikipedia.org/wiki/Iris_flower_data_set

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| 0 | 4.9 | 3.6 |
| 0 | 5.3 | 3.7 |
| 1 | 4.9 | 2.4 |
| 1 | 5.7 | 2.8 |
| 1 | 6.3 | 3.3 |
| 1 | 6.7 | 3.0 |

Deleted two of the four features, so that input space is 2D

Full dataset: https://en.wikipedia.org/wiki/Iris_flower_data_set

# Fisher Iris Dataset