DSC40B: Theoretical Foundations of Data Science II

Lecture 1: *Welcome, introduction and examples*

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Prelude

Course Information

- Course webpage:
  - http://dsc40b.com
- Office hours:
  - Thursdays *12:30pm – 1:30pm (Same zoom link as class)*
  - always feel free to send me emails with questions / concerns
    - yusuwang@ucsd.edu
  - using *Campuswire* message board may be faster to get an answer
- Zoom info:
  - You should have received an email.

Course Information

- Homework and Exams:
  - 8 homework (roughly one per week other than the last)
    - Check out Homework Redemption policy on course webpage
  - 2 midterms:
    - Midterm 1: Feb 4th ; Midterm 2: Feb. 25th
    - Check out Midterm Redemption policy on course webpage
  - Redepmtion midterms
    - March 13th
  - 1 Super-homework (as substitute for final exam):
    - Due in the final exam week

Course Information

- Grading:
  - 40%: Homework Assignments (lowest dropped)
  - 25%: Midterm 01
    - (or Redemption Midterm 01, whichever is larger)
  - 25%: Midterm 02
    - (or Redemption Midterm 02, whichever is larger)
  - 10%: Final super-homework
  - Passing threshold: ≥60% in each midterm in order to pass!

Course Information

- Slip Days
  - You have four "slip days" to use throughout the quarter. A slip day extends the deadline of any one homework by 24 hours. Slip days can't be "stacked“. Slip days are applied automatically at the end of the quarter, but it's your responsibility to keep track of how many you have left.
- Homework collaboration
  - You may discuss homework with your classmates – in fact, it is sometimes encouraged. It is very important that you write up your solutions individually.

Course Materials

- Couse note by *Justin Eldridge* (*JE*)
  - https://ucsd-ets.github.io/dsc40b-2021-wi-public/published/default/notes/book.pdf

- Textbooks:
  - Cormen, Leiserson, Rivest, Stein (*CLRS*), *Intruction to Algorithms*
  - Dasgupta, Papadimitriou, Vazirani, *Algorithms*

Introduction to the course

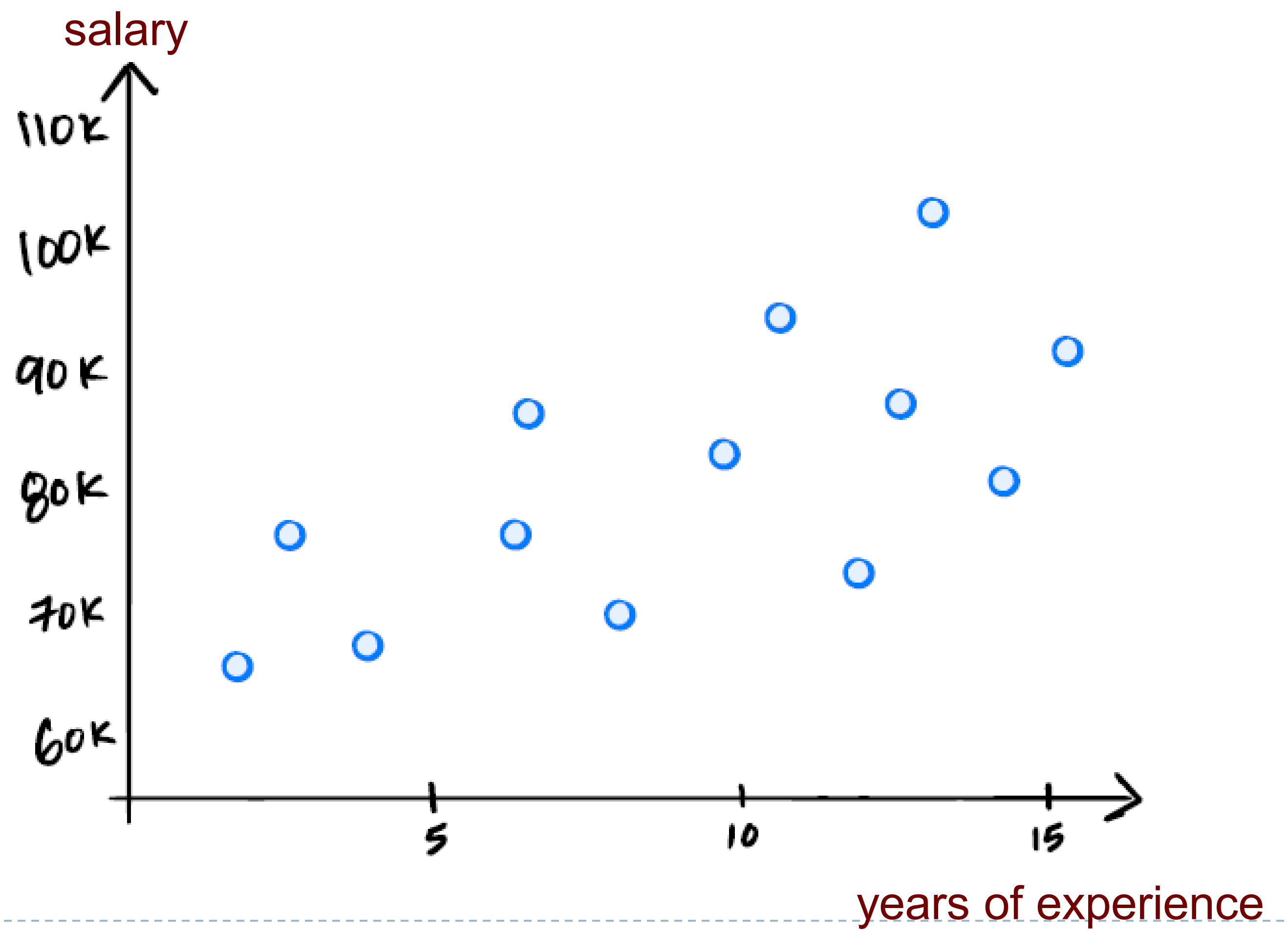
Recall in DSC 40 A

- How do we formalize learning from data

- How do we model it in a precise way so that a computer could potentially tackle it

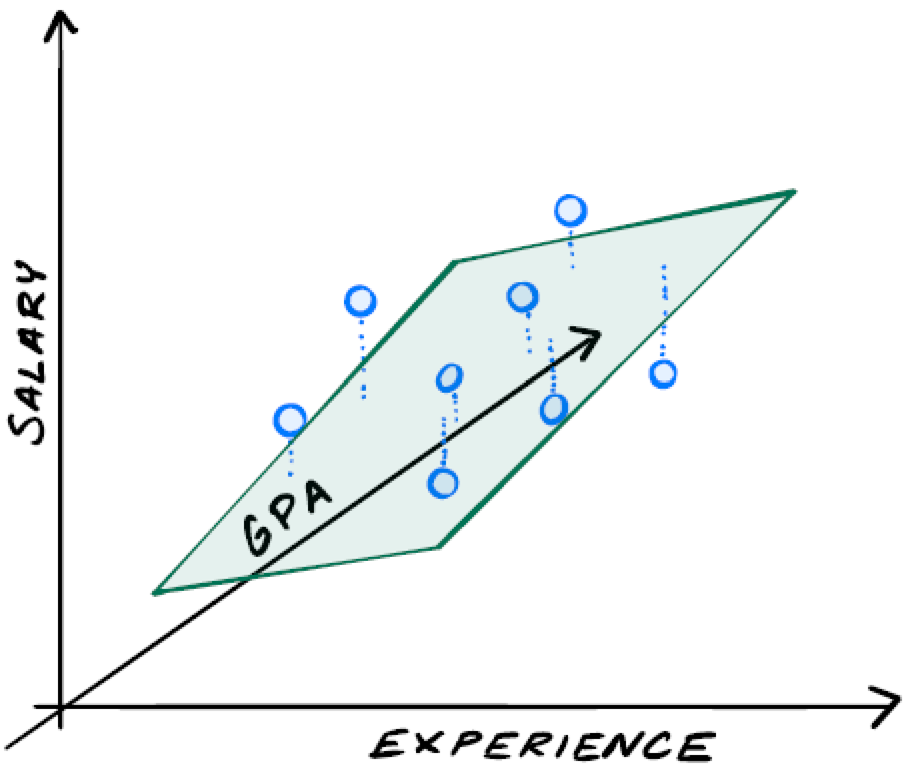
A simple example

- Salary prediction from existing data



A simple example

- Salary prediction from existing data



- Formulation (linear regression):
  - Find the best (hyper-)plane fitting these points with least total error (sum-square distances)
  - $(X^T X)^{-1}\vec{w} = X^T\vec{b}$

But ….

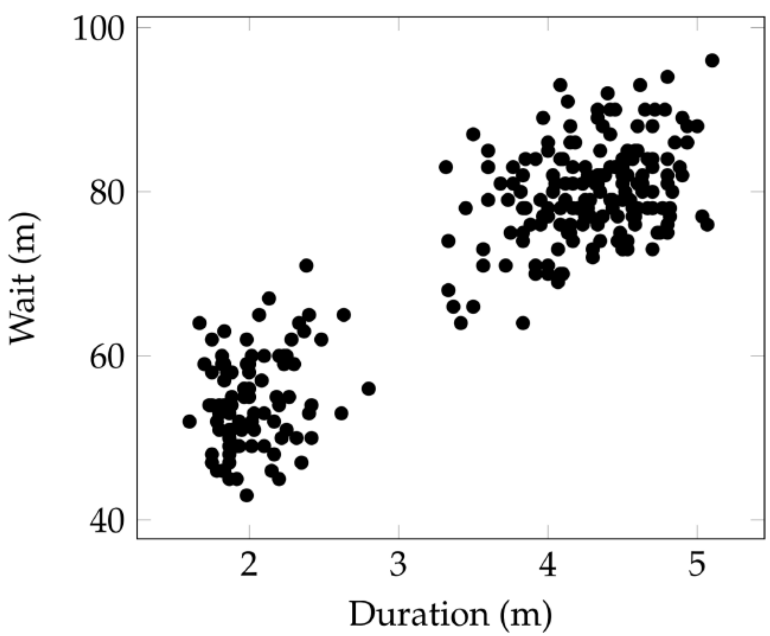
- How do we really compute it?
- How do we ask the computer to compute it for us?

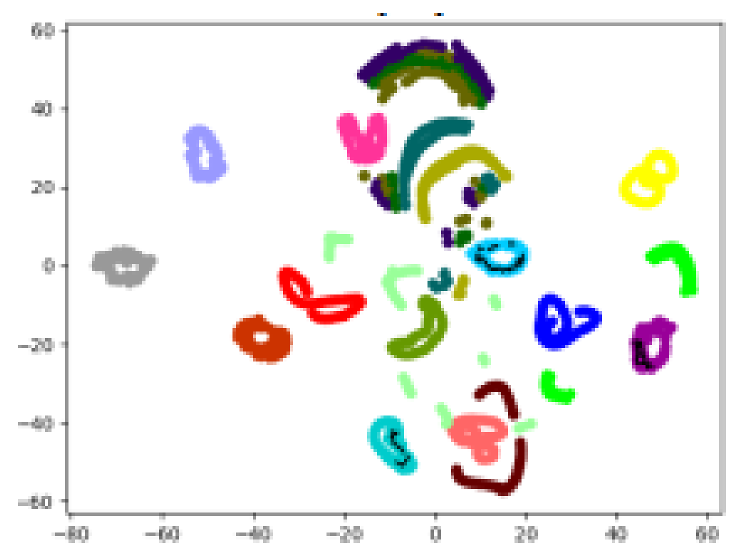
```
>>> import numpy as np
>>> w = np.linalg.solve(X.T @ X, X.T @ b)
```

- This is an algorithm
  - a sequence of steps / operations to achieve a goal
- How do we know this is a "good" algorithm?
  - How fast does it run on 1,000 points?
  - How does it scale to 1,000,000 points?
  - Can we come up with better algorithms for this?

A second example

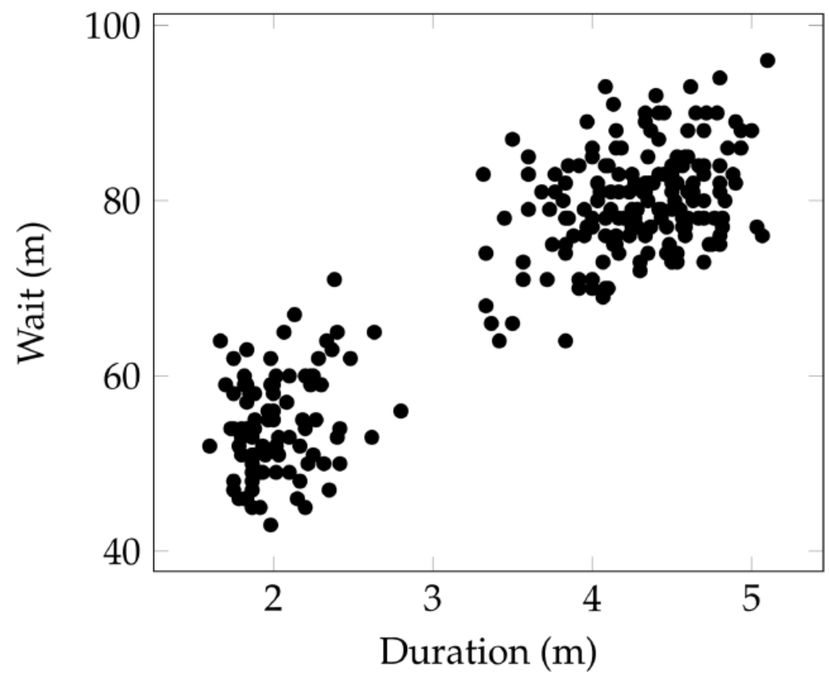
- Clustering
  - Given a set of data, identify "groups" (clusters) such that "similar" data points are grouped together
  - Ubiquitous across science and engineering





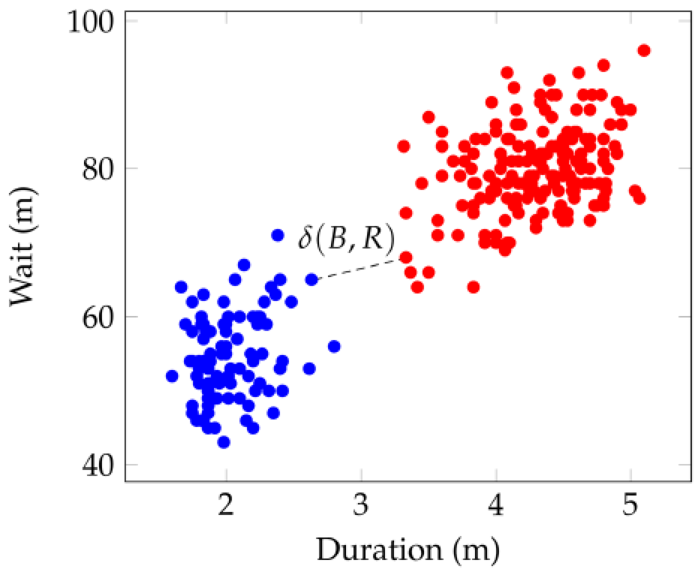
Old Faithful Geyser

- What's the pattern behind its eruption?
- How to find the two clusters?



DSC40A says

- Let's model this as an optimization problem
  - develop a way to measure / quantify the "goodness" of different grouping
  - then compute the best grouping with highest goodness score



- A grouping candidate:
  - assign each point to be either blue or red
- Quality (goodness):
  - min separation distance $\delta(B, R)$
    - smallest distance between a red or blue point
- Goal:
  - given points $X = \{x_1, \ldots, x_n\}$
  - return the assignment of $X = B \cup R$ with largest separation distance $\delta(B, R)$

What remains

- What is an algorithm to achieve this?
  - The algorithm needs to be correct
- Is our algorithm good?
  - How do we know? (aka: how to analyze our algorithm?)
- How do we design better algorithms?

A first algorithm for clustering

- Intuition: to compute min-separation grouping
  - try all possible assignment of all input data points
  - compute separation distance for each assignment (grouping)
  - return the one with largest separation distance (the best)

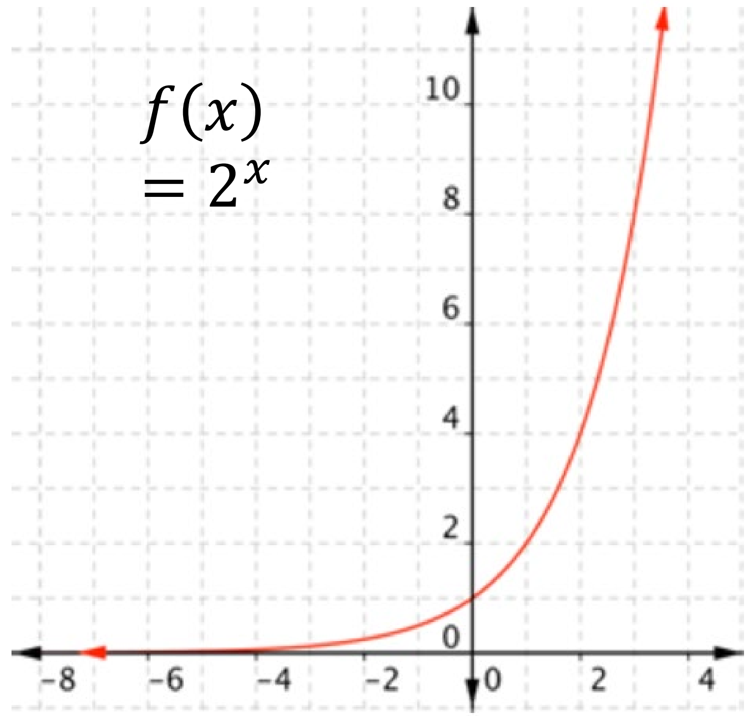
```
best_separation = float('inf') # Python for "infinity"
best_clustering = None

for clustering in all_clusterings(data):
    sep = calculate_separation(clustering)
    if sep < best_separation:
        best_separation = sep
        best_clustering = clustering

print(best_clustering)
```

Running time?

- Precise time:
  - depends on the computer
  - rough idea:
    - How many possible assignment do we have?
      - assigning *R* or *B* to each input point
      - $2 \times 2 \times \cdots \times 2 = 2^n$
    - Suppose it takes 1 nanosecond to check one grouping
    - Takes 2^n nanoseconds in total

- Time needed

n	Time
1	1 nanosecond
10	1 microsecond
20	1 millisecond
30	1 second
40	18 minutes
50	13 days
60	36 years
70	37,000 years



- Clearly not efficient. Can we do better? How to design better algorithms?

This course: DSC40B

- Focus on algorithms
  - What is an algorithm?
    - step by step strategy to solve problems
    - should terminate and return correct answer for any input instance

- Various issues involved in designing good algorithms
  - What do we mean by “good”?
    - algorithm analysis, asymptotic language used to measure performance
  - How to design good algorithms
    - data structures, algorithm paradigms
  - Fundamental problems
    - graph traversal, shortest path etc.

How to measure efficiency?
Time complexity

Efficiency

- An algorithm takes an input and performs a task (which could produce an output)
- Efficiency matters!
  - Running time?
  - How much memory it needs?
  - An algorithm is only useful when it is efficient enough

- How do we measure time efficiency?
- Note: running time
  - depends on size of input
  - depends on specific input too

Scenario

- Suppose you are building a least-square regression model to predict oxygen level of a patient based on various parameters measured about her
- You developed an algorithm and trained it on 1,000 patients
  - it runs 1 second
- What if you now want to train on 1,000,000 patients?
  - is it 1000 seconds?
- Growth of running time w.r.t. input size

A first try

- How about we time it
  - e.g, using Jupyter tools: *time* and *timeit*

- Disadvantages:
  - depending on the machine
  - to get the growth, need to perform multiple runs and plot the time to obtain the pattern
    - one timing doesn't tell how the algorithm scales
  - even then, the time may depend on specific input
    - input of the same size could incur different running time

Time complexity analysis

- Count intuitively just operations
  - eliminate the precise running time of a specific computer
- Determine it by analyzing the code without running it
- Obtain a function (a formula) on how the ``count” changes with input size (i.e, growth w.r.t input size)
  - instead of timing or plotting to find how time scales

An example

- Consider the following code
  - input is an array A

```
def mean(A):
        total = 0
        n = len(A)
        for i in range(n):
                total += A[i]
        return total / n
```

Time complexity

- First abstraction: depending on input size
  - Consider function $T(n)$, and aim to obtain a formula for $T(n)$ to capture growth of the running time w.r.t input size

- Second abstraction:
  - Assume that basic operations take constant time
    - e.g, all operations such as addition/multiplication/division takes constant time each
    - e.g, for an array A, access $A[i]$ takes constant time

An example

- Consider the following code
  - input is an array A

```
def mean(A):
        total = 0
        n = len(A)
    for i in [0,n-1]:
            total += A[i]
    return total / n
```

c_1

c_2

c_3

- $T(n) = c_1 + \sum_{i=0}^{n-1} c_2 + c_3 = \mathrm{c}_2\mathrm{n} + \mathrm{c}_1 + \mathrm{c}_3$

Time complexity

- First abstraction: depending on input size
  - Consider function $T(n)$, and aim to obtain a formula for $T(n)$
- Second abstraction:
  - Assume that basic operations take constant time
    - e.g, all operations such as addition/multiplication/division takes constant time each
    - for an array A and index i, access $A[i]$ takes constant time
- Third abstraction:
  - Ignore constants as well as lower order terms,
    - focus on dominating terms to capture relative growth w.r.t. n
  - $T(n) = c_1 + \sum_{i=1}^{n} c_2 \ + c_3 = \mathrm{c}_2\mathrm{n} + \mathrm{c}_1 + \mathrm{c}_3 = \Theta(n)$

An example

- Consider the following code
  - input is an array A

```
def mean(A):
        total = 0
        n = len(A)
    for i in [0,n-1]:
            total += A[i]
        return total / n
```

c_1

c_2

c_3

Algorithm mean(A) has time complexity $T(n) = \Theta(n)$

- $T(n) = c_1 + \sum_{i=0}^{n-1} c_2 \ + c_3 = \mathrm{c}_2\mathrm{n} + \mathrm{c}_1 + \mathrm{c}_3 = \Theta(n)$

Caution

- Note, it is not true that each single command line in the code will take constant time
- Example:

```
def mean_2(A):
        total = sum(A)
        n = len(A)
        return total / n
```

- $T(n) = a_1 n + a_2 + a_3 = \Theta(n)$

A simple exercise

- Input: an array A of n numbers
- Output: return the largest number in A
- What is the time complexity of your algorithm?

```
def maximum(A):
        current_max = -float('inf')
        for x in A:
        if x > current_max:
                current_max = x
        return current_max
```

Time complexity

- First abstraction:
  - aim to obtain $T(n)$ where n is size of input
- Second abstraction:
  - assume that basic operations take constant time
- Third abstraction:
  - Ignore constants as well as lower order terms,
  - $T(n) = \Theta(n)$ for previous example
- $\Theta(\cdot)$ is ca… …plexity of this fo…

Next time
We will learn what exactly are asymptotic time complexity and go through more examples

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