DSC 190

DATA STRUCTURES & ALGORITHMS

Lecture 9 | Part 1

Today's Lecture

Algorithms

- We’ve been studying data structures.
- We’ll now move towards algorithm design.
- Data scientists do design algorithms.
- But perhaps more important to understand solutions to common problems and which problems are difficult.

Today

- We'll introduce the idea of an **optimization problem**.
- Talk about one easy strategy that sometimes works.

DSC 190

Data Structures & Algorithms

Lecture 9 | Part 2

Optimization Problems and Design Strategies

Optimization Problems

- We often want to find the **best**.
  - Shortest path between two nodes.
  - Minimum spanning tree.
  - Schedule that maximizes tasks completed.
  - Line of best fit.

- These are **optimization problems**.

Example: Regression

- Given a set of n points in $\mathbb{R}^2$, find a straight line $y = mx + b$ which minimizes the Sum of Squared Errors.

- **Given**: set of n points $\{(x_i, y_i)\}$ in $\mathbb{R}^2$

- **Search Space**: all straight lines of form $y = mx + b$

- **Objective Function**: $\phi(m, b) = \sum_{i=1}^{n}(y_i - (mx_i + b))^2$

Continuous Optimization

- Here, the search space is continuous, often **infinite**.
- Methods for solving often use calculus.

Discrete Optimization

- Here, the search space is discrete, typically **finite**.
- Example: shortest path between two nodes.
- Methods for solving (usually) can't use calculus.
- We will focus on these problems.

Brute Force

- If search space is finite, can employ **brute force search**.
- Typically search space is too large to be feasible.

Design Strategies

- Focus on **design strategies** for discrete optimization.:
  - **Greedy Algorithms**
  - **Backtracking**
  - **Dynamic Programming**

DSC 190

DATA STRUCTURES & ALGORITHMS

Lecture 9 | Part 3

The Greedy Approach by Example

Problem

- **Choose**: 4 numbers with largest sum.

95	83	80	77
62	65	55	75
85	91	70	74
88	72	59	79

Specification

- **Given**: A set X of n numbers and an integer k.
- **Search Space**: Subsets $S \subset X$ of size k.
- **Objective**: maximize sum of numbers in S,

$$\phi(S) = \sum_{s \in S} s$$

Brute Force

- Brute force: try every possible subset of size k.
- How many are there?

$$\binom{n}{k} = \Theta(n^k)$$

- Time complexity is $\Theta(k \cdot n^k)$

The Greedy Approach

95	83	80	77
62	65	55	75
85	91	70	74
88	72	59	79

The Greedy Approach

- At every step, make the best decision at that moment.
- Is this optimal? Not always, but it is here.

Proof

Let $x_1 \geq \cdots \geq x_k$ be the k largest numbers. Let $y_1 \geq \cdots \geq y_k$ be some other solution. Since $x_1, \ldots, x_k$ are the k largest:

$$x_1 \geq y_1, \quad x_2 \geq y_2, \quad \ldots, \quad x_k \geq y_k.$$

Therefore:

$$\sum_{i=1}^{k} x_i \geq \sum_{i=1}^{k} y_i$$

Since the other solution was arbitrary, this shows that the greedy solution is at least as good as anything else; therefore it is maximal.

Efficiency

- Algorithm: loop through once, find k largest numbers.
- Linear time, $\Theta(n)$.
- Much faster than $\Theta(k \cdot n^k)$!

A Variation

- Now you can only choose one number from each row.

95	83	80	77
62	65	55	75
85	91	70	74
88	72	59	79

Specification

- **Given**: An $n \times n$ matrix X of numbers and an integer k.
- **Search Space**: Subsets $S \subset X$ of size k where each element is from a different row of X.
- **Objective**: maximize sum of numbers in S.

$$\phi(S) = \sum_{s \in S} s$$

Optimality

- The greedy approach of choosing largest within each row is optimal.

Another Variation

- Now you can only choose one from each row/column.

95	83	80	77
62	65	55	75
85	91	70	74
88	72	59	79

Specification

- **Given**: An $n \times n$ matrix X of numbers and an integer k.
- **Search Space**: all subsets of entries of X of size k such that each element is in a different row/column of X.
- **Objective**: maximize sum of numbers in subset.

$$\phi(S) = \sum_{s \in S} s$$

Greedy is not Optimal

- The optimal solution is: 80 + 75 + 91 + 88 = 334

95	83	80	77
62	65	55	75
85	91	70	74
88	72	59	79

Main Idea

For some problems, a greedy approach is guaranteed to find the optimal solution. For other problems, it is not.

Main Idea

Coming up with a greedy algorithm is usually simple – proving that it finds the optimal may not be so easy.

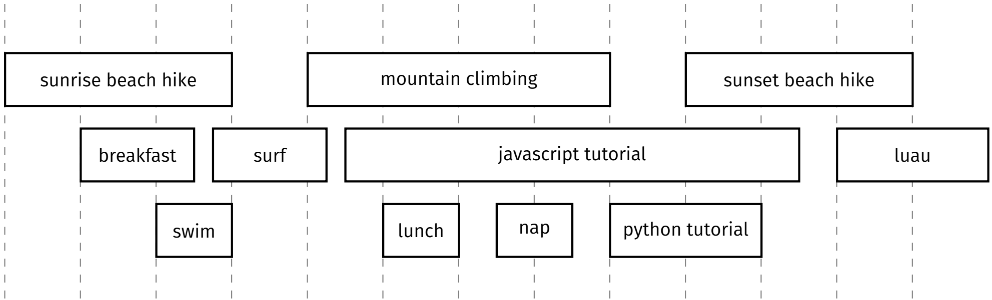
DSC 190

Data Structures & Algorithms

Lecture 9 | Part 4

Activity Selection Problem

Vacation Planning



Formalized

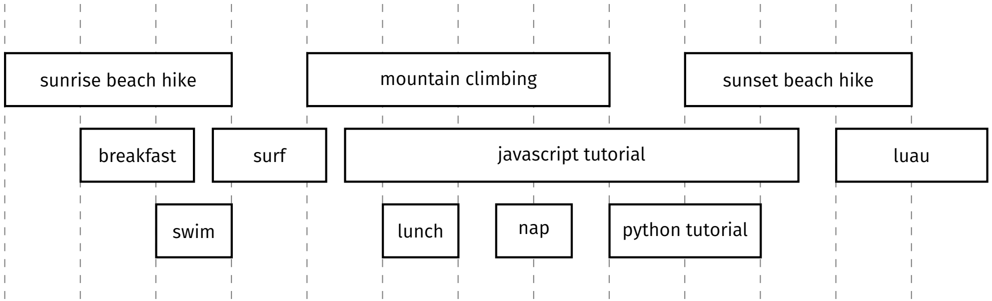
- This is called the **activity selection** problem.
- **Given**: a set of start/finish times (s_i, f_i) for n events
- **Search Space**: all schedules S with non-overlapping events
  - Format: S is a set of event indices $e_1, e_2, \ldots, e_k$
- **Objective**: maximize $|S|$ (number of events)

$$\phi(S) = |S|$$

Greedy Strategies

- There are several strategies we might call "greedy".
- Approach #1: in order of duration, shortest events first.

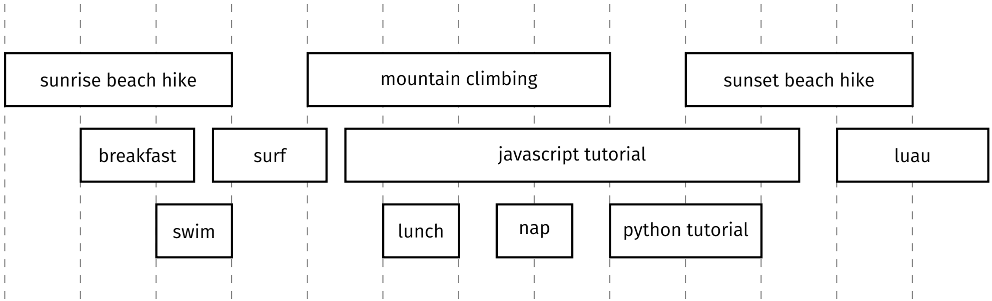
In Order of Duration



Greedy Strategies

- Approach #2: in order of start time.

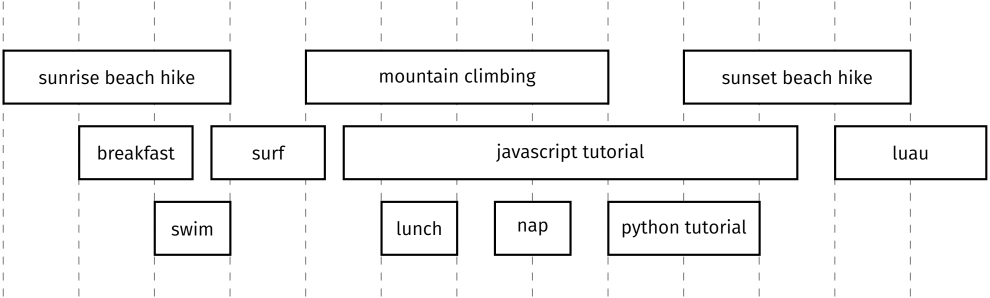
In Order of Start Time



Greedy Strategies

- Approach #3: in order of finish time.

In Order of Finish Time



In Order of Finish Time

- Choose event with earliest finish time as first event.
- Choose subsequent events in order of finish time.
  - provided that they are non-overlapping.
- This is **guaranteed** to find global optimum.
- But how do we know this?

DSC 190

Data Structures & Algorithms

Lecture 9 | Part 5

Exchange Arguments

Convincing Yourself

- Designing a greedy algorithm is usually easy.
- It can be hard to convince yourself that it is optimal.
- Now, one proof technique: **exchange arguments**.

First: Proving **Non-Optimality**

- To show that a strategy is **non-optimal**, find a counterexample.

Proving Optimality

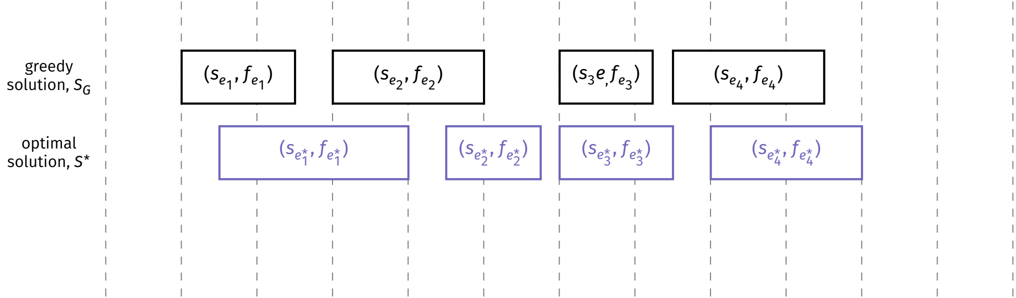
- There may be many optimal solutions – we want to show that the greedy solution S_G is always one of them.

Exchange Arguments

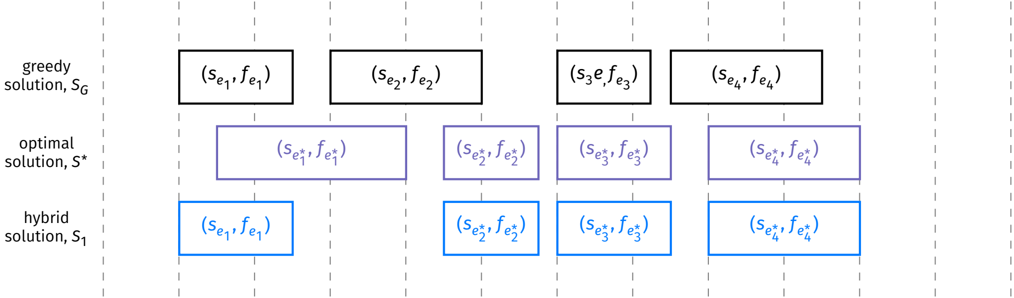
- Start with an arbitrary optimal solution, S^*.
- Make a **chain** of optimal solutions $S^*, S_1, S_2, \dots, S_G$
- At every step from S_{k-1} to S_k:
  - construct solution S_k by **exchanging** part of S_{k-1} with S_G
  - argue that S_k is **valid**[1]
  - argue that S_k is **also optimal**
- Proves S_G is optimal, as $\phi(S^*) = \phi(S_1) = \phi(S_2) = \dots = \phi(S_G)$

[1] It is part of the search space and meets all constraints.

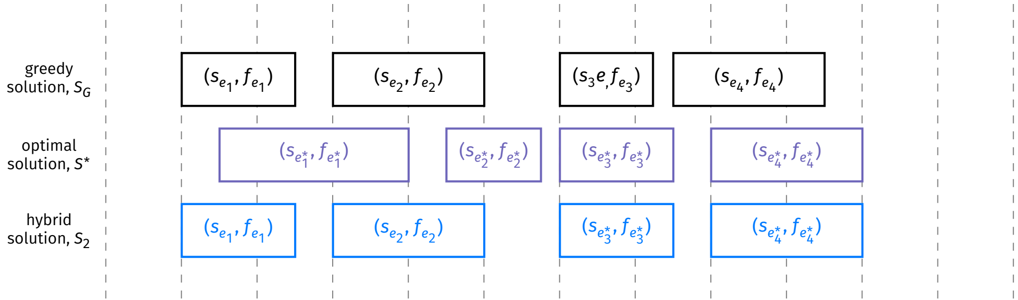
Exchange Argument for Activities



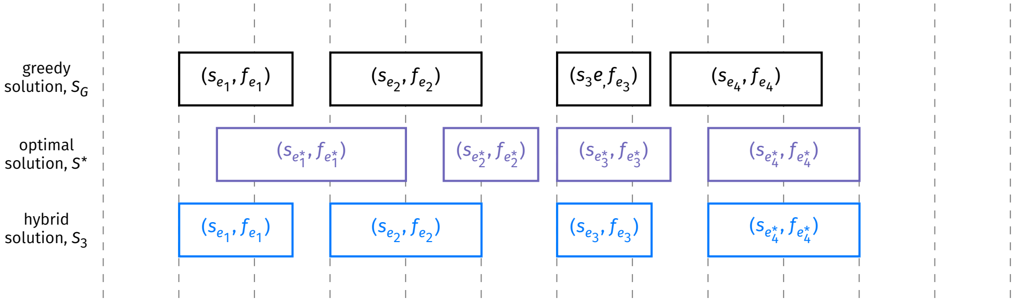
Exchange Argument for Activities



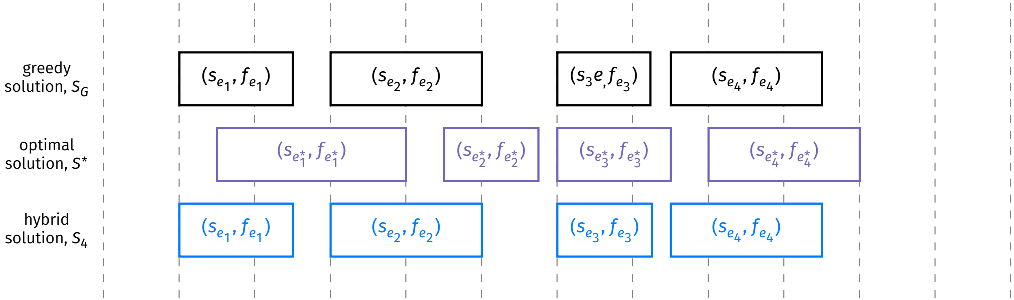
Exchange Argument for Activities



Exchange Argument for Activities



Exchange Argument for Activities



Exchange Argument for Activities

Take an arbitrary optimal solution S^*. Suppose it is different from the greedy solution, S_G (as otherwise we're done).

If it's different, it has to be different *somewhere*. Let's look at the first event in S^* that is not in S; call this the ith event in S^*.

We'll exchange the ith event in S^* with the ith event in S_G, but we have to be a little careful: what if $|S^*| > |S_G|$, so that it's possible that S_G has no ith element? So there are two cases: $i \leq |S_G|$ and $i > |S_G|$.

Exchange Argument for Activities

First case: $i \leq |S_G|$. Then exchange the ith event in S^* with the ith event in S_G, creating a new solution S'.

This is **valid**: the event from S_G cannot overlap with any of the events in S^*, since the previous $i - 1$ events in S^* are the same as in S_G (and they didn't overlap), and the finish time of the greedy event is ≤ the finish time of event it is replacing, so it cannot overlap with the remaining events.

It is also **optimal**, since $|S'| = |S^*|$.

Exchange Argument for Activities

Second case: $i > |S_G|$. This means that there is at least one “extra” event in S^* than in S_G.

But this cannot happen: this extra event does not overlap with the events in S_G (since S_G is equal to the first $i - 1$ elements of S^*, and the “extra” event doesn’t overlap with them). Its finish time is larger than any event in S_G. So the greedy approach would have included this event. Thus this case is not possible.

Exchange Argument for Activities

In either case, S' is a valid optimal schedule.

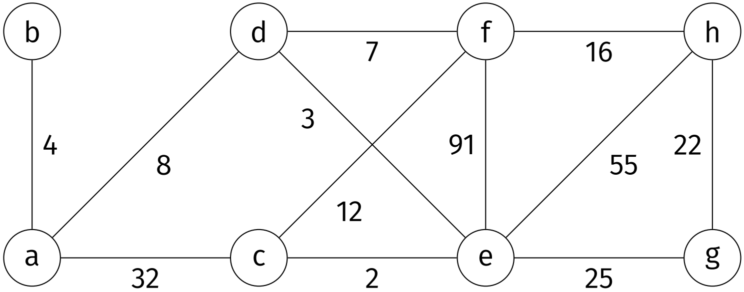
S^* and S_G can differ in only a finite number of places; therefore, repeating this procedure a finite number of times produces a chain of optimal solutions where each solution is more similar to S_G. The chain terminates when S_G is reached, which shows that S_G is optimal ($|S_G| = |S^*|$).

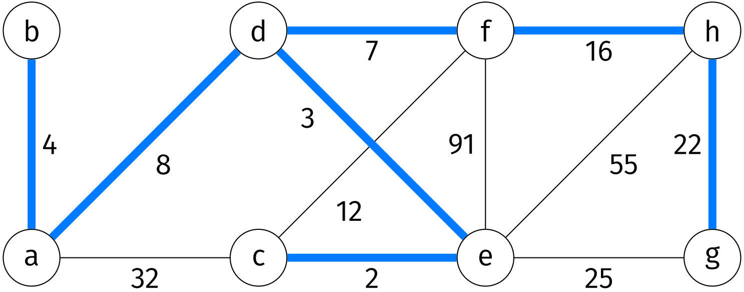
DSC 190

Data Structures & Algorithms

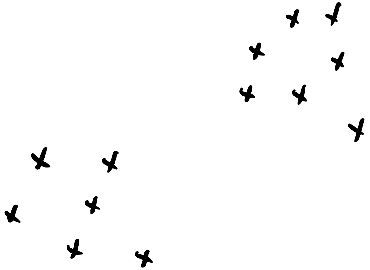
Lecture 9 | Part 6

Minimum Spanning Trees

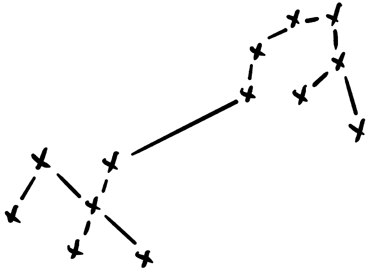

b
d
f
h
7
16
3
4
91
22
8
55
12
a
c
e
g
32
2
25


b
d
f
h
7
16
4
3
91
22
8
55
12
a
c
e
g
32
2
25

MSTs and Clustering



MSTs and Clustering



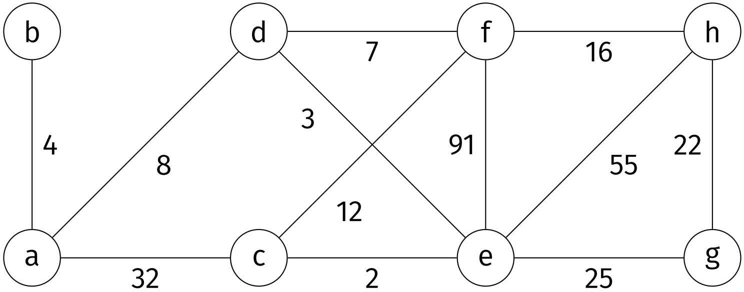
Minimum Spanning Trees

- **Given**: a weighted graph $G = (V, E, \omega)$, where $\omega : E \to \mathbb{R}$.
- **Search Space:** all **spanning trees** $T = (V, E')$, where $E' \subset E$.
- **Objective**: minimize total edge weight

$$\phi(T) = \sum_{e \in E'} \omega(e)$$

Kruskal's Algorithm

- **Kruskal's Algorithm** is a **greedy** algorithm for computing a MST.
- Idea: add edges one-by-one in order of weight.
  - But only if edge does not make a cycle!


b
d
f
h
a
c
e
g
7
16
4
8
3
91
22
55
12
32
2
25

Kruskal's Algorithm (Pseudocode)

```
def kruskals(graph, weight):
    mst = UndirectedGraph()
    edges = sorted(graph.edges, key=weight)

    for (u, v) in edges:
        if u and v are not connected in mst:
            mst.add_edge(u, v)

    return mst
```

Implementing Kruskal's Algorithm

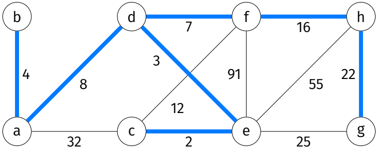
```
def kruskals(graph, weight):
    mst = UndirectedGraph()
    edges = sorted(graph.edges, key=weight)

    dsf = DisjointSetForest()
    for i in range(len(graph.nodes)):
        dsf.make_set()

    for (u, v) in edges:
        if dsf.find_set(u) != dsf.find_set(v):
            mst.add_edge(u, v)
            dsf.union(u, v)

    return mst
```

Optimality

- Kruskal’s Algorithm find an optimal solution.
- We can prove this with an **exchange argument**.

Notes

- The greedy approach produces a valid spanning tree.
- Any two spanning trees have same number of edges.
- Removing an edge from a MST partitions nodes in two.



Exchange Idea

- Suppose $e^* = (u, v)$ is in T^*, but not in T.
- We'll find a node e on the path from u to v in T.
- Make a new tree, T', by taking T^*, removing e^*, replacing it with e.

Exchange Argument

Let T^* be any minimum spanning tree, and let T_G be a tree produced by Kruskal's algorithm. Suppose that T^* and T_G are different, and let $e^* = (u, v)$ be an edge in T^* that is not in T_G.

Consider the path from u to v in T_G. Adding e^* to T_G would create two different paths from (u, v), and thus a cycle. Let (A, B) be the cut produced if e^* were removed from T^*, and let e be an edge along the cycle that crosses the cut (A, B) (there must be at least one).

We will exchange e^* in T^* for the edge e.

Exchange Argument

First, this will create a **valid** spanning tree. Removing e^* in T^* breaks the tree into two connected components with disjoint node sets A and B. Since e crosses (A, B), adding it will re-connected the disconnected components, and thus form a spanning tree, T'.

Second, the new tree is **also optimal**. We claim that $\omega(e') \geq \omega(e)$. At the time e' was considered by Kruskal's, it was rejected because it would create a cycle. Meaning that edge e was already added, implying that $\omega(e) \leq \omega(e^*)$. As such, replacing e^* with e can only decrease or maintain[2] the total edge weight. Thus T' must be optimal.

Repeat this process, creating a chain of trees $T^*, T_1, T_2, \ldots, T_G$. Since each tree is optimal, T_G is as well.

---

[2] In fact, it must maintain. Decreasing would contradict fact that T^* is optimal.

DSC 190

Data Structures & Algorithms

Lecture 9 | Part 7

Designing Greedy Algorithms

Designing Algorithms

- When do we know to use a greedy algorithm?
- It isn’t always obvious.

A Pattern

- Our examples have a common pattern: sort by some attribute, then loop through.
  - Number grid: take numbers in descending order.
  - Activities: take activities in increasing order of finish time.
  - MST: take edges in increasing order of weight.

- This is a new justification for value of sorting.

- Suggestion: when tackling a problem, try sorting first.

Greedy Approximations

- A greedy algorithm can be useful, even if not guaranteed to produce optimal answer.
- Especially true if exact algorithms are **slow**.
- Example: k-means clustering (Lloyd's algorithm)

k-means Problem

- **Given**: n data points X in $\mathbb{R}^d$, parameter k.
- **Search Space**: all clusterings $C = \{X_1, \ldots, X_k\}$ of X into k disjoint sets.
- **Objective function**: minimize

$$\phi(C) = \sum_{i=1}^{k} \sum_{x \in X_i} (x - \text{mean}(X_i))^2$$

Greedy Algorithm

- Lloyd's algorithm (a.k.a., the "k-means algorithm") is a greedy algorithm for minimizing the *k*-means objective.
- Start with k centroids, $\mu_1, \ldots, \mu_k$.
- At each step, let X_i be set of points closest to μ_i, update μ_i to be mean(X_i), repeat until convergence.
- Each step decreases value of objective function.

Optimality

- Lloyd's algorithm is **not** guaranteed to find optimum.
- Then again, no feasible algorithm is.
- Used in practice because it is fast and "good enough".