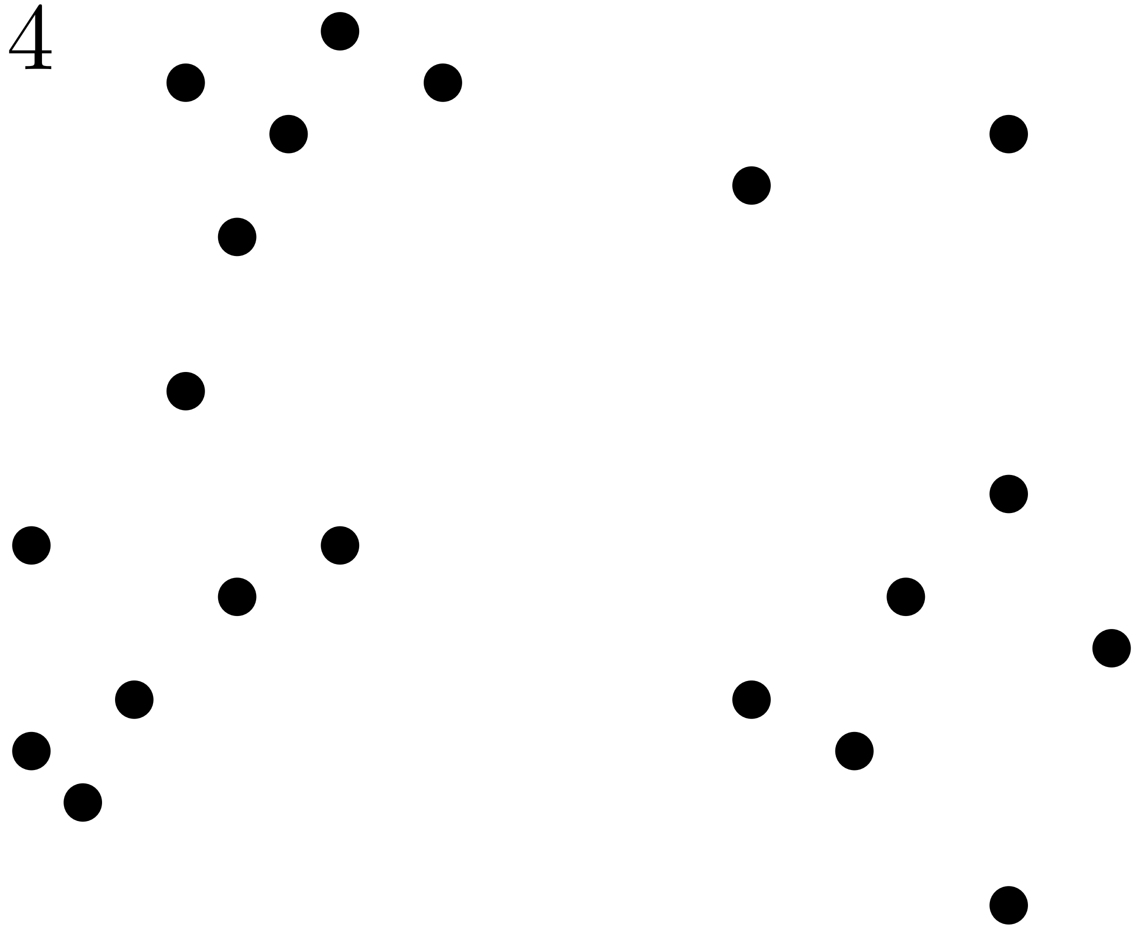
Center-based Clustering

2-approximation for k-center clustering
5-approximation for k-median clustering
k-means clustering

Center-based clustering – intuition

Given: integer k, point set P

$k = 4$



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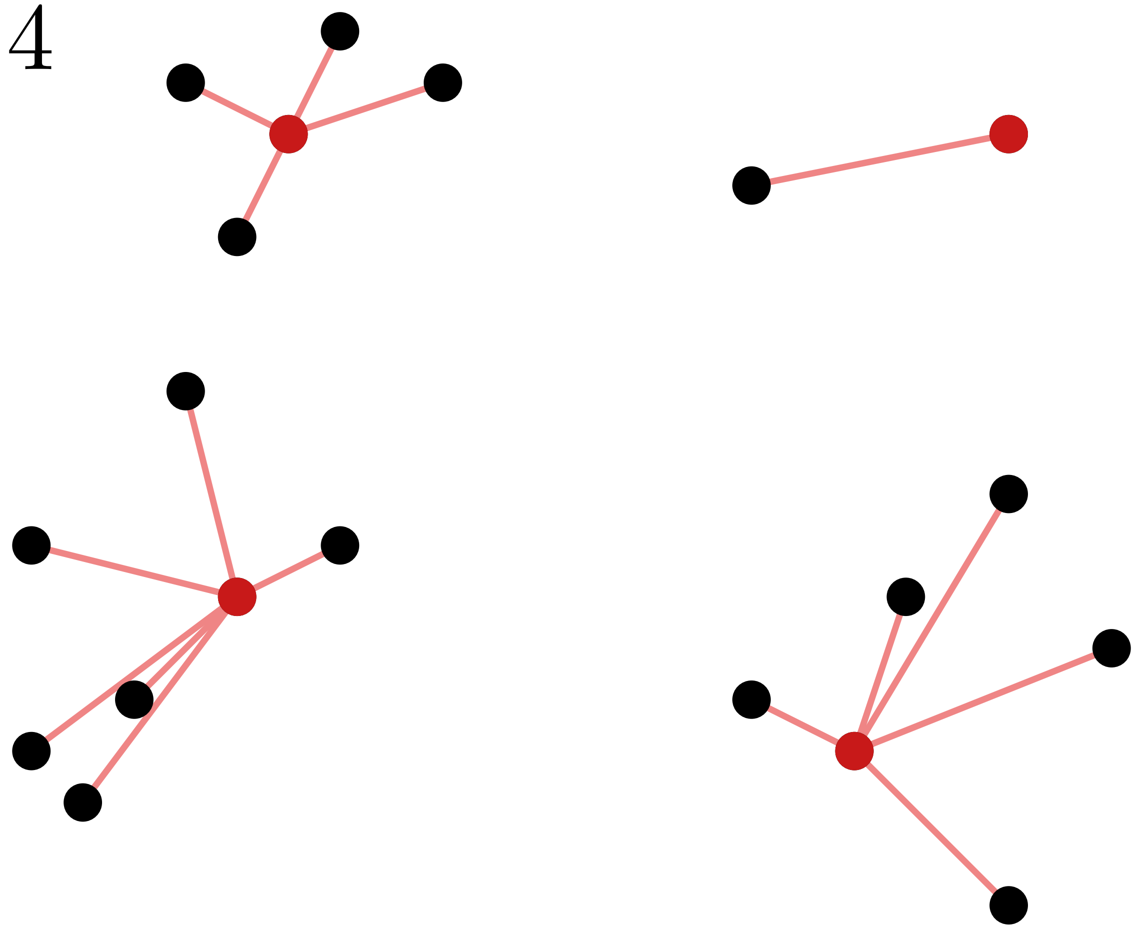

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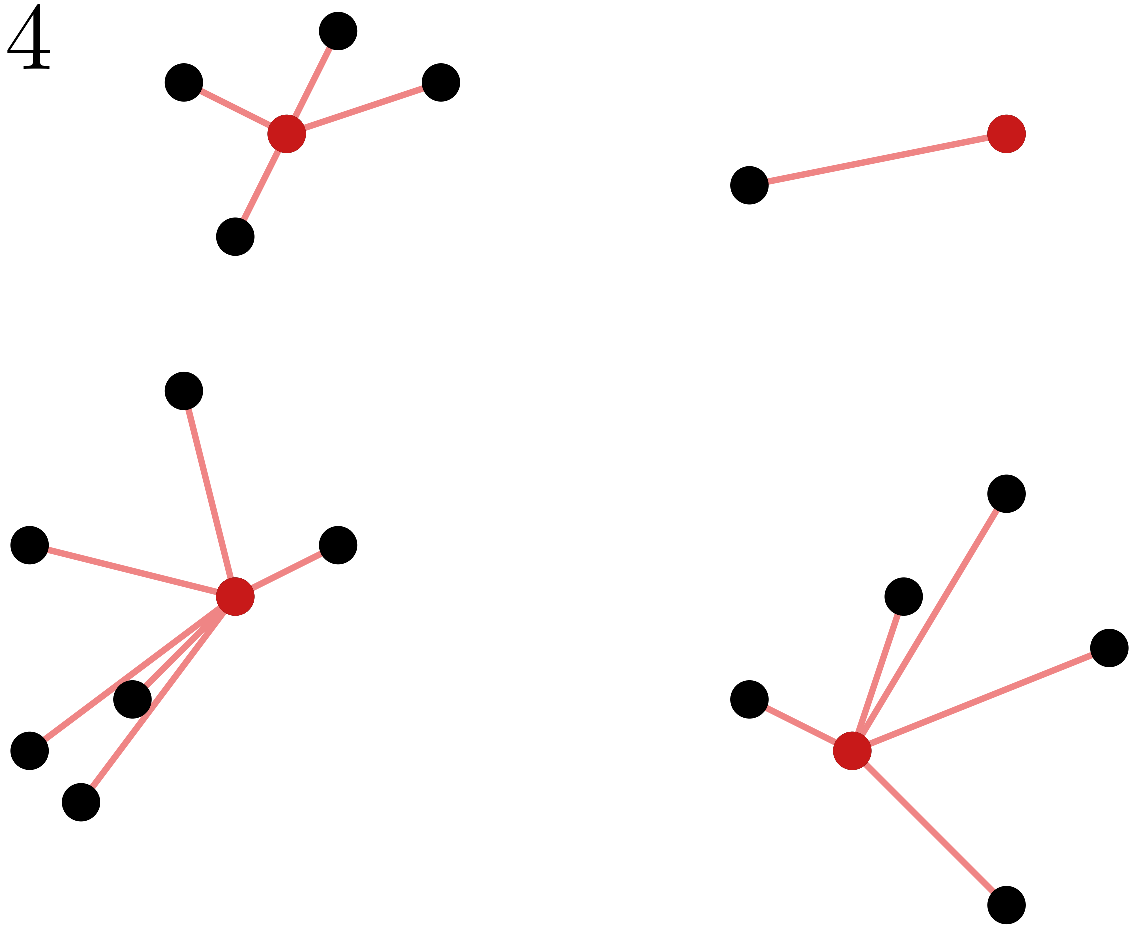

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- finding groups of nearby points

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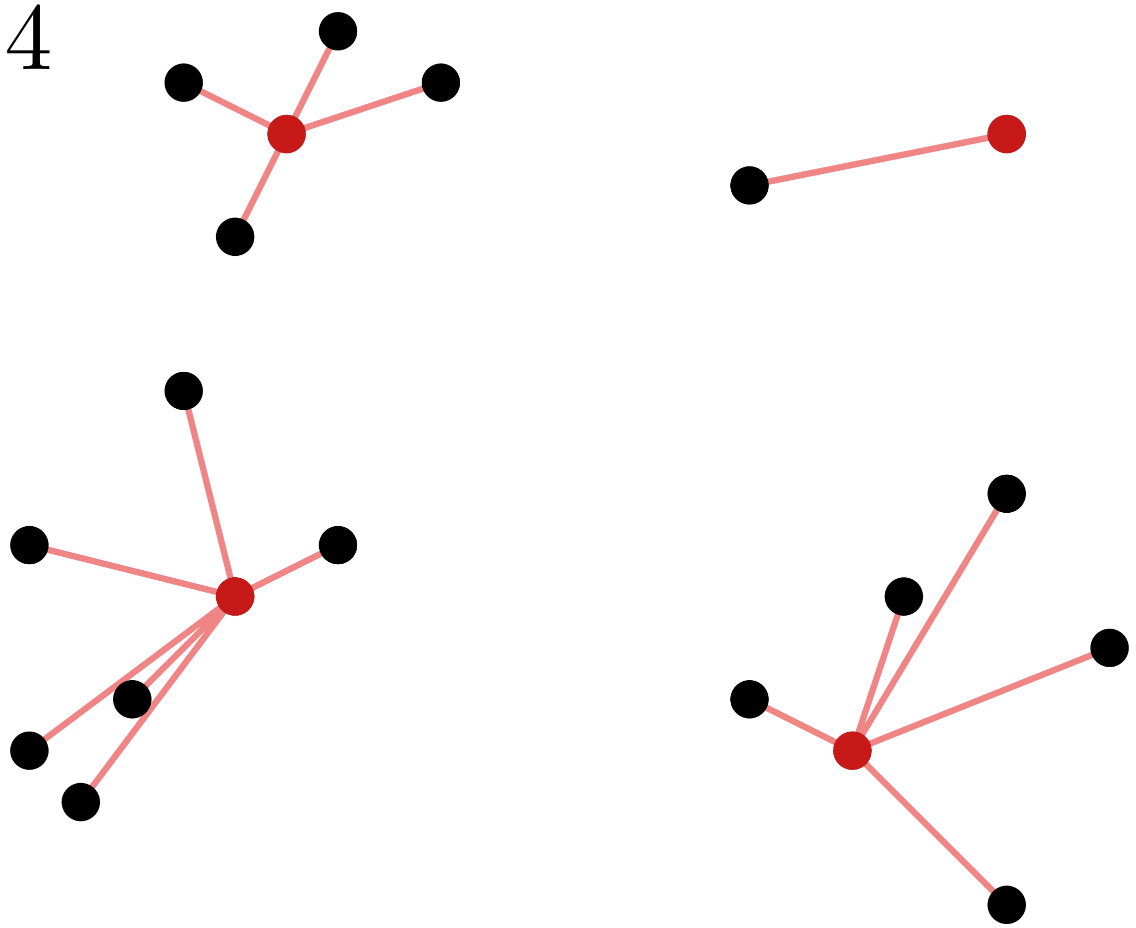

Given: integer k, point set P in metric space

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Preliminaries

metric space: pair (X, d) with X a set, and $d\colon X \times X \to [0, \infty)$ satisfying

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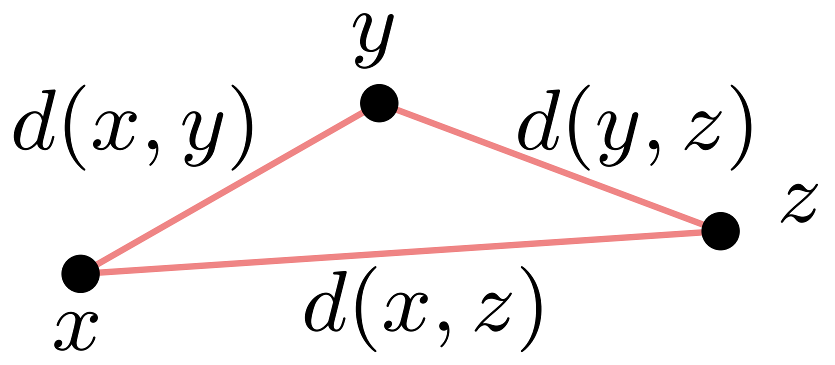

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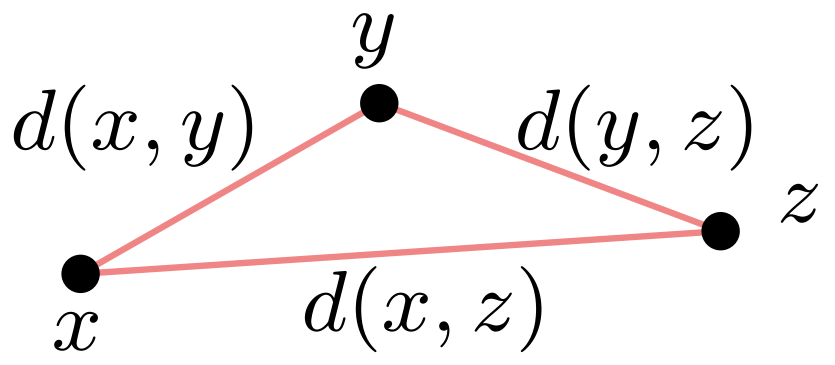
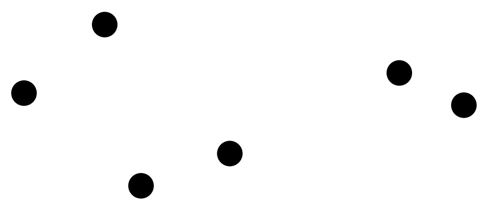


examples:

R^2 with Euclidean distance



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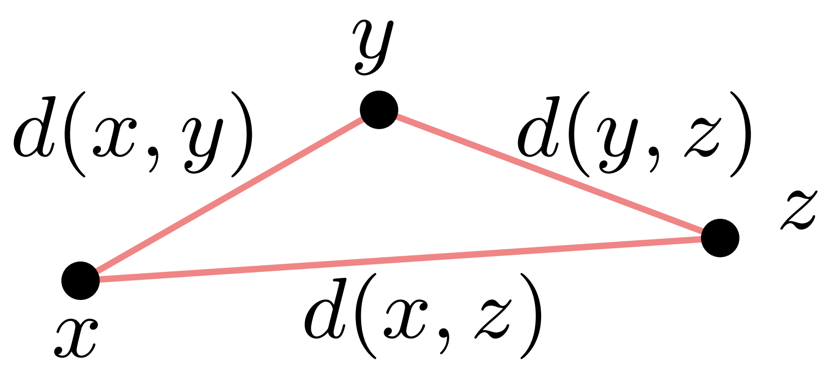

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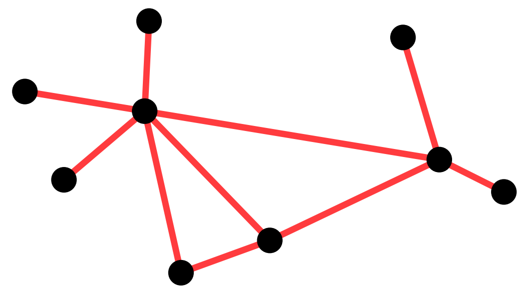

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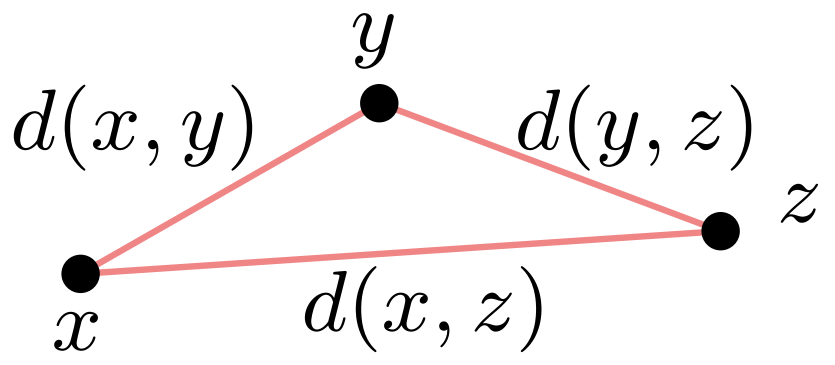

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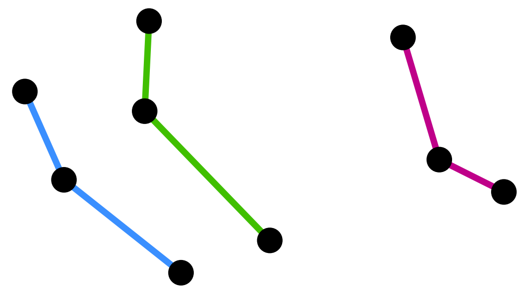
curves with Fréchet distance



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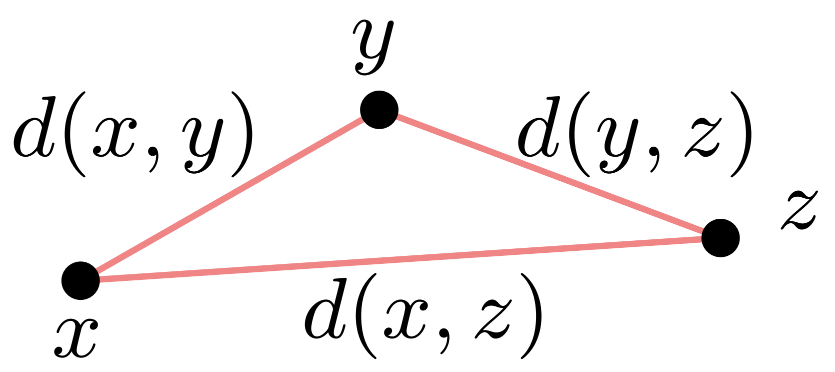

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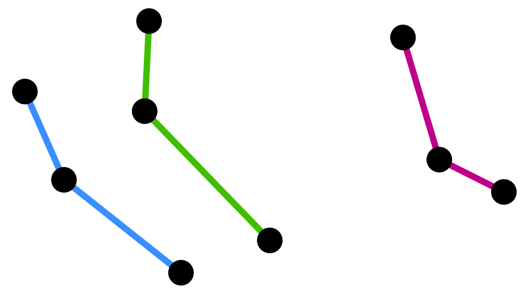

notation: $d(p, C) := \min_{q \in C} d(p, q)$

k-center clustering in metric space (X, d)

Given: $P \subset X$ and integer k

Goal: Find $C \subset X$ of size k such that

$$\max_{p \in P} d(p, C)$$

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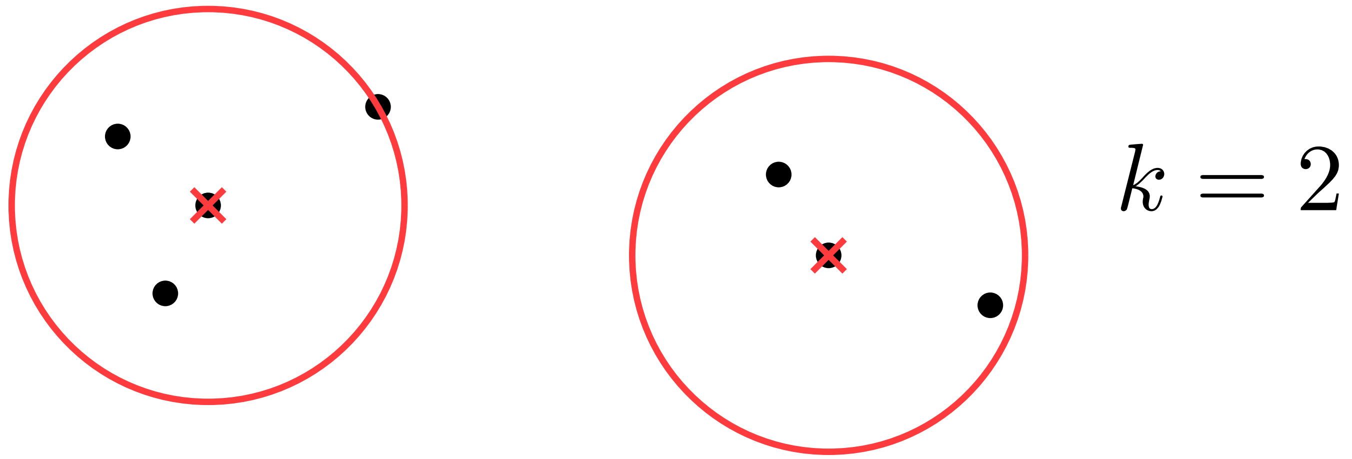

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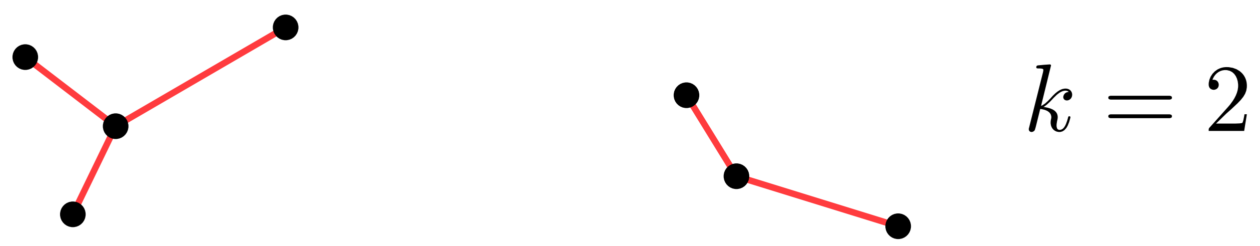


discrete k-center problem: $C \subset P$

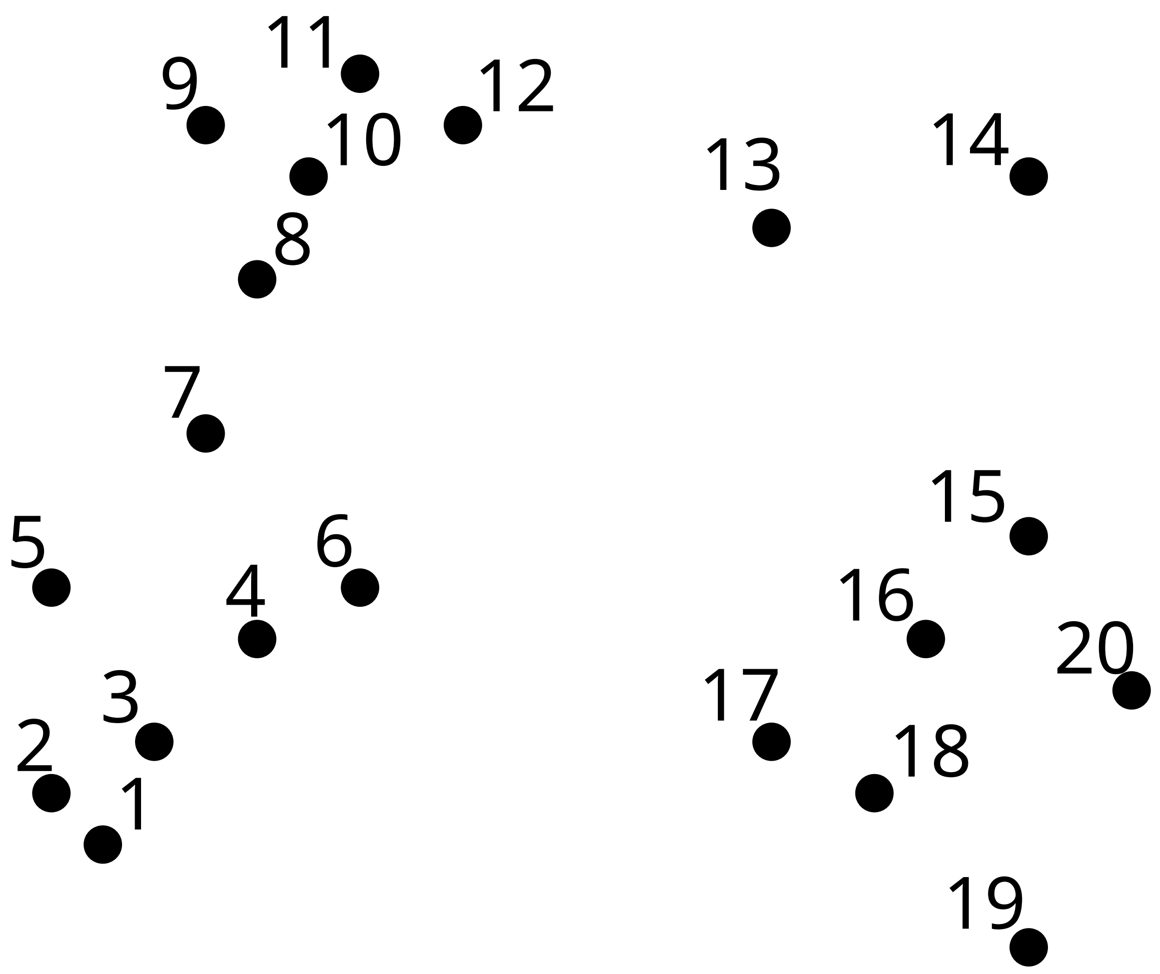
later:

(discrete) k-median problem: sum instead of $\max$

k-means: sum of squares

Quiz

Which of the following is an optimal set of centers for $k = 3$?



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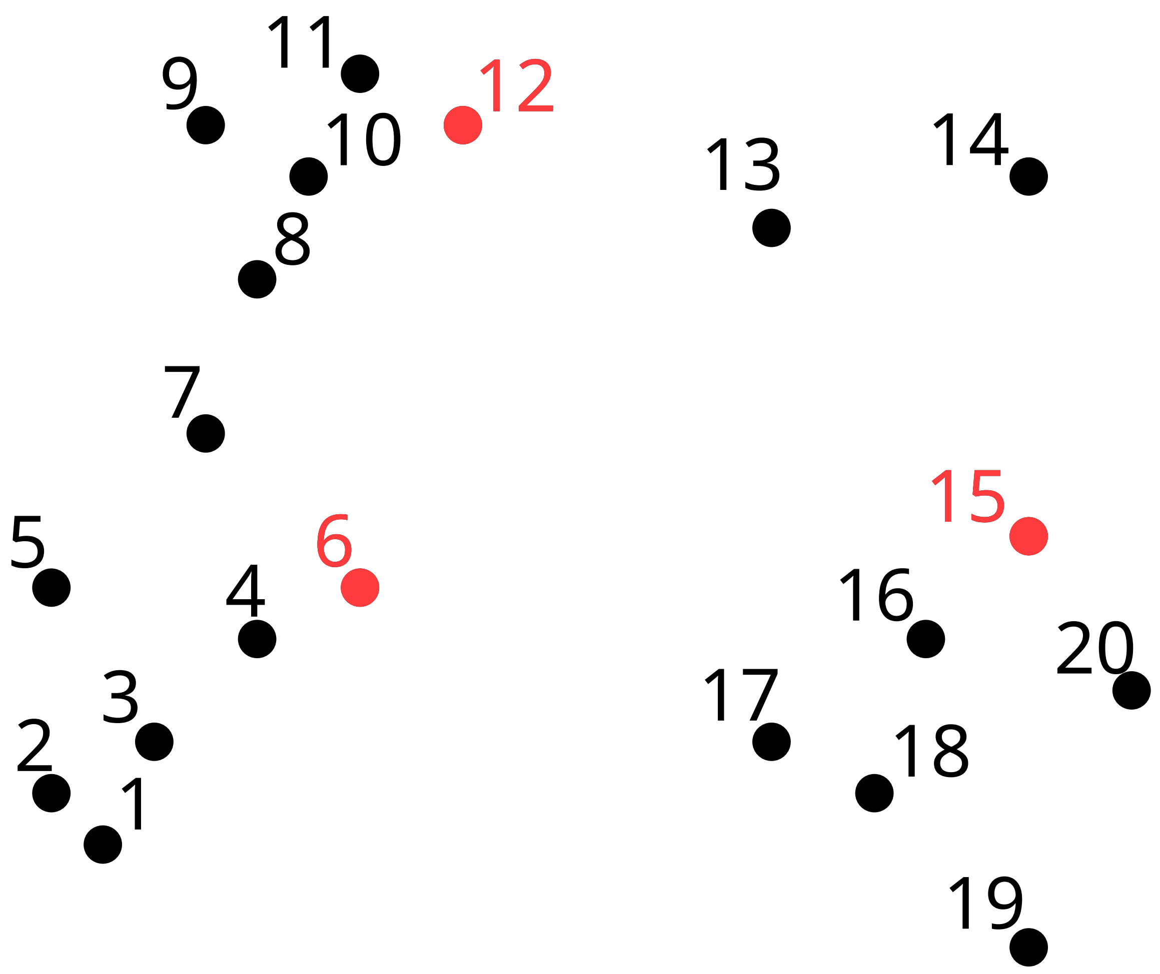

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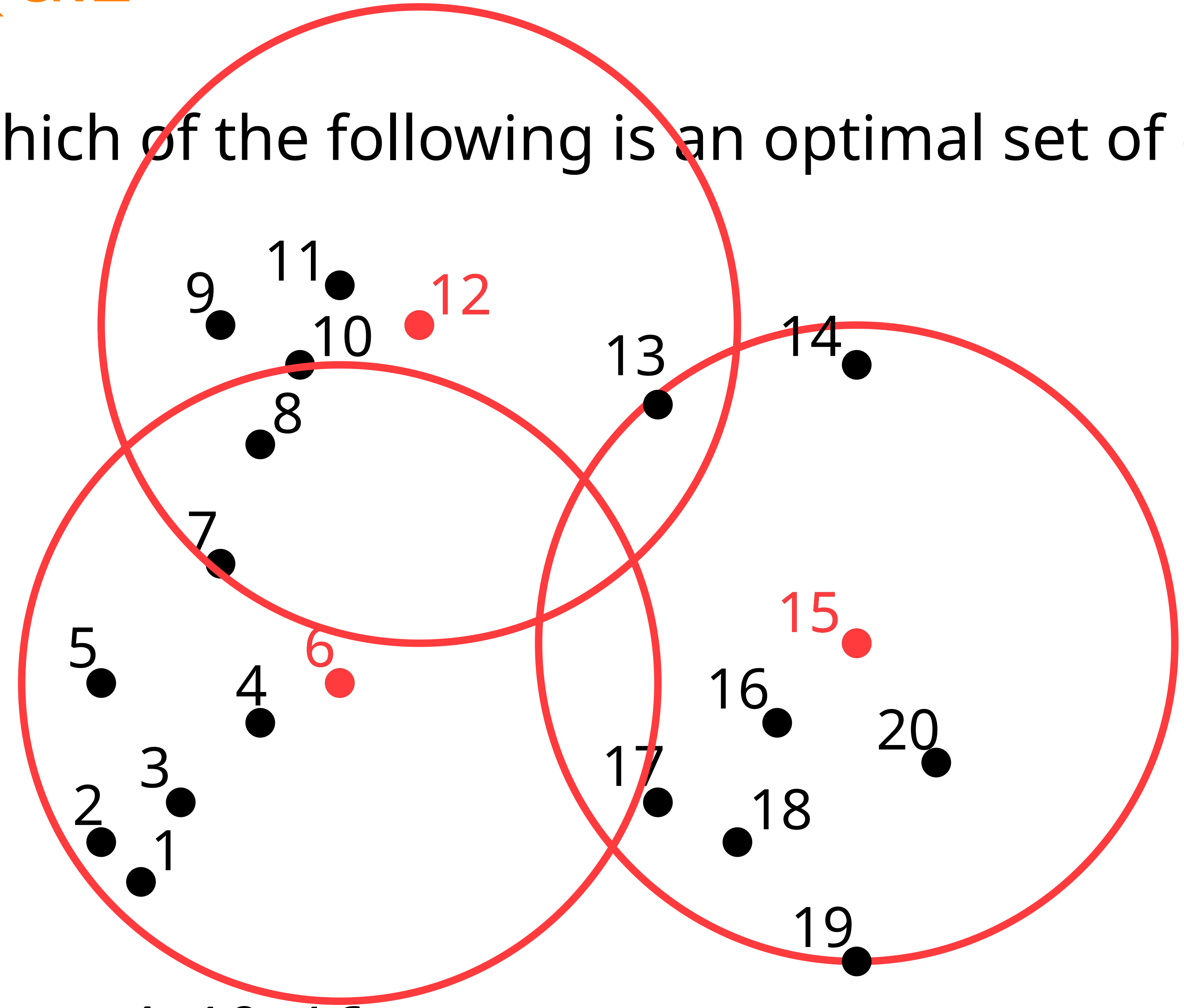

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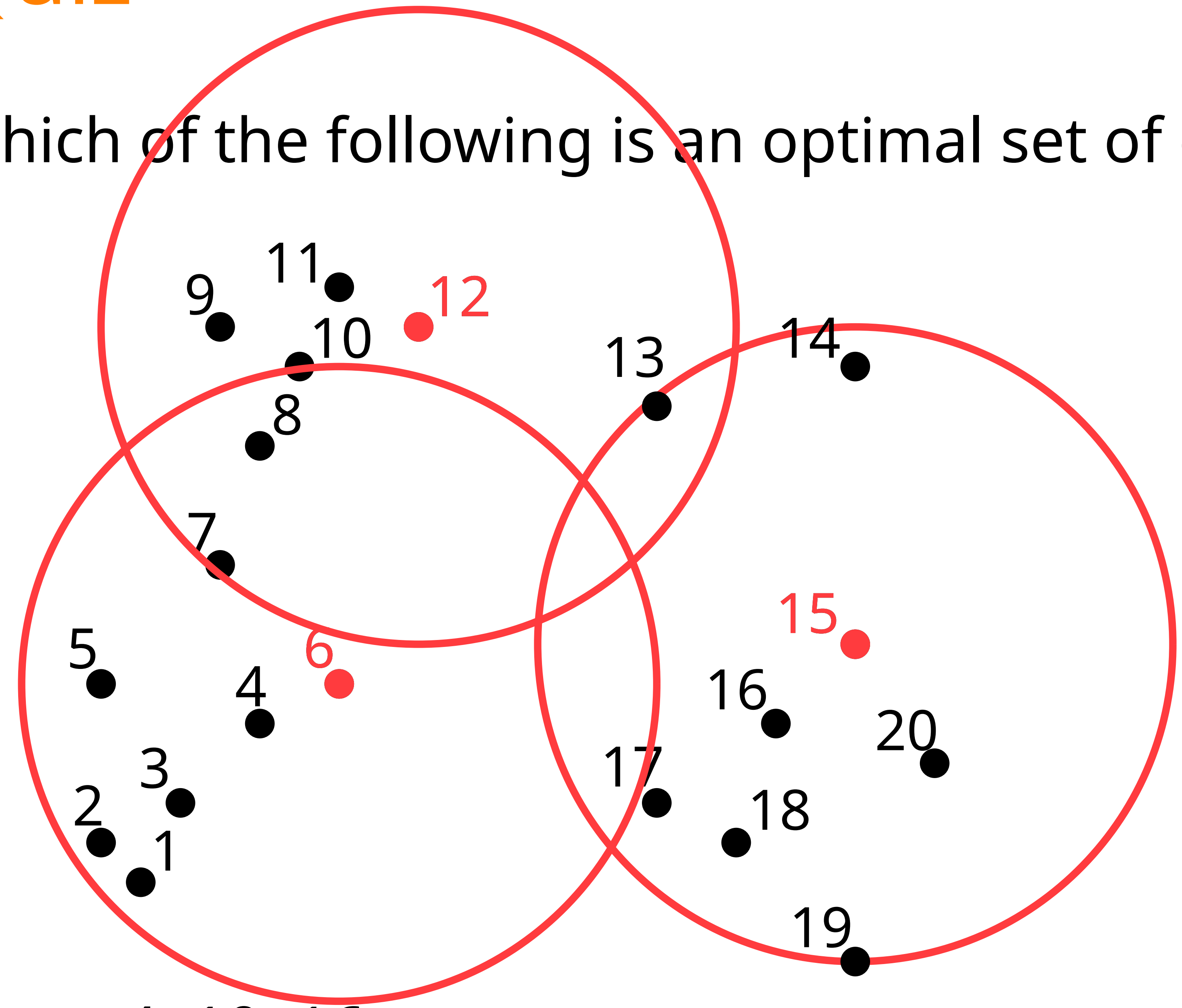

This problem is NP-hard

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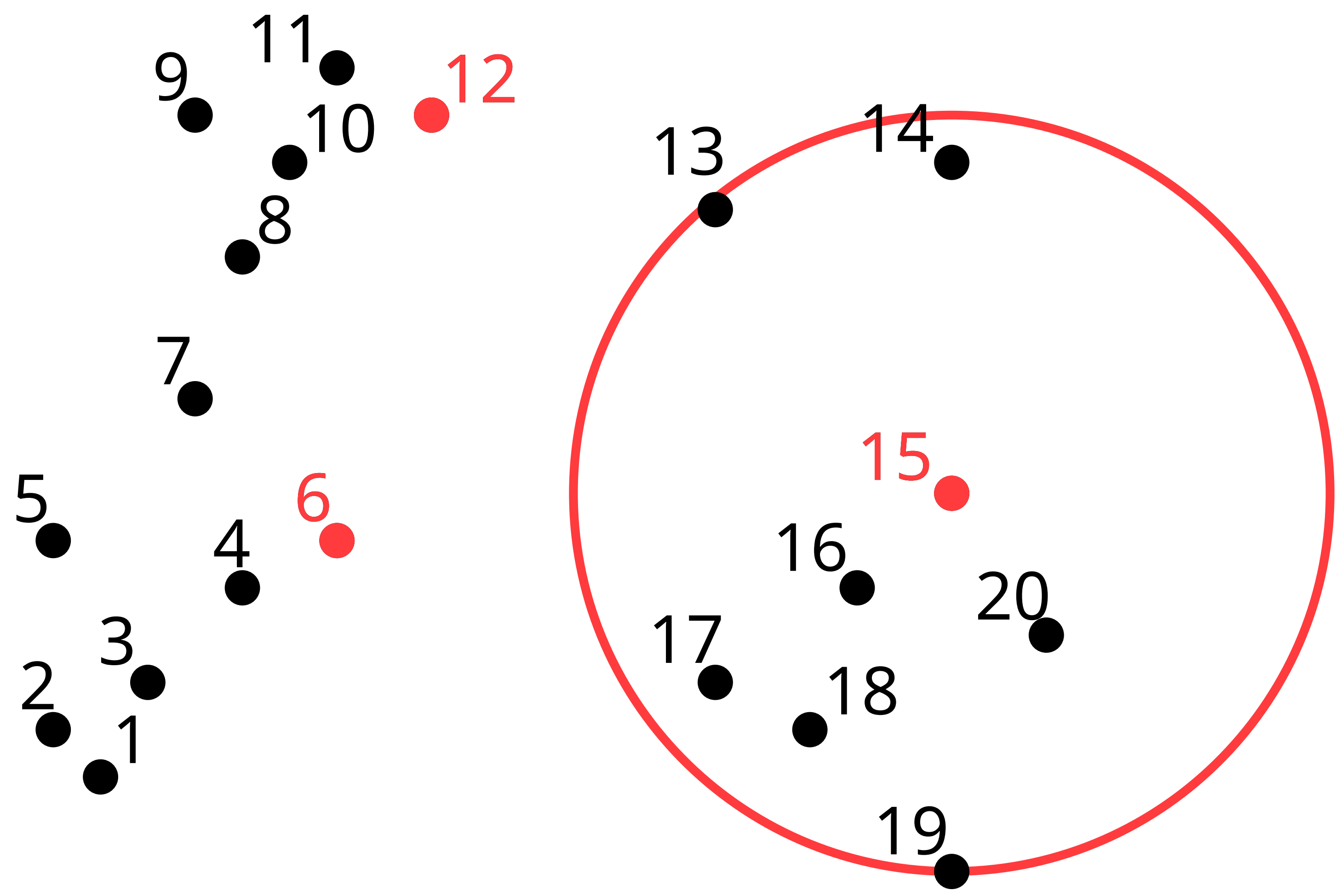
k-center clustering

approximation algorithm

Algorithm GreedyKCenter(P, k)

Incrementally add points to C. How can we guarantee to reduce the maximum?



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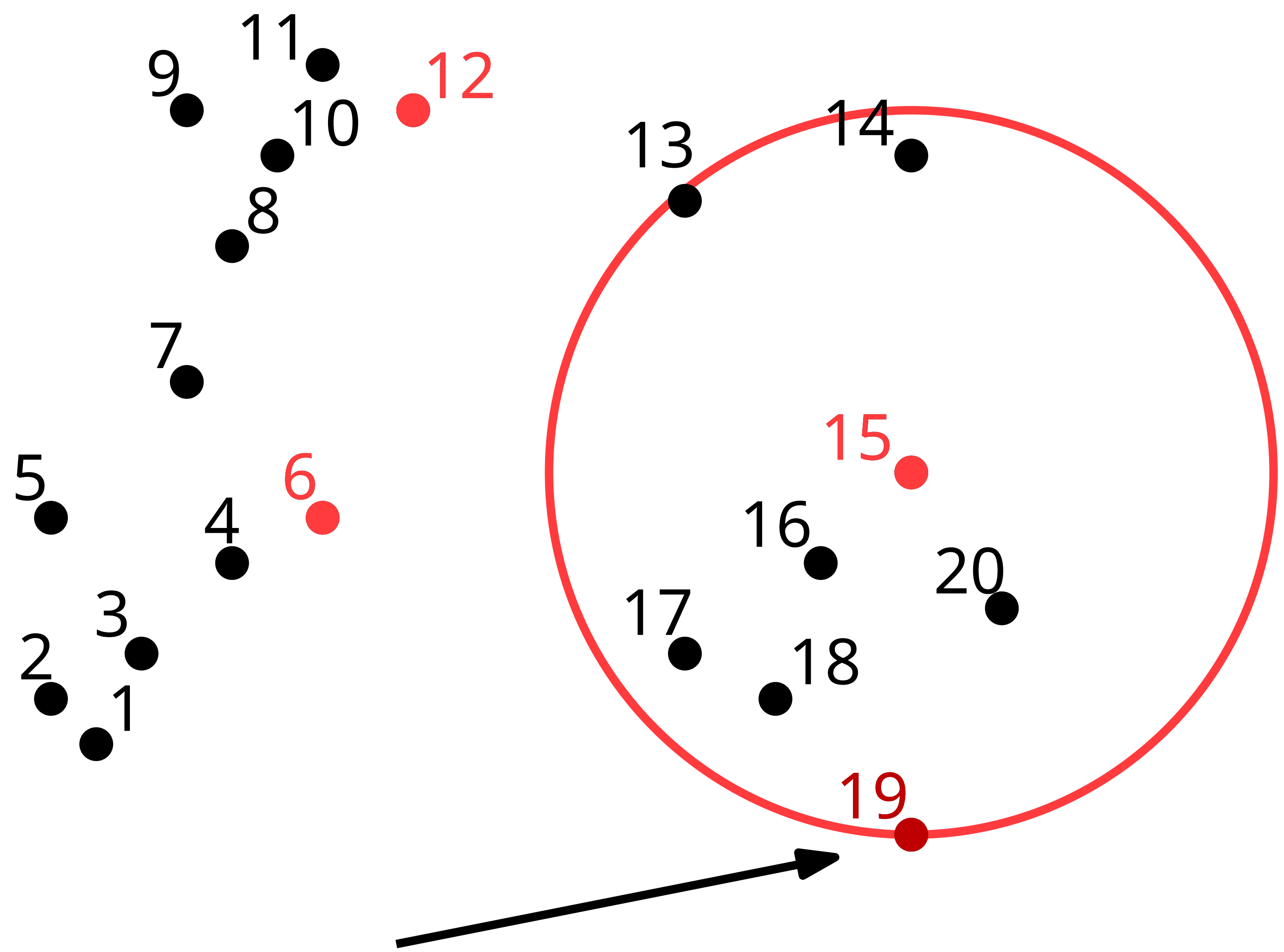

Add the point p with maximum $d(p, C)$!

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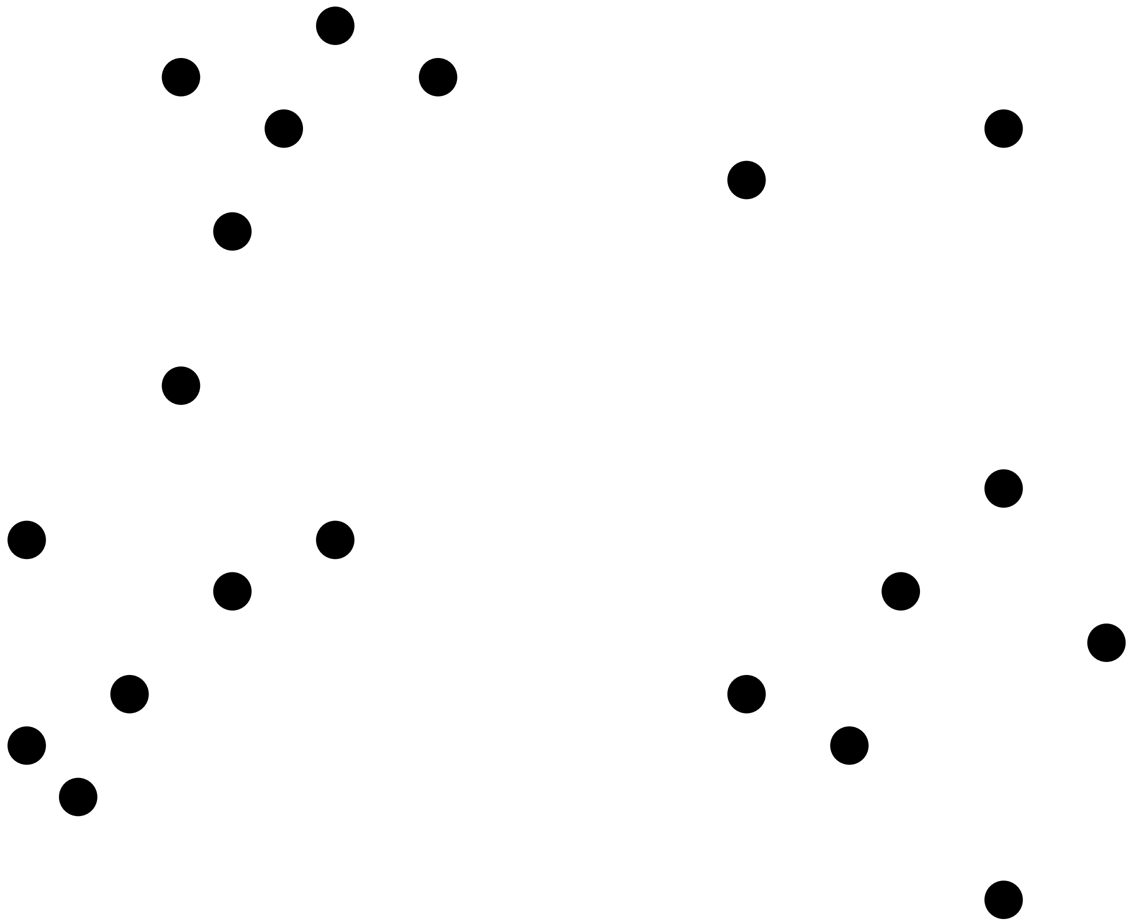

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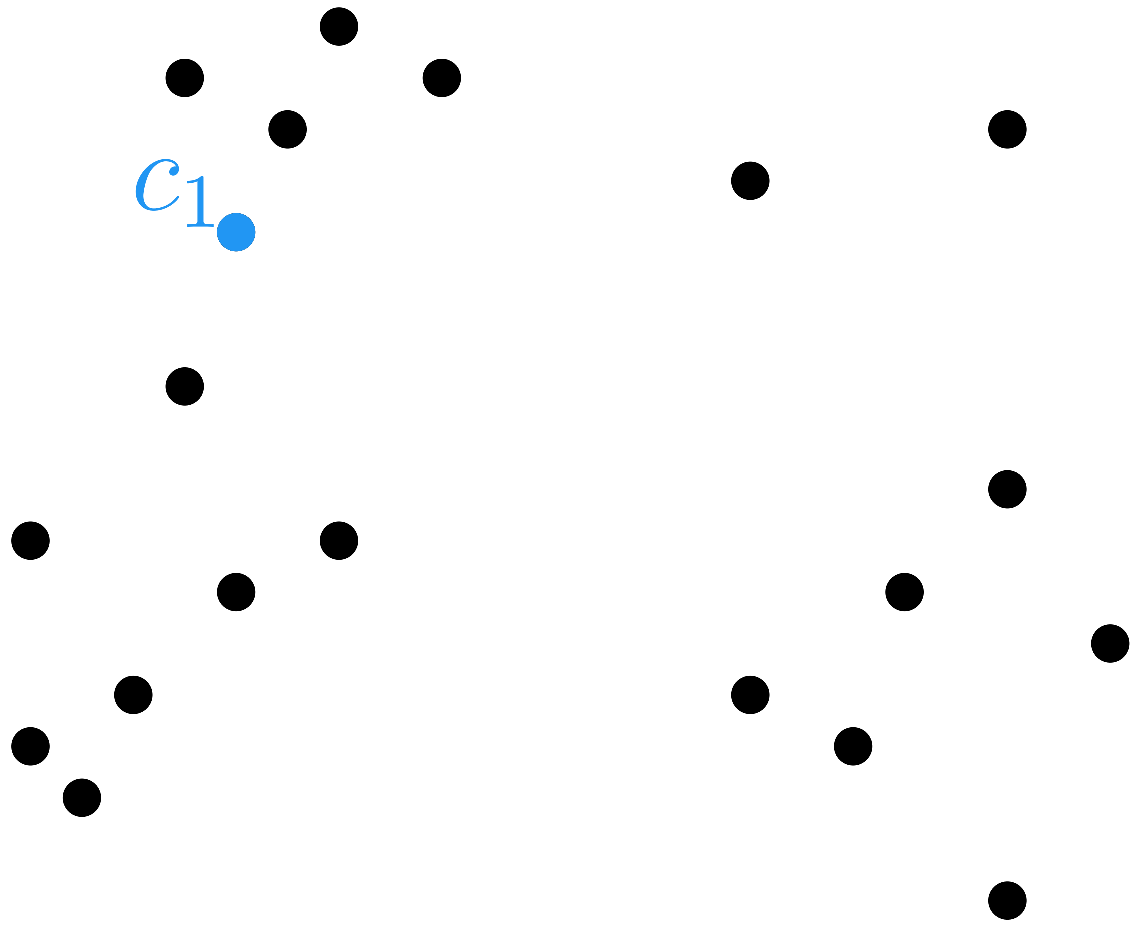

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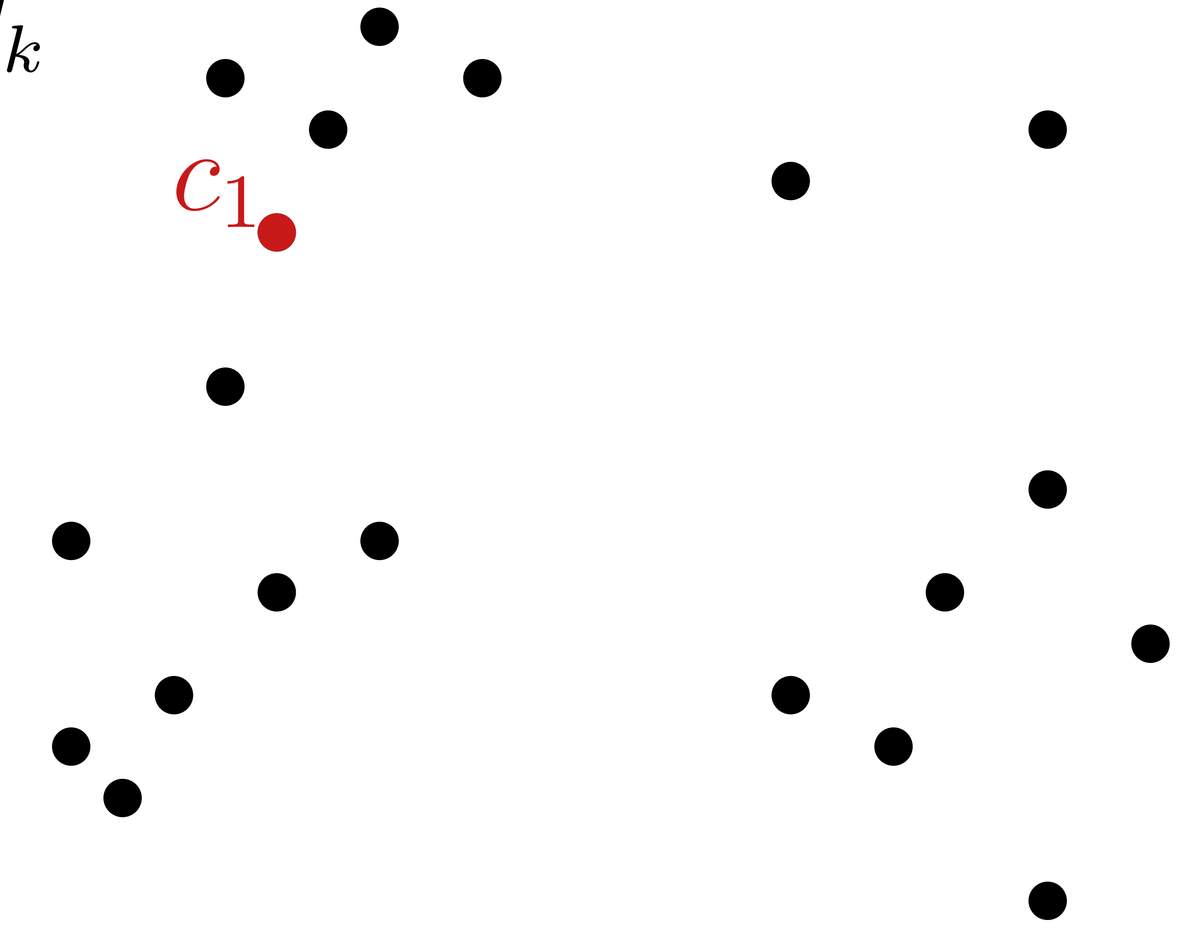

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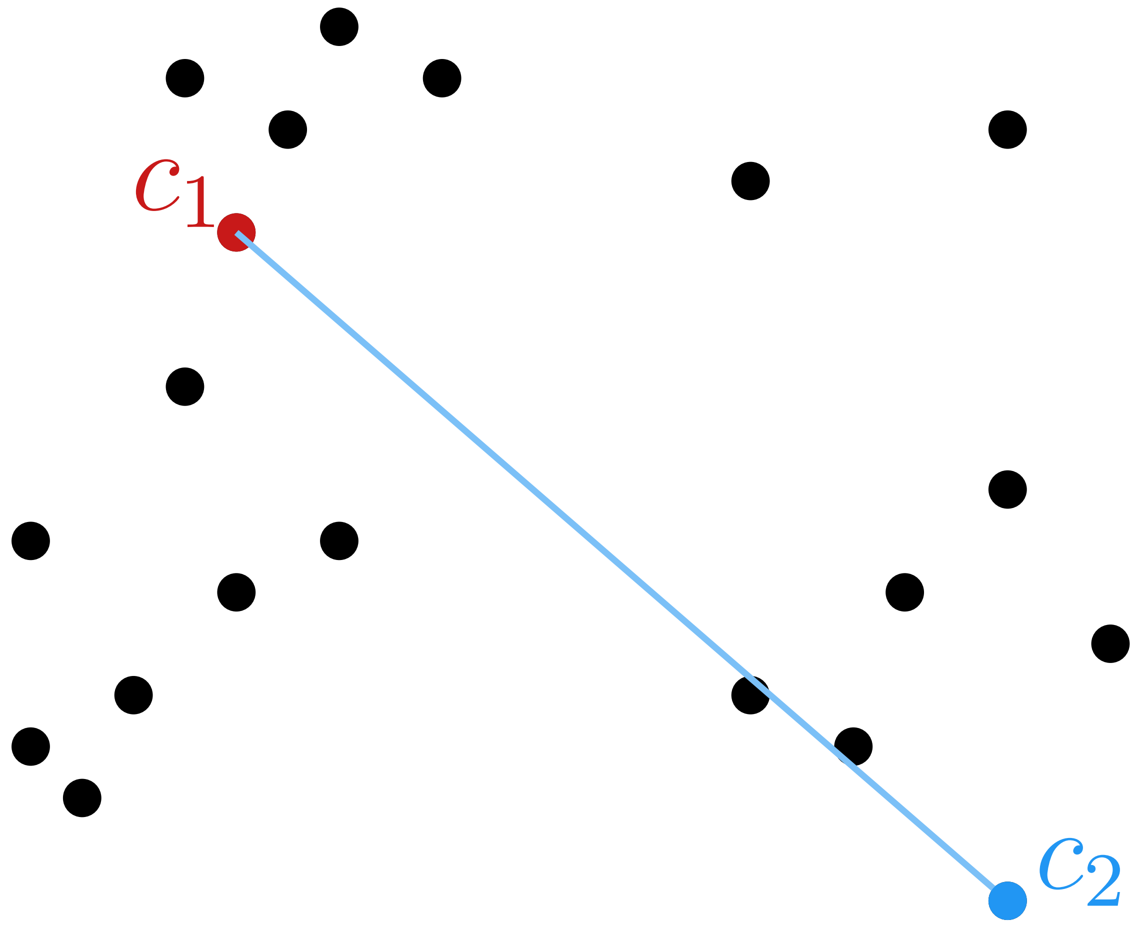

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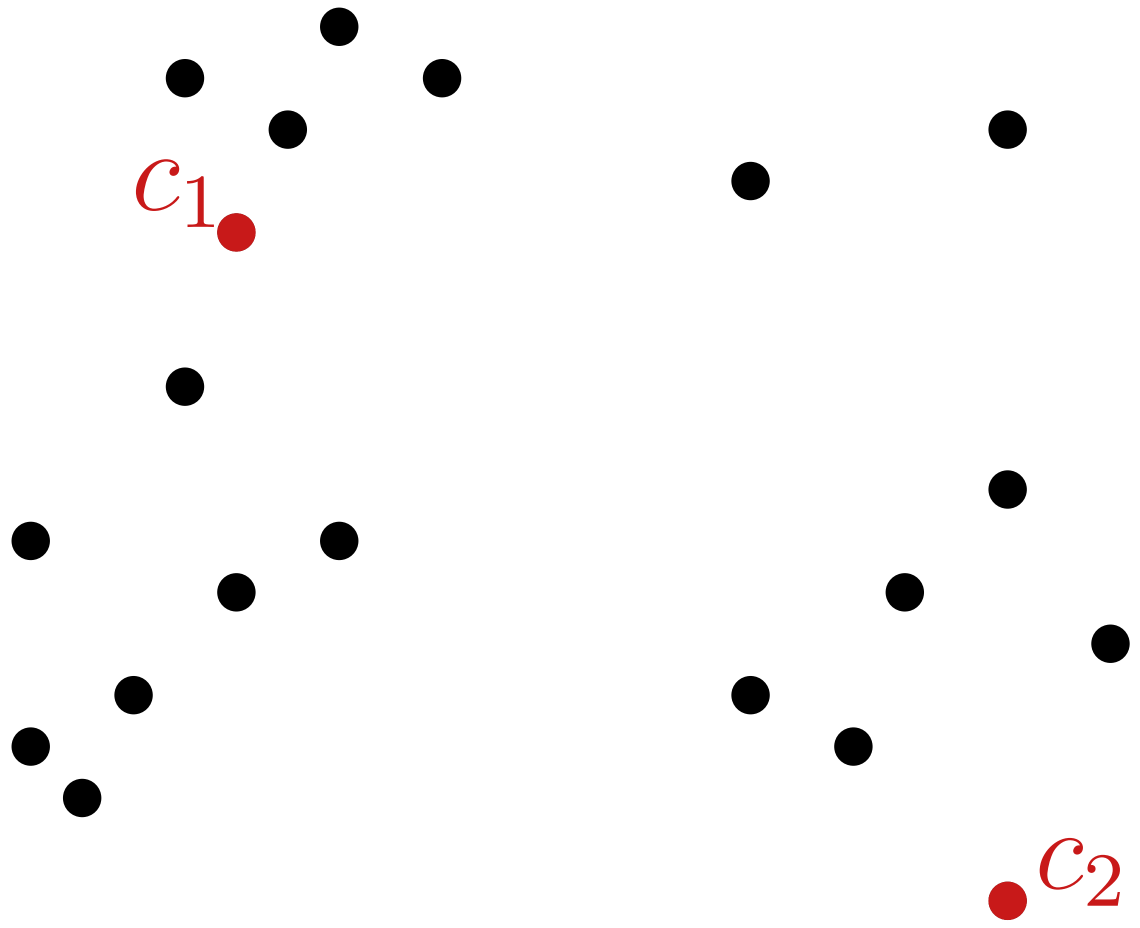

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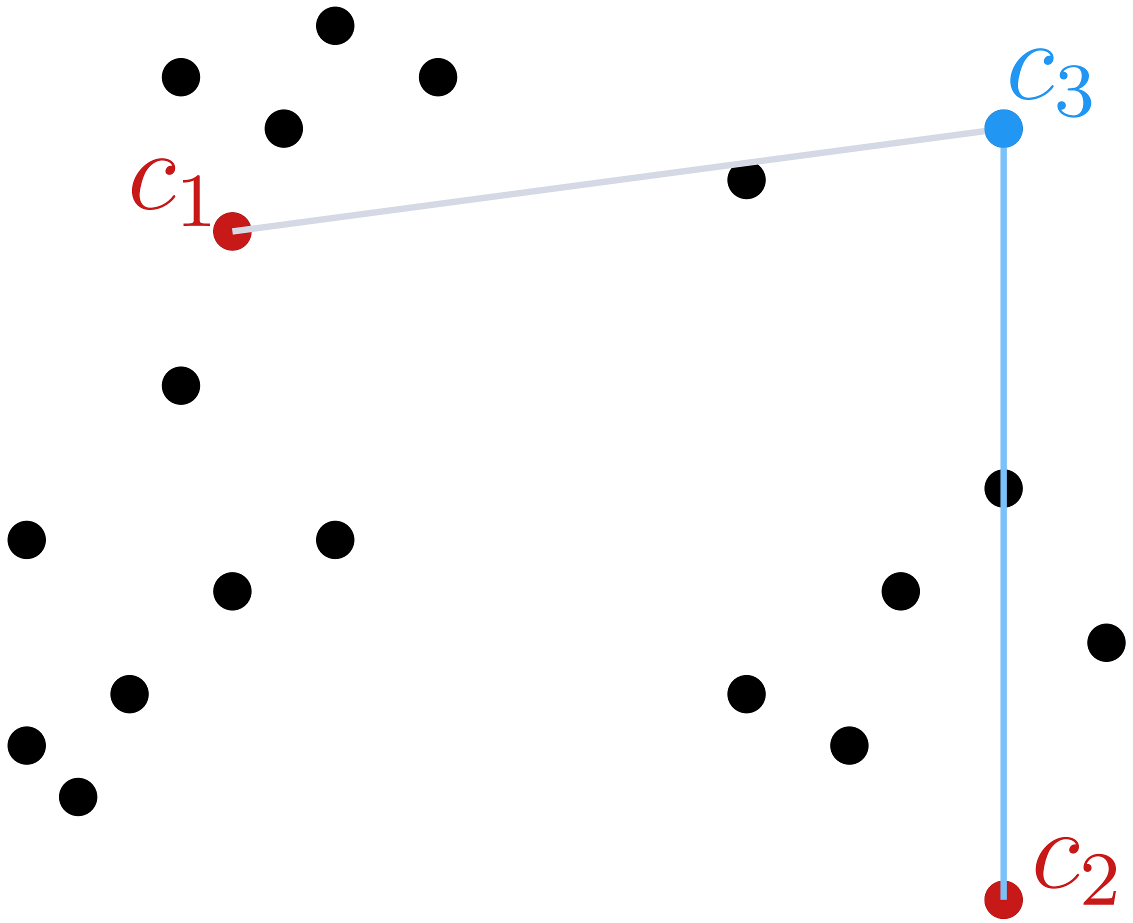

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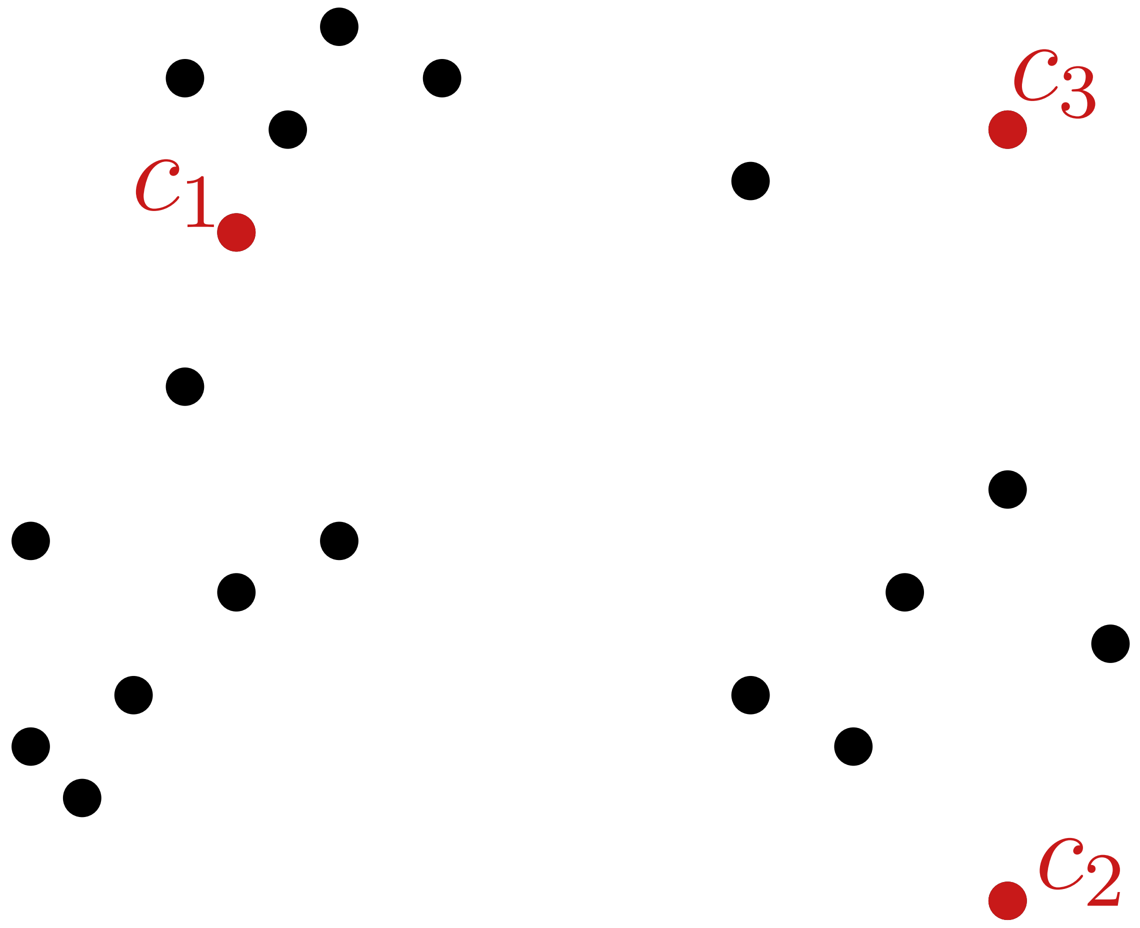

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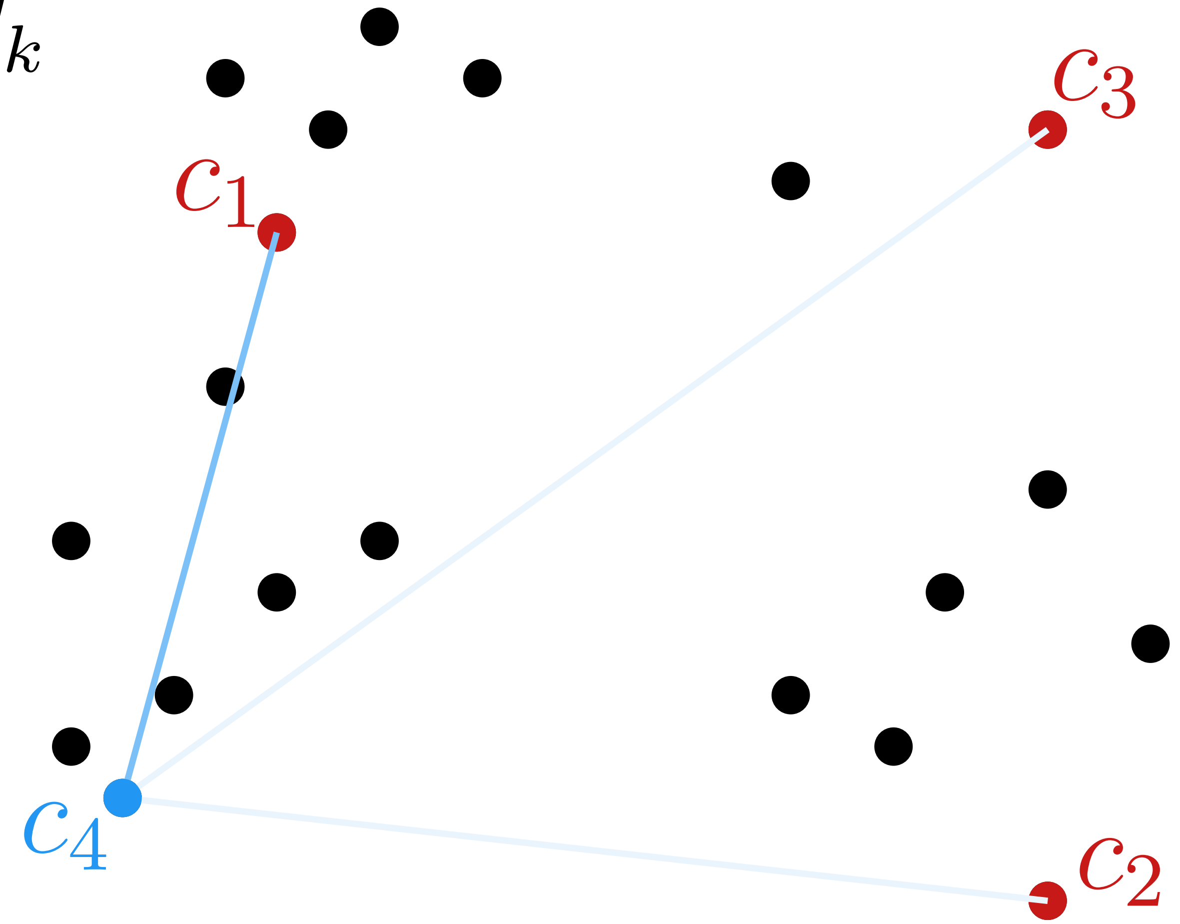

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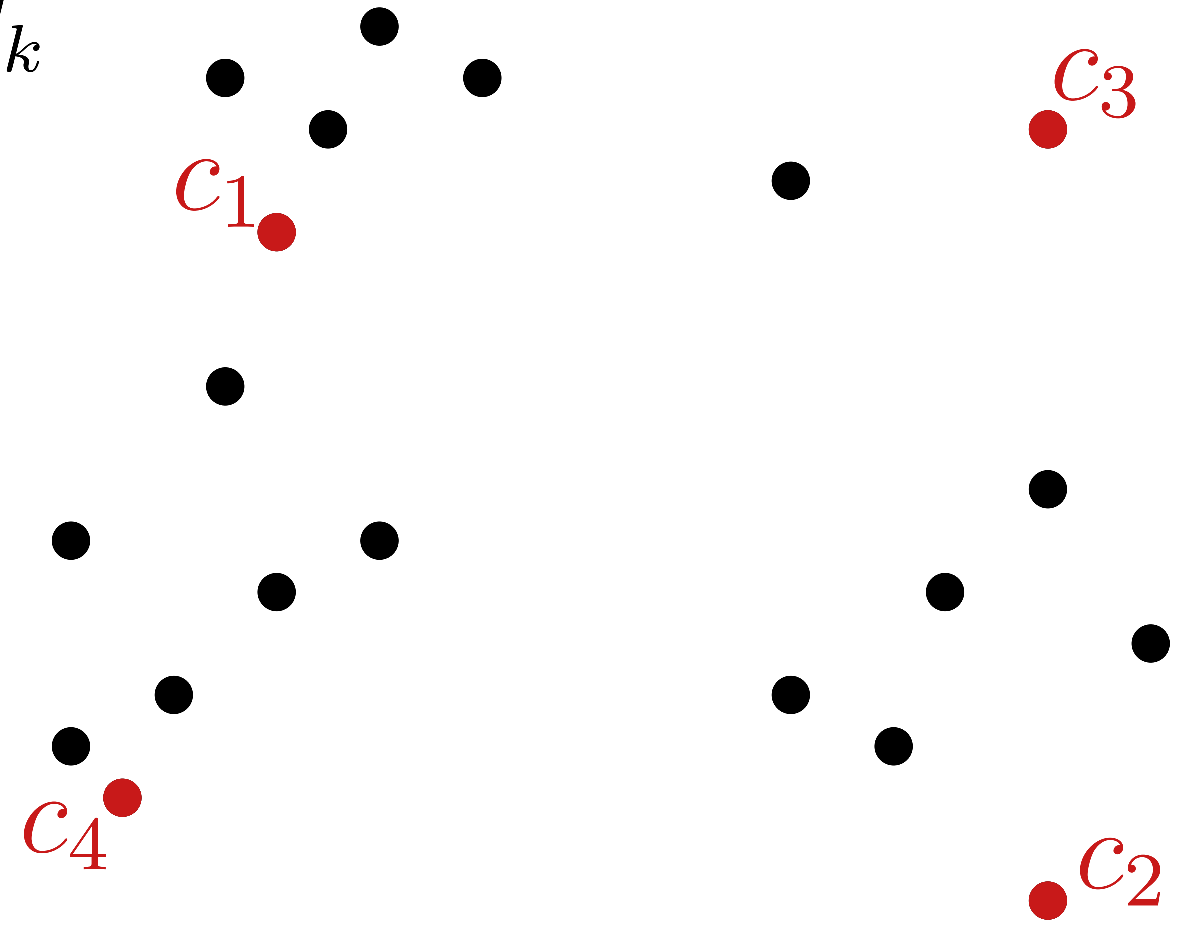

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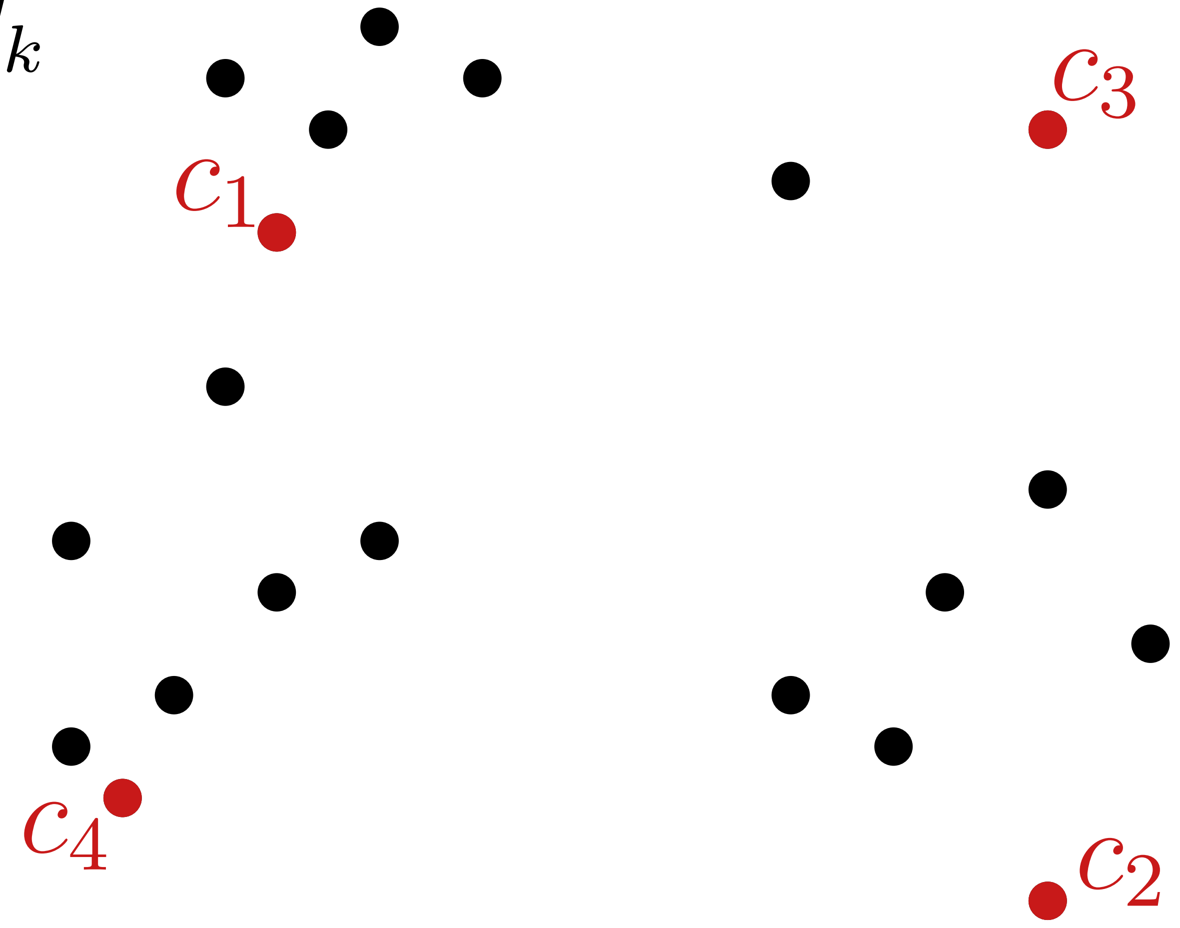

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GreedyKCenter(P, k) computes a 2-approximation for k-center clustering.

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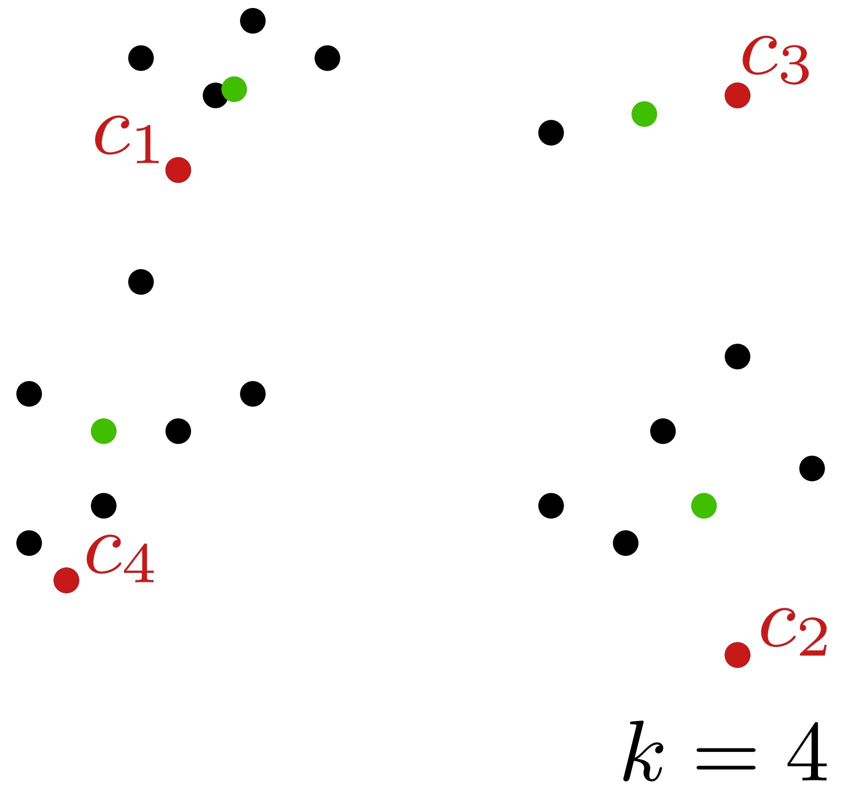

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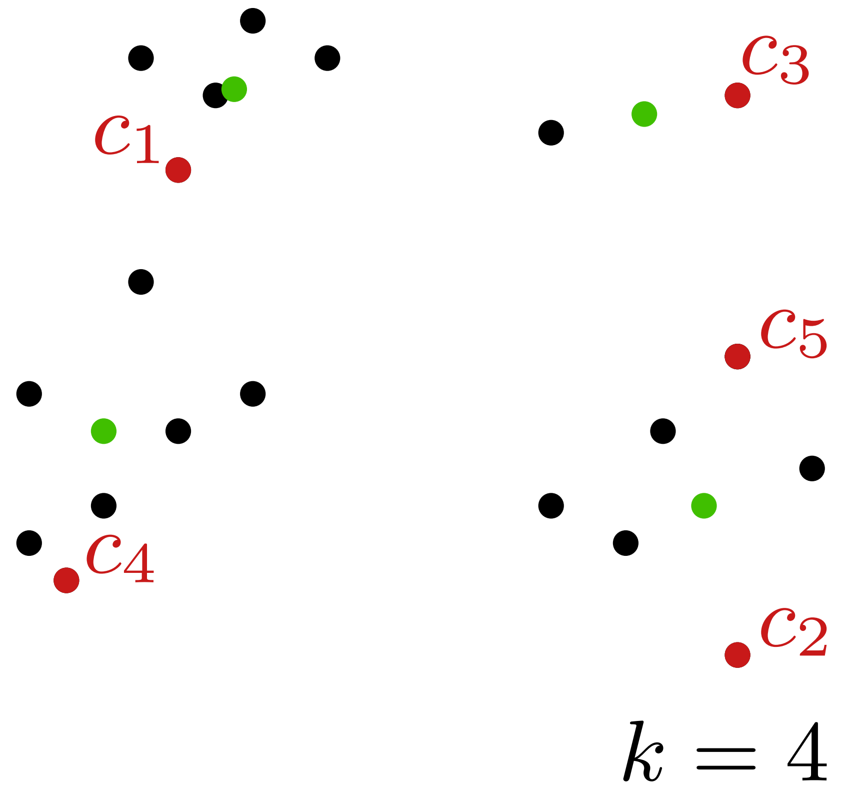

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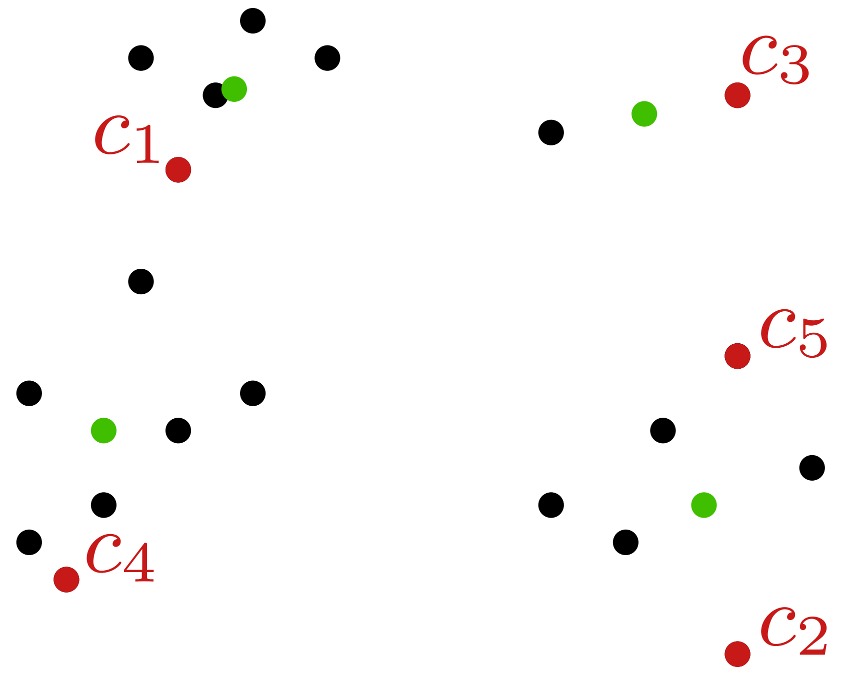

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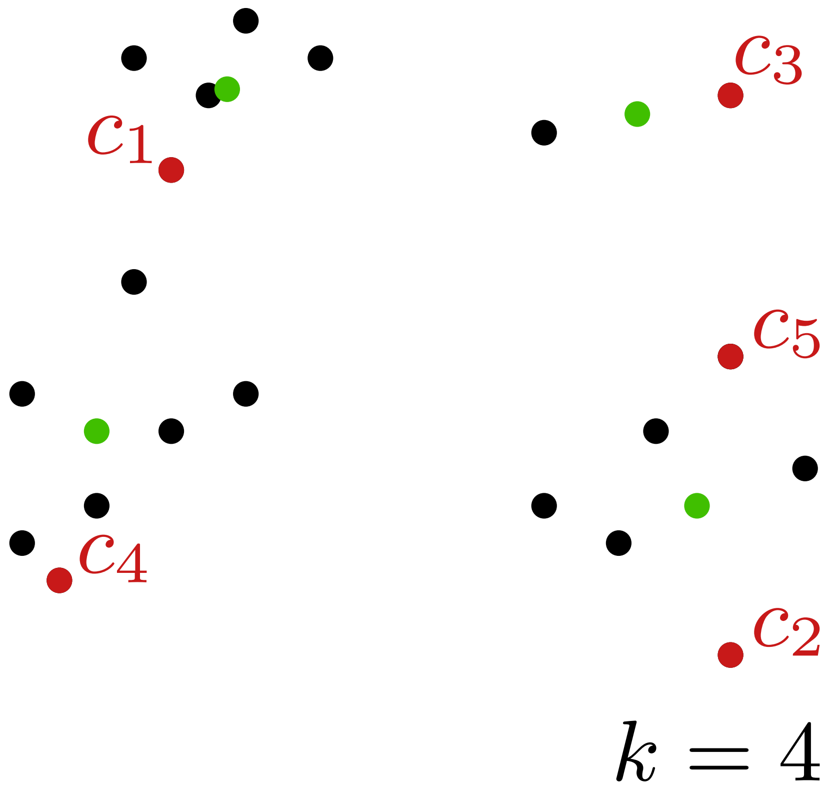

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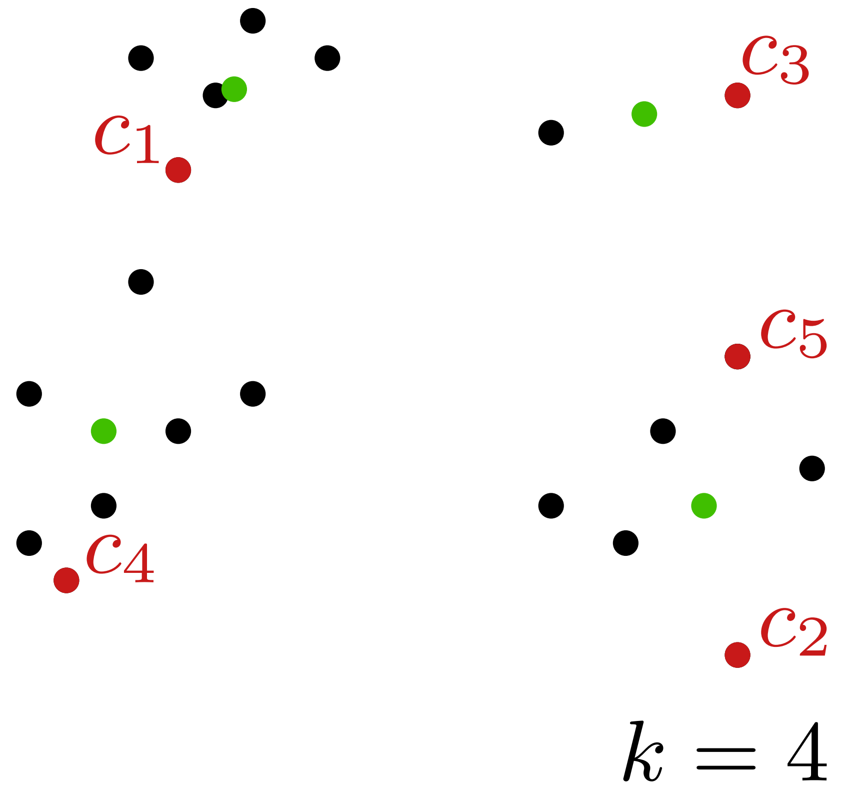

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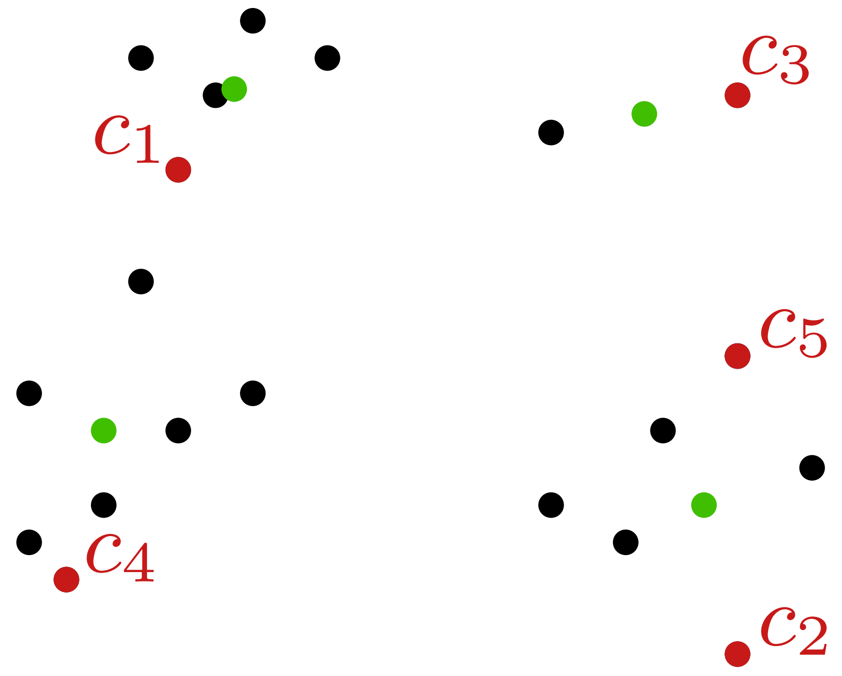
$C_{j-1} \subset C_k$



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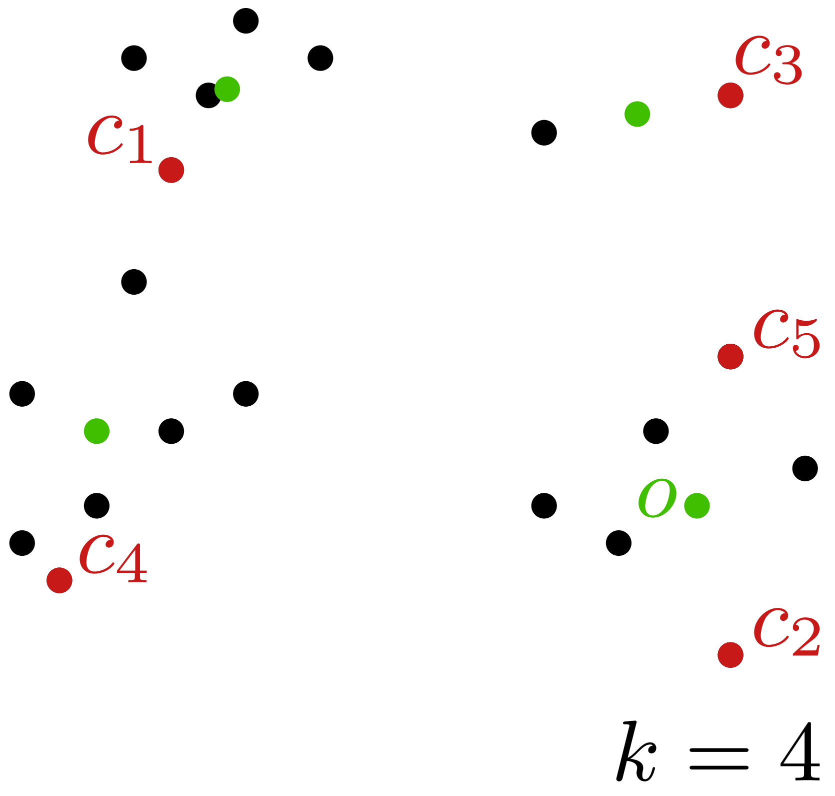
pigeonhole principle:

$\exists c_i, c_j$ in the same cluster of C^*; $o :=$ corresponding center



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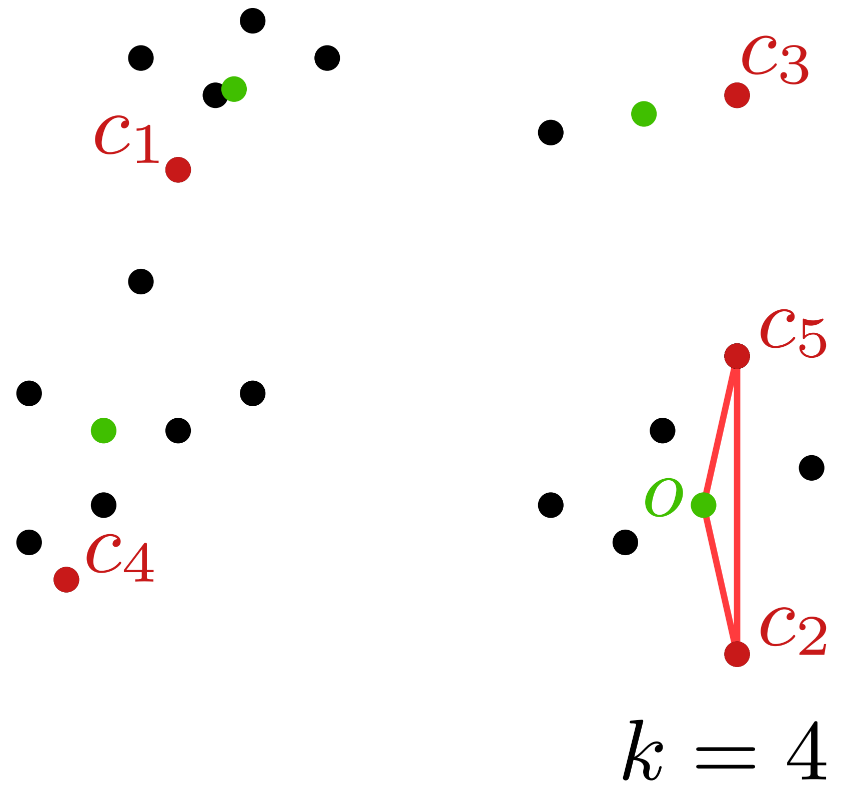
$d(c_j, c_i) \geq d(c_j, C_{j-1}) \geq d(c_{k+1}, C_{j-1}) \geq d(c_{k+1}, C_k) = r$



pigeonhole principle:

$\exists c_i, c_j$ in the same cluster of C^*; $o :=$ corresponding center

triangle inequality:

$r \leq d(c_j, c_i) \leq d(c_j, o) + d(o, c_i) \leq 2OPT$

Quiz

The proof that GreedyKCenter gives a 2-approximation works . . .

A only in R^2 with Euclidean distance

B in R^d but only with Euclidean distance

C in any metric space

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- $2 - \varepsilon$ for general metric spaces
- 1.82 for R^2 with Euclidean distance
- $2 - \varepsilon$ for R^2 with L_1- or L_∞- distance

discrete k-median clustering

approximation algorithm

discrete k-median clustering in metric space (X, d)

Given: $P \subset X$ and integer k

Goal: Find $C \subset P$ of size k such that

$$\sum_{p \in P} d(p, C)$$

is minimized.

$k = 2$

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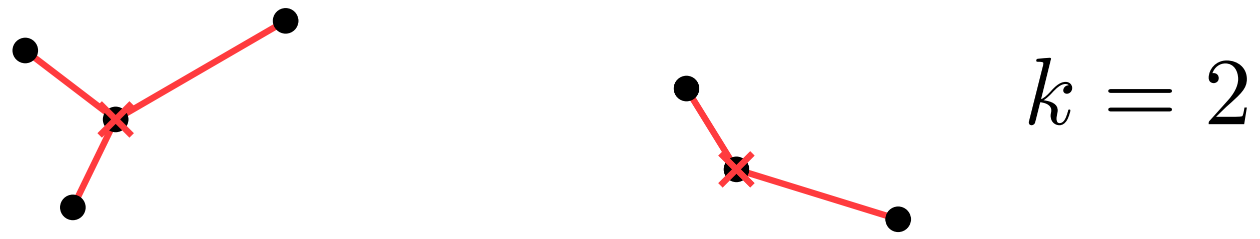
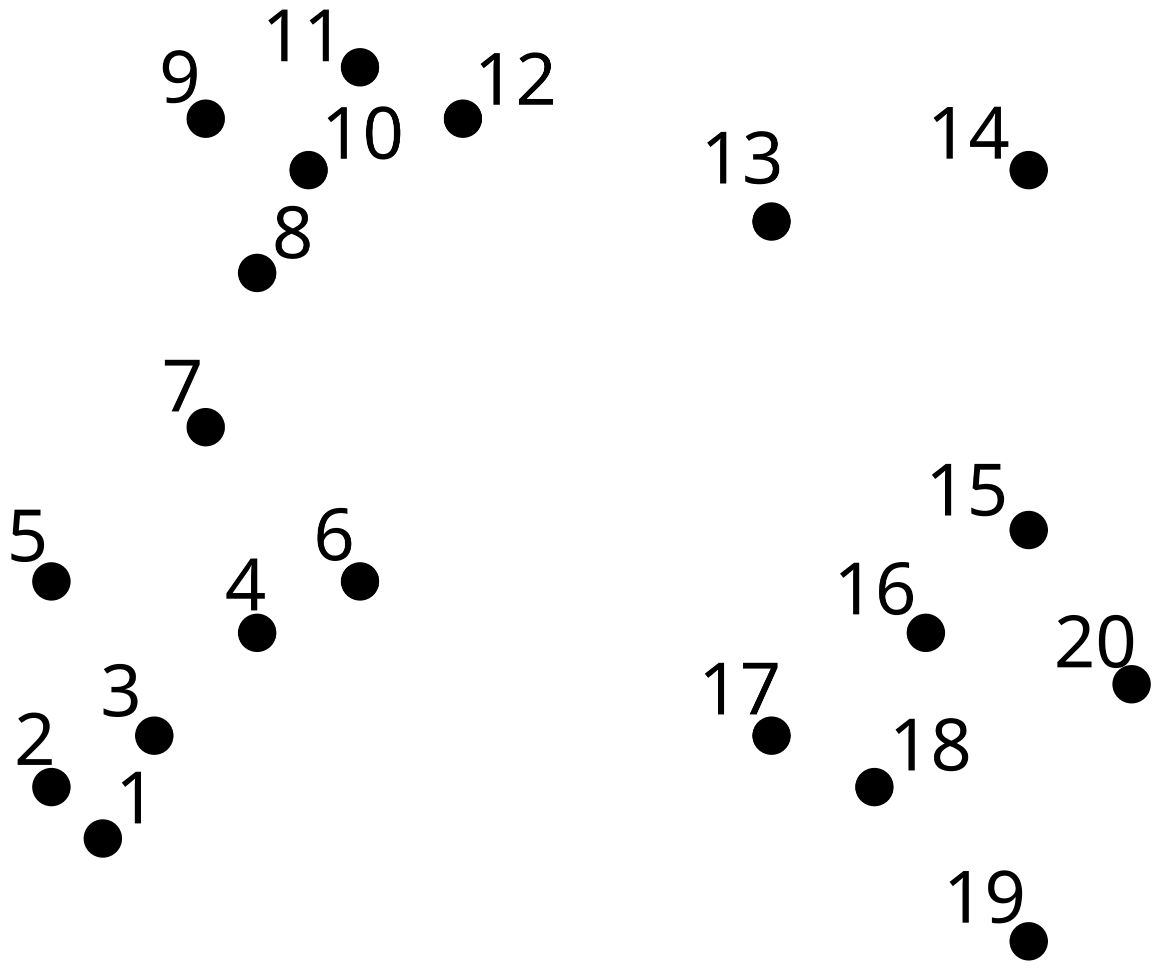


Question ($k = 3$)

Which set C of 3 points minimizes $\sum_{p \in P} d(p, C)$?



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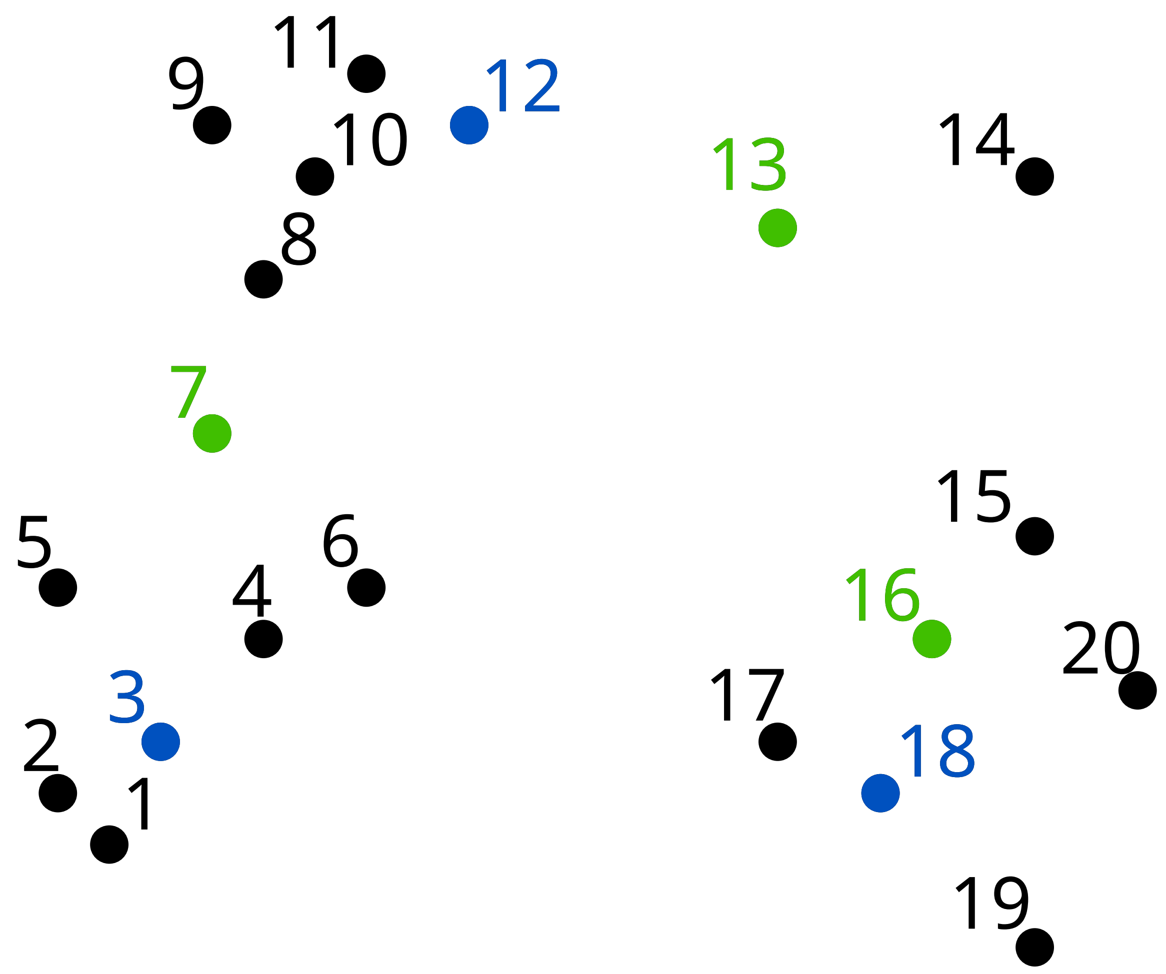

good? $\{3, 12, 18\}$, $\{7, 13, 16\}$

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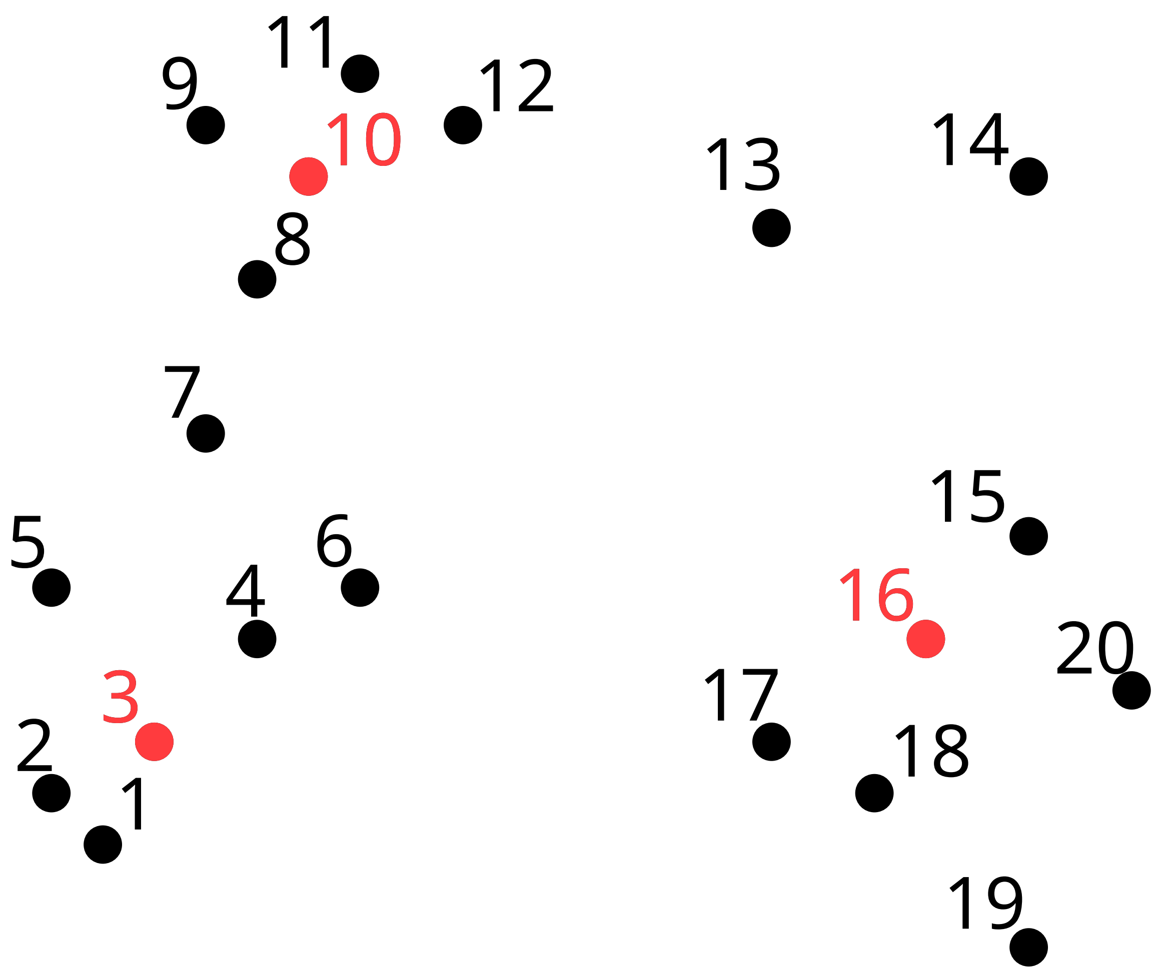

good? $\{3, 12, 18\}$, $\{7, 13, 16\}$

optimal: $\{3, 10, 16\}$

GreedyKCenter for k-median?

Use 2-approximation for k-center clustering (?) on n points

$$\max_{p \in P} d(p, C) \leq \sum_{p \in P} d(p, C) \leq \sum_{p \in P} \max_{p \in P} = n \cdot \max_{p \in P}$$

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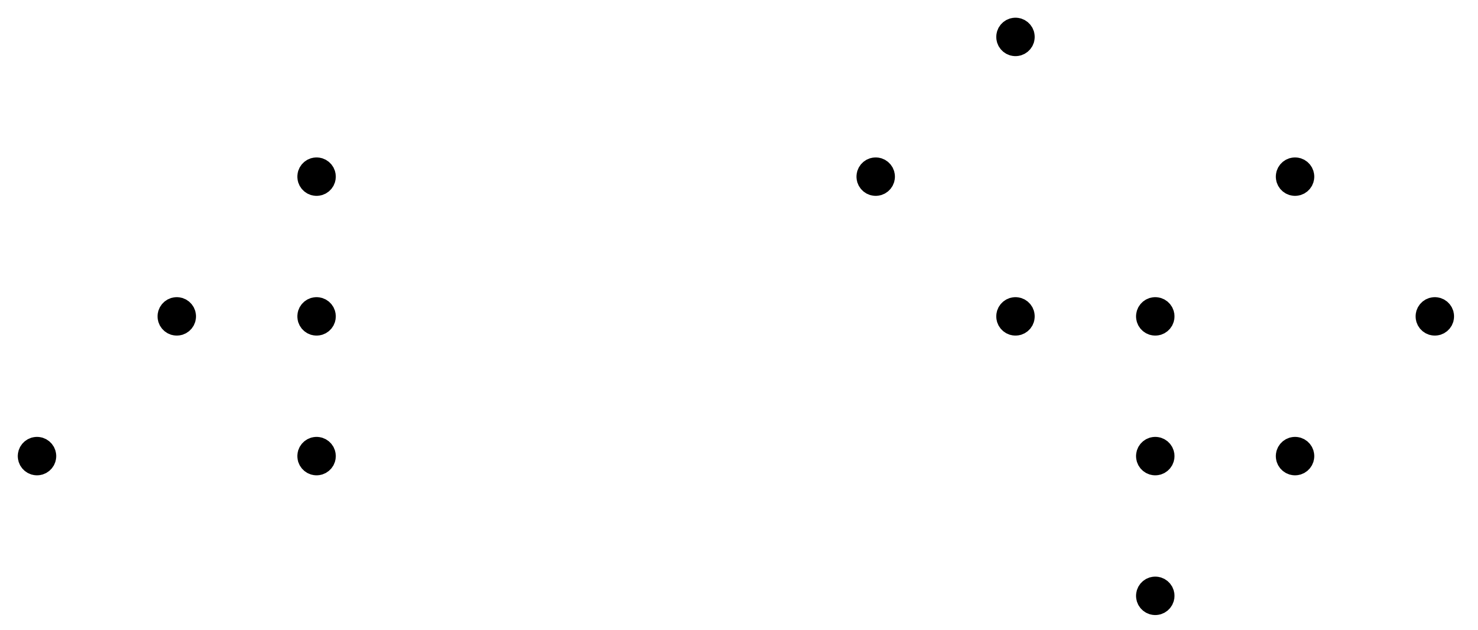
We can do better with local search!

LocalSearchKMedian(P, k)

```
C ← GreedyKCenter(P, k)
while ∃p ∈ P \ C, c ∈ C s.t. replacing c by p in C reduces ∑_{p∈P} d(p, C)
by factor 1 − τ:
    C ← C ∪ {p} \ {c}
return C
```



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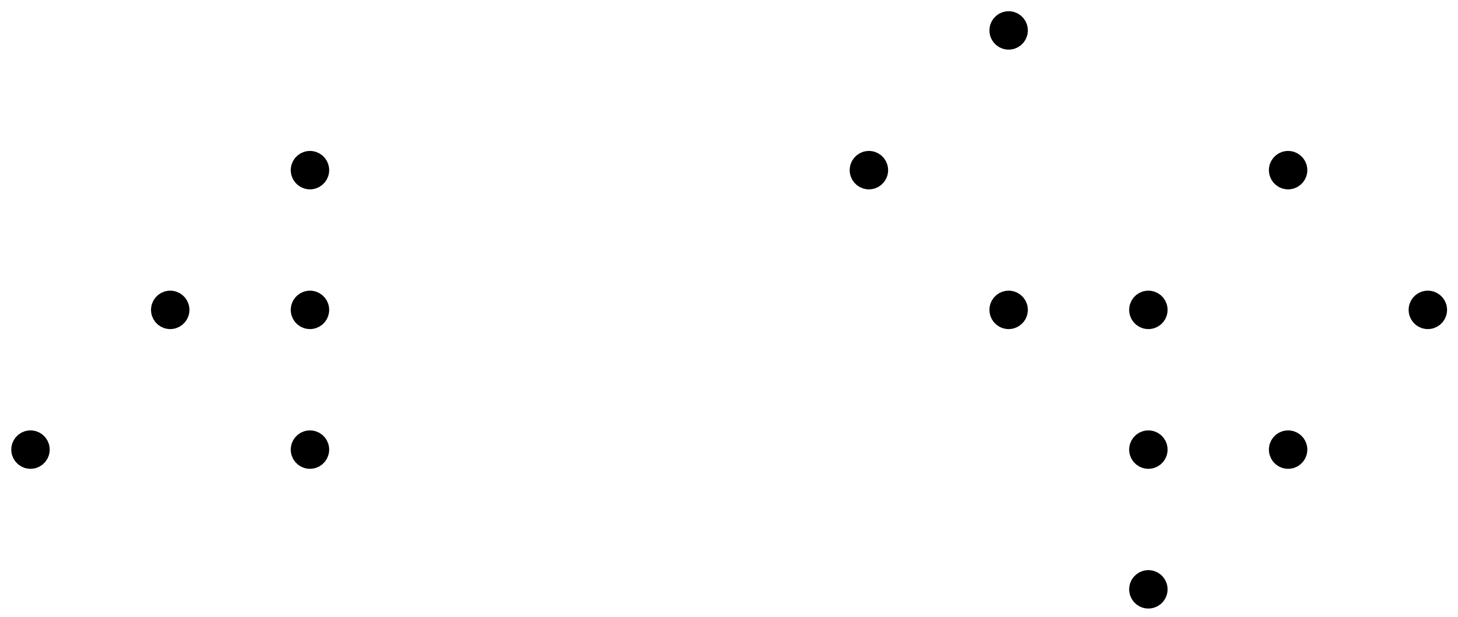
we choose τ later.



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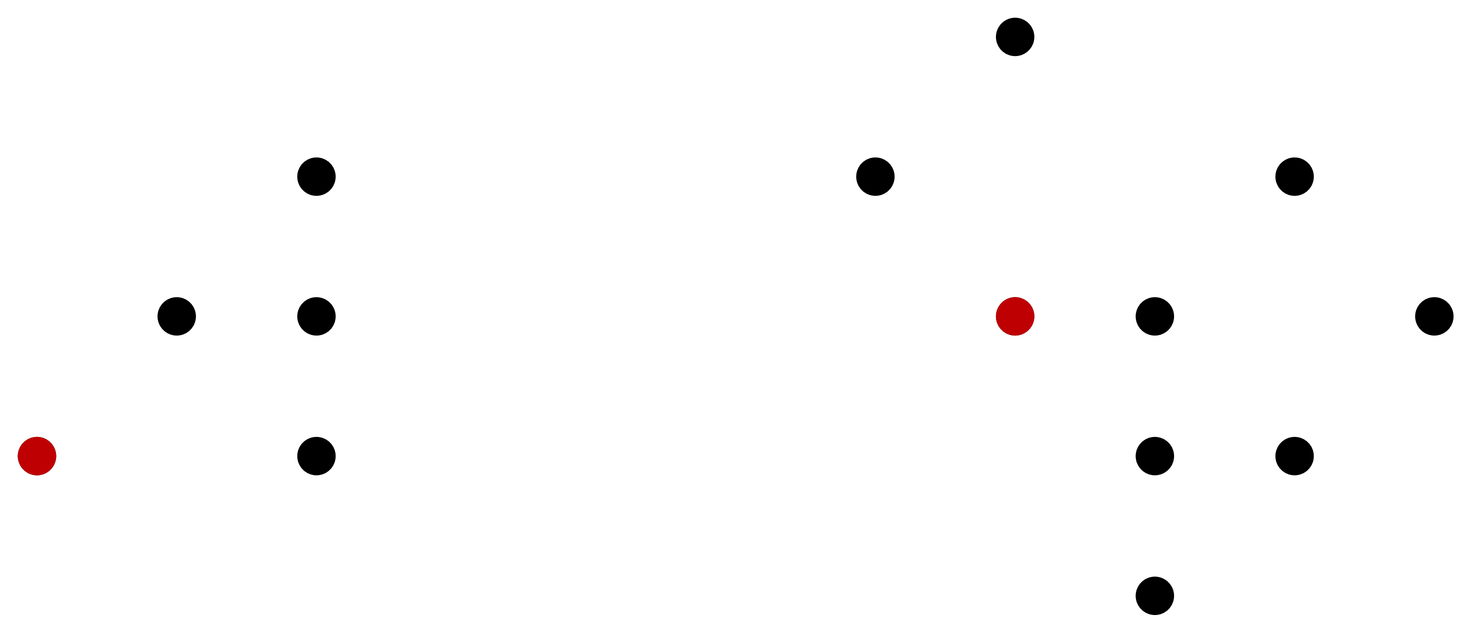

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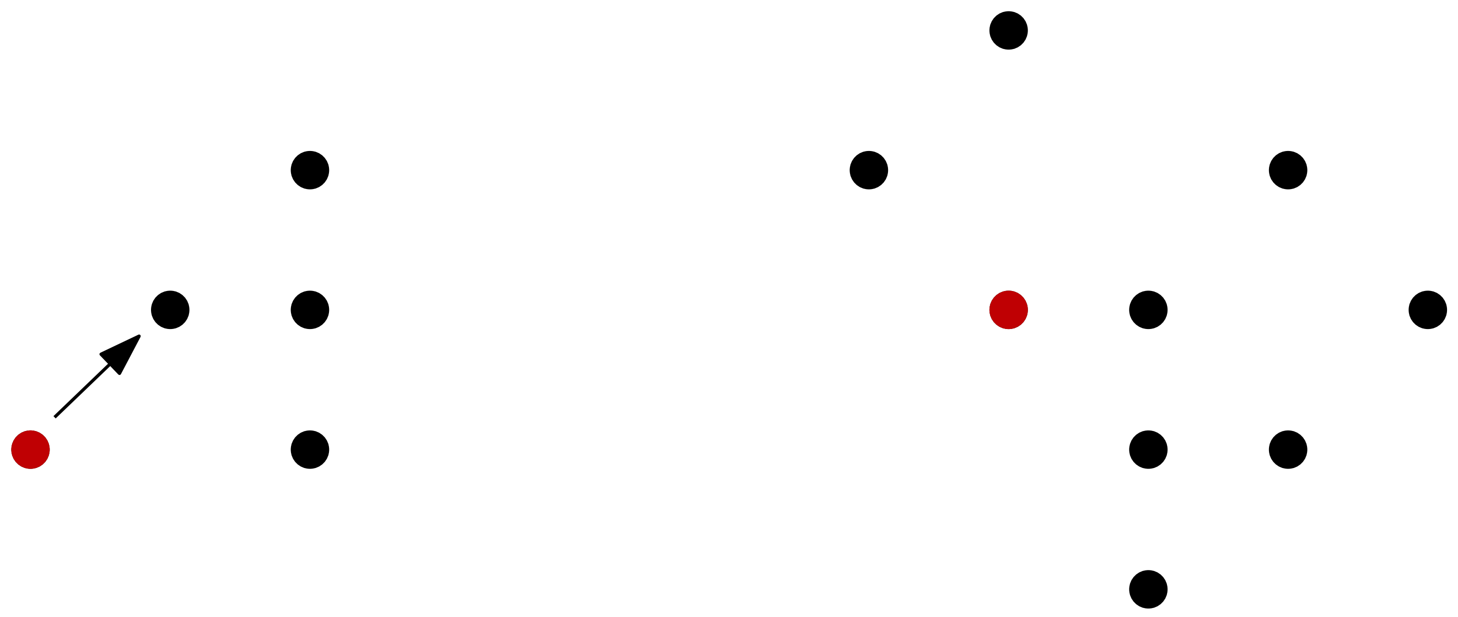

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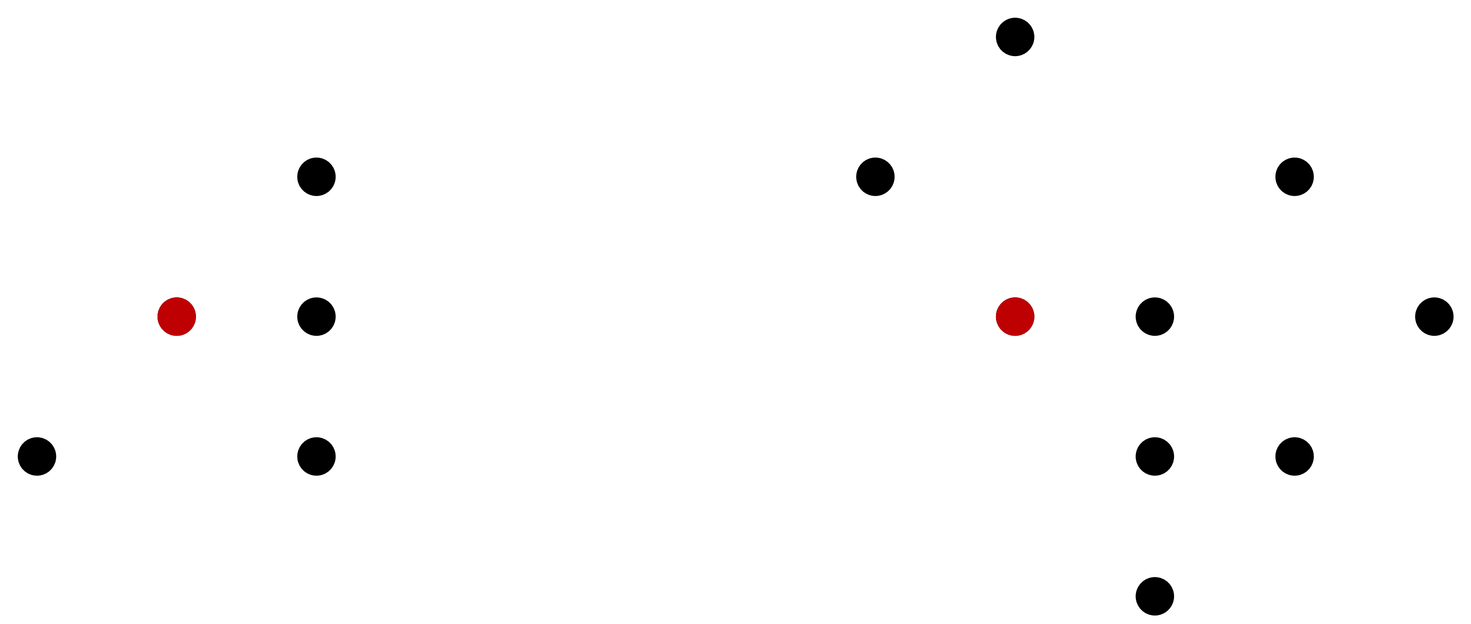

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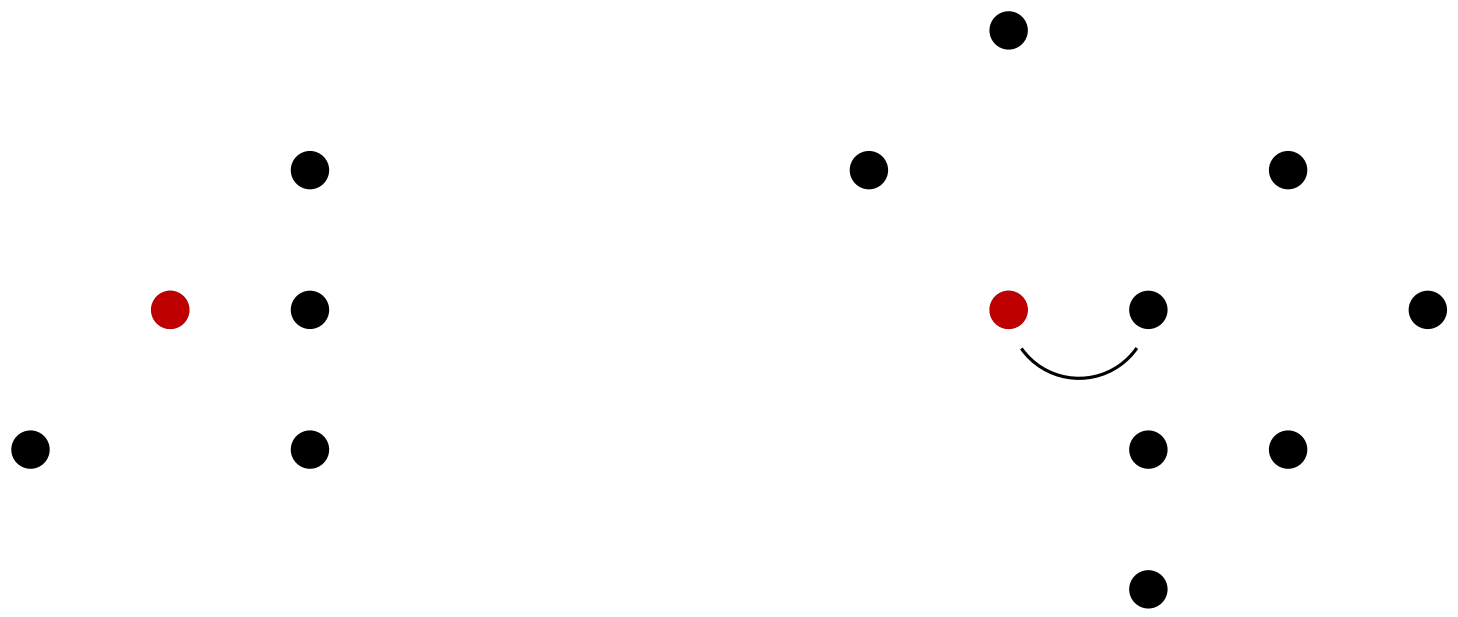

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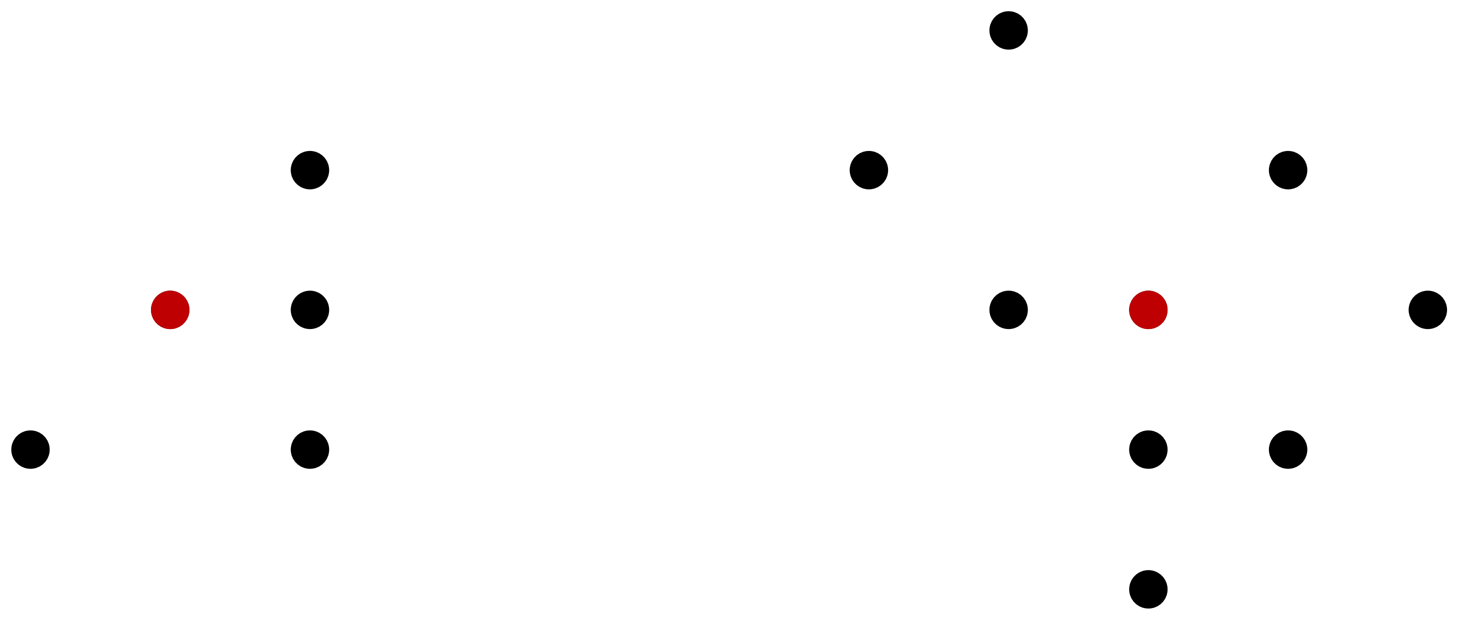

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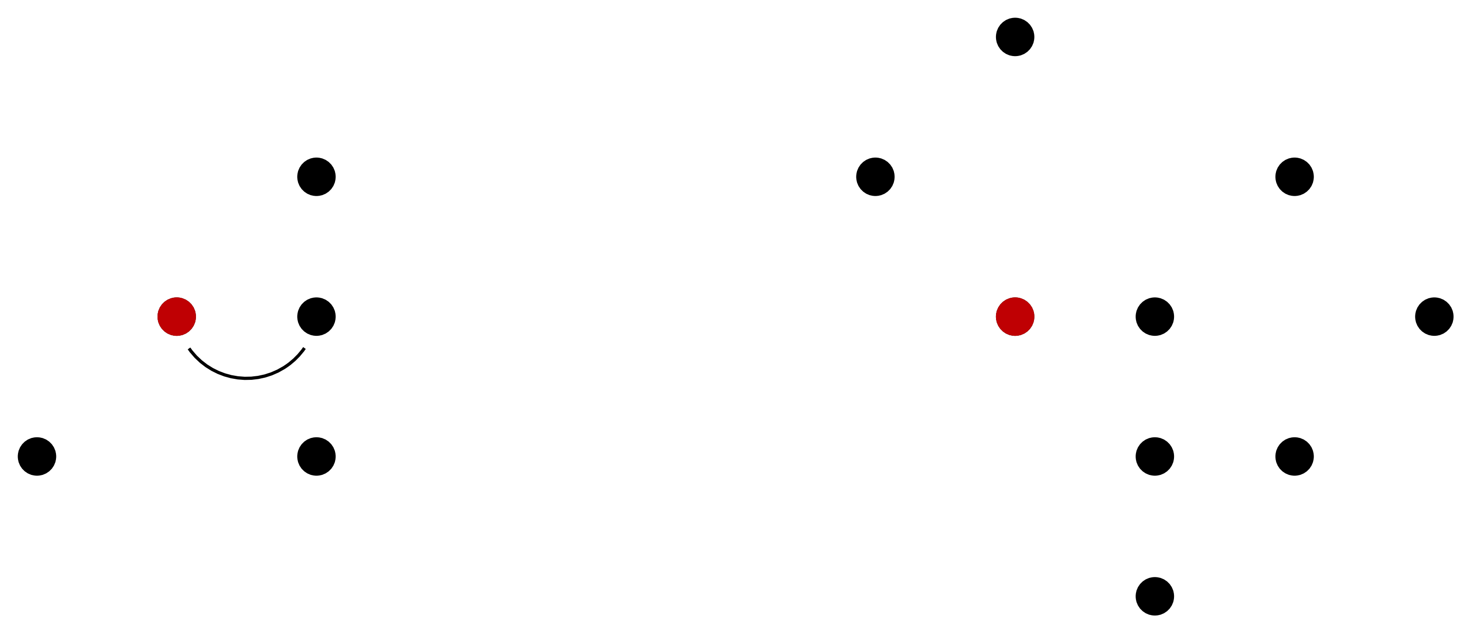

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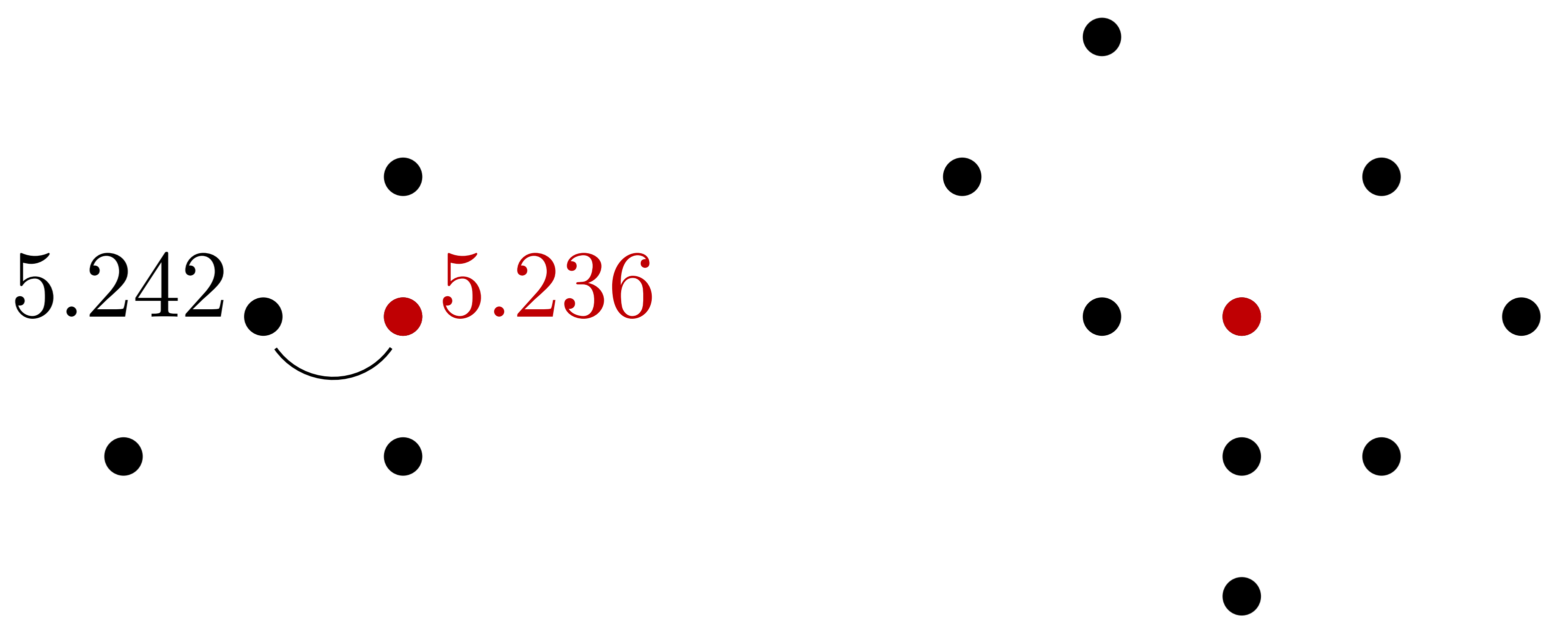

Running time

Try swapping every $p \in P \setminus c$ with every $c \in C$:

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time per iteration of **while**-loop: $O((nk)^2)$

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Can be simplified to $O(\frac{\log n}{\tau})$ [without proof but elementary maths]

Approximation factor

LocalSearchKMedian(P, k): $(5 + \varepsilon)$ - approximation for discrete k-median

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Warning: proof tedious (but fun (?) and insightful)

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I will sketch the core ideas

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I will show: if we replace until no improvement (aka: ignore τ),
we get 5-approximation

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C: computed centers, C^* opt. centers

$A_p := d(p, C)$, $O_p := d(p, C^*)$

$\gamma(p) =$ center of $p \in C$, $\gamma^*(p)$ same in C^*

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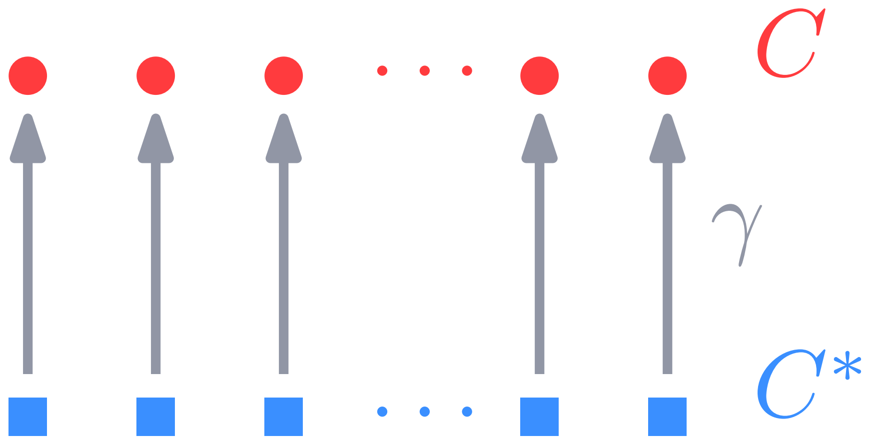

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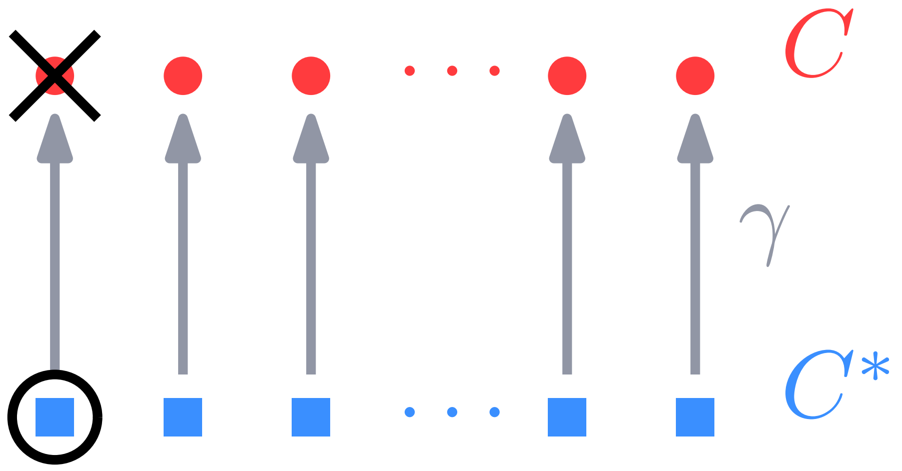

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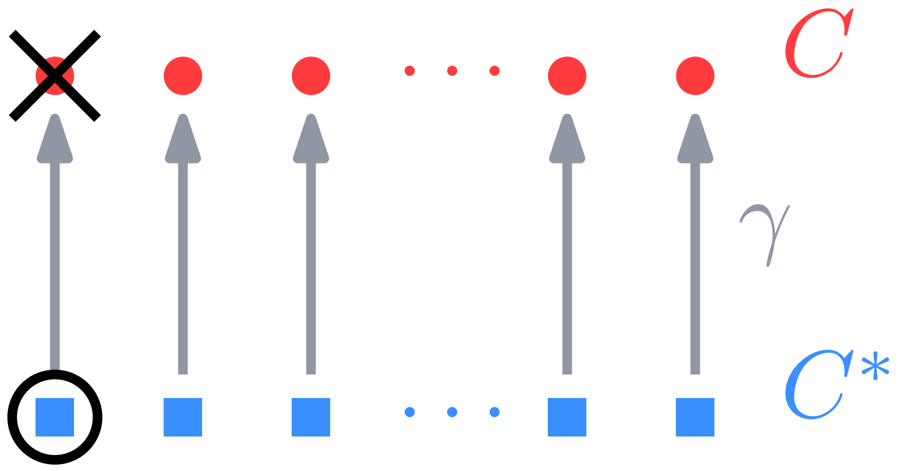

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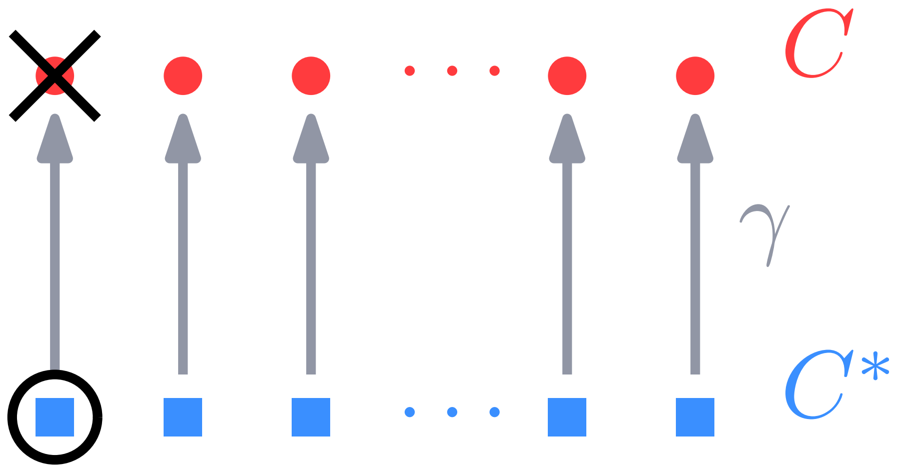

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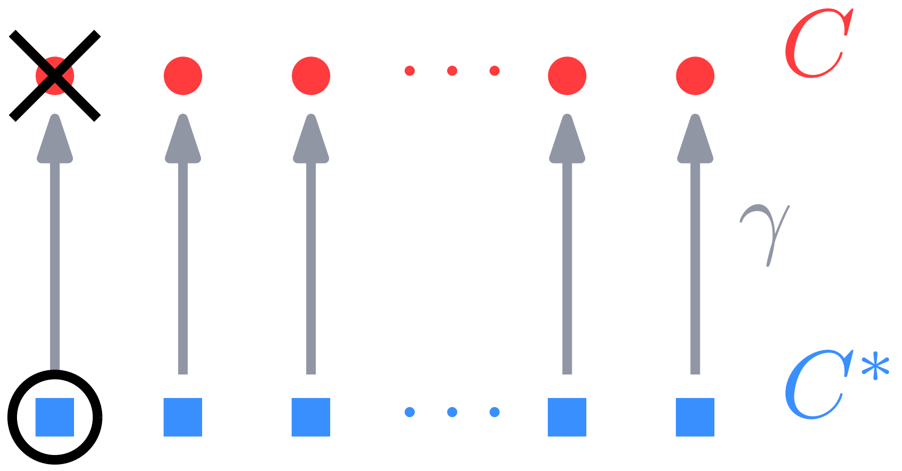

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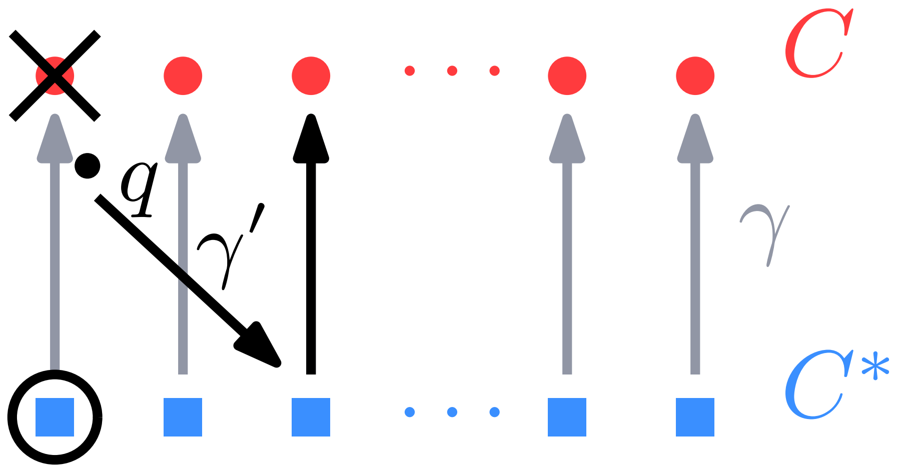

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$d(p, C') \leq$
$d(p, o) = O_p$

bound cost for $q \in N(\gamma(o)) \setminus N^*(o)$
by taking $d(q, \gamma(\gamma^*(q)))$

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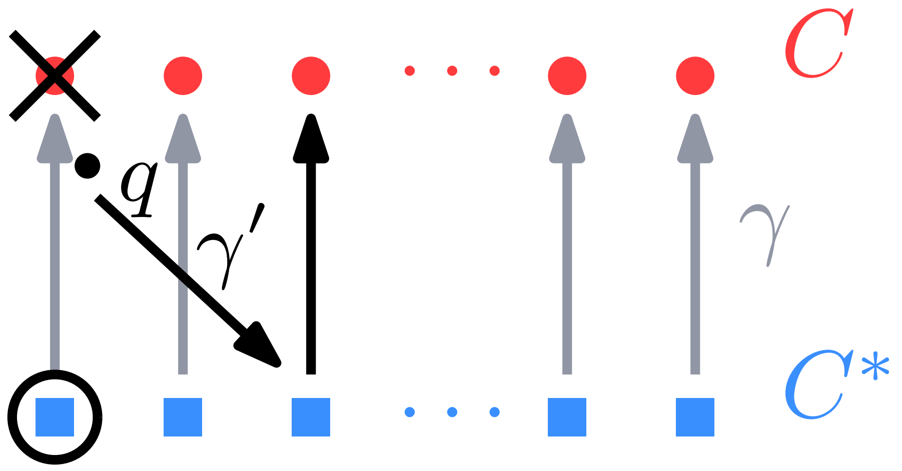

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by triangle ineq. (proof later): $\leq \sum_{q \in N(\gamma(o))} 2O_q$

By doing this for all $o \in C^*$ and summing: $\sum A_p \leq 3 \sum O_p$

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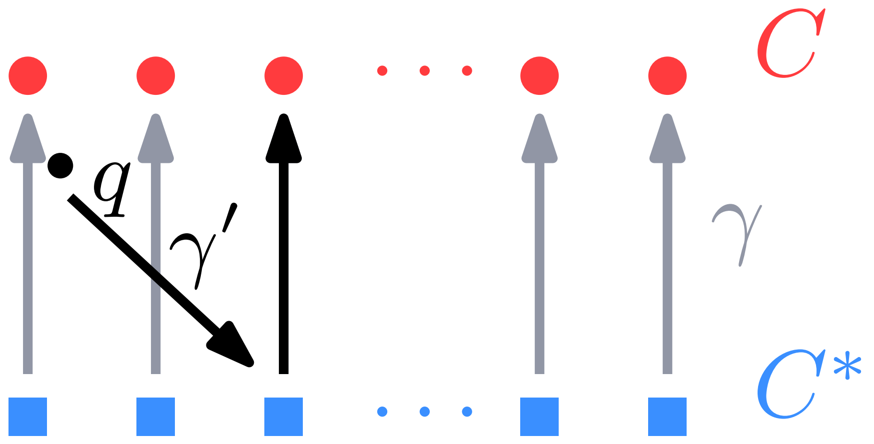

proof of $d(q, \gamma(\gamma^*(q))) - A_q \leq 2O_q$:

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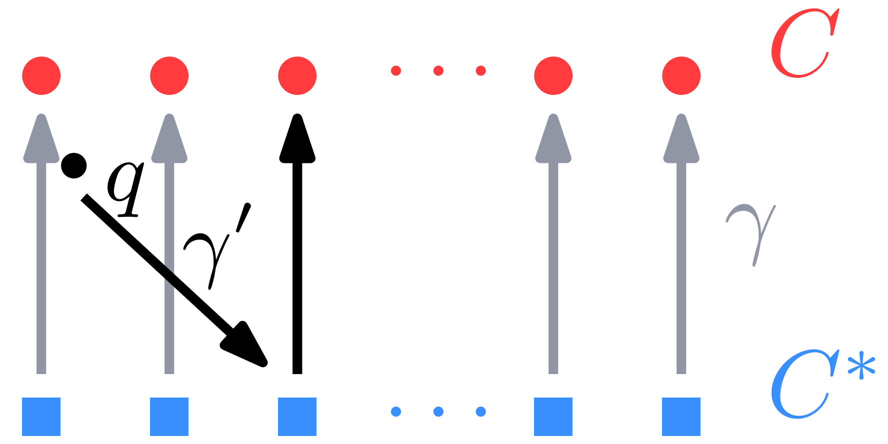

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$$d(q, \gamma(\gamma^*(q))) \leq d(q, \gamma^*(q)) + d(\gamma^*(q), \gamma(\gamma^*(q)))$$

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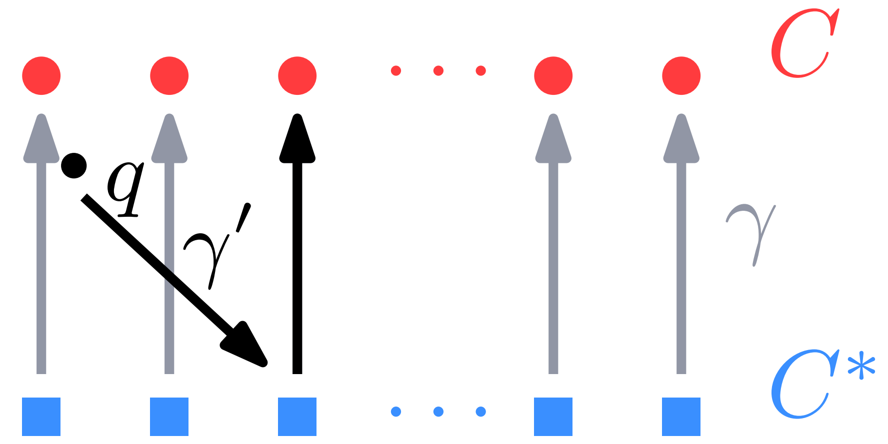

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$A_p := d(p, C)$, $O_p := d(p, C^*)$

$\gamma(p) =$ center of $p \in C$, $\gamma^*(p)$ same in C^*

$N(c)$: cluster of $c \in C$, $N^*(c^*)$ likewise

proof of $d(q, \gamma(\gamma^*(q))) - A_q \leq 2O_q$:

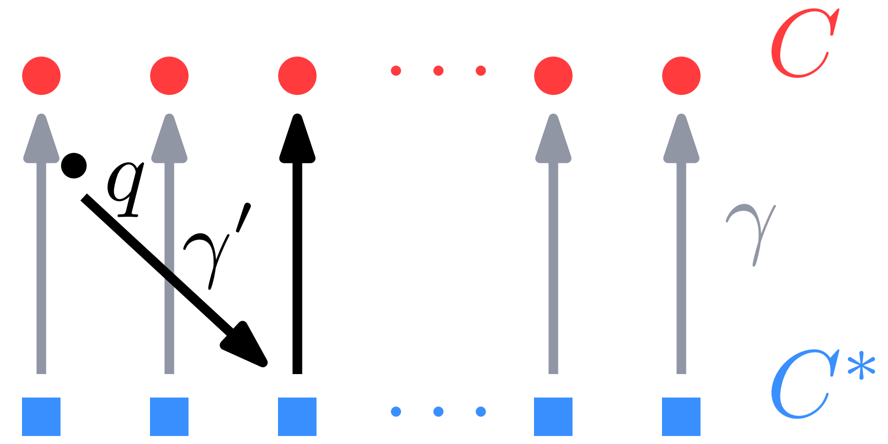
$$d(q, \gamma(\gamma^*(q))) \leq d(q, \gamma^*(q)) + d(\gamma^*(q), \gamma(\gamma^*(q)))$$
$$\leq O_q + d(\gamma^*(q), \gamma(\gamma^*(q)))$$

Approximation factor

LocalSearchKMedian(P, k): $(5+\varepsilon)$ - approximation for discrete k-median

simple case: for all $o, o' \in C^*$:

$o \neq o' \rightarrow \gamma(o) \neq \gamma(o')$



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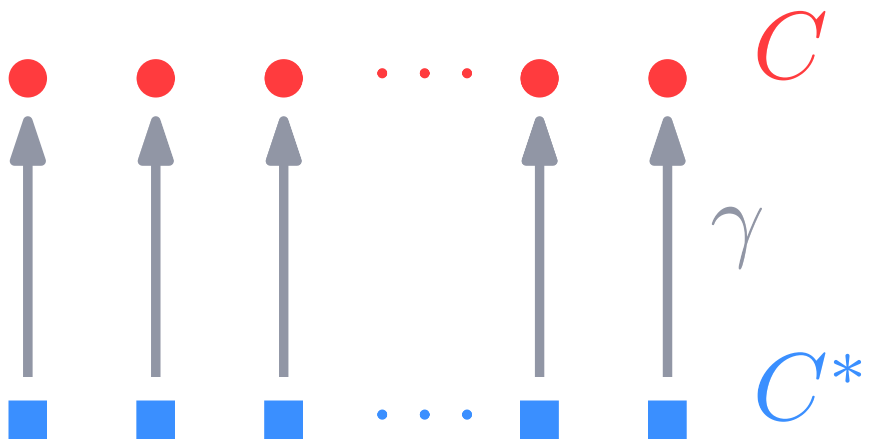
Approximation factor (general case)

so far



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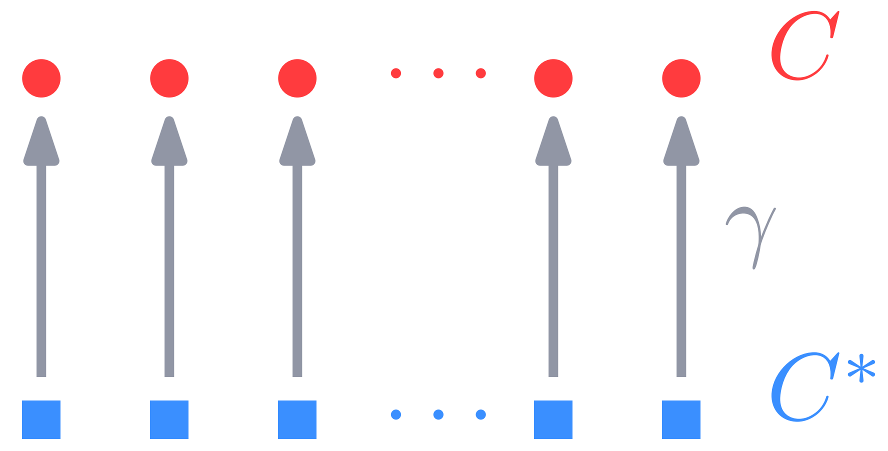
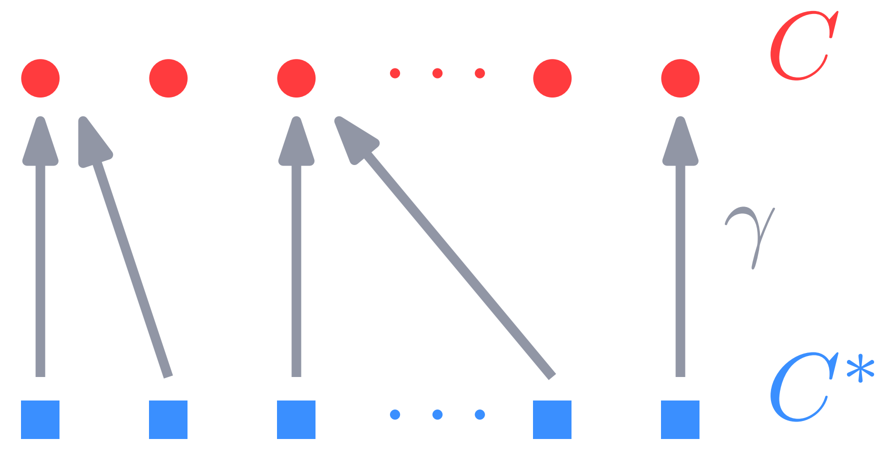


in general



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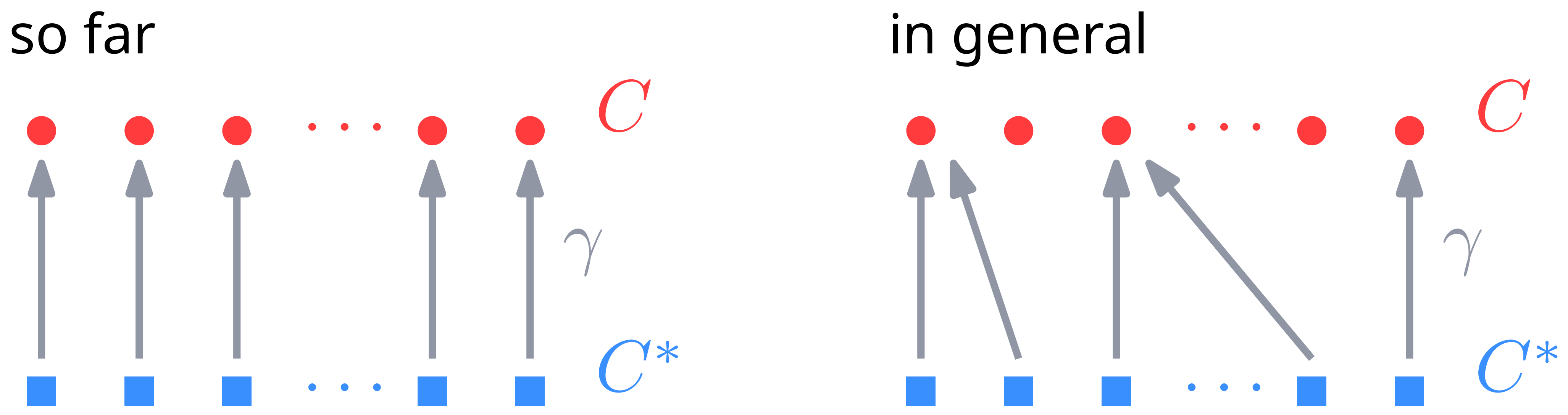

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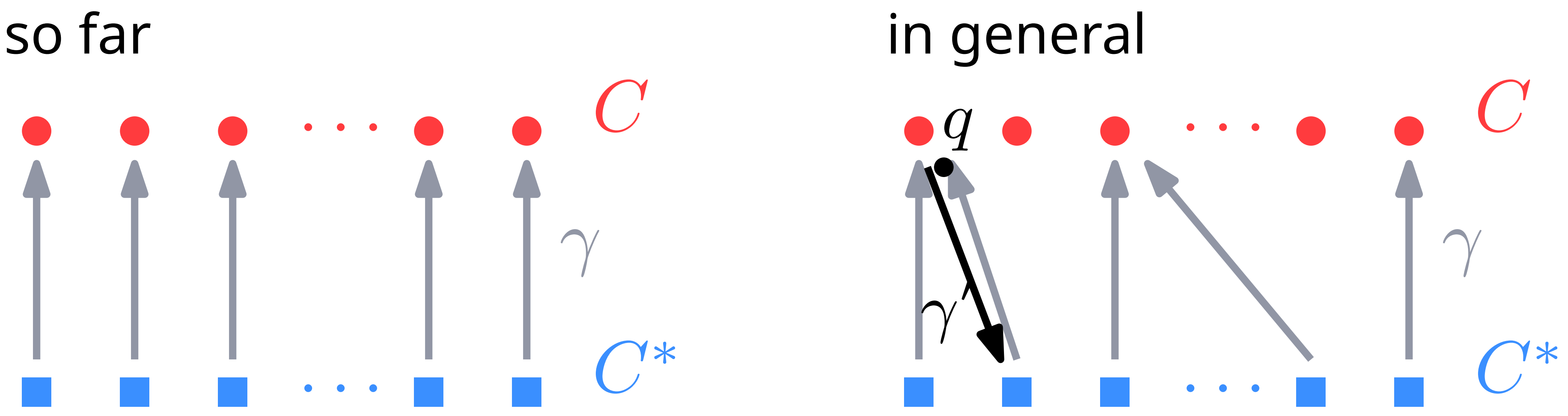
Approximation factor (general case)



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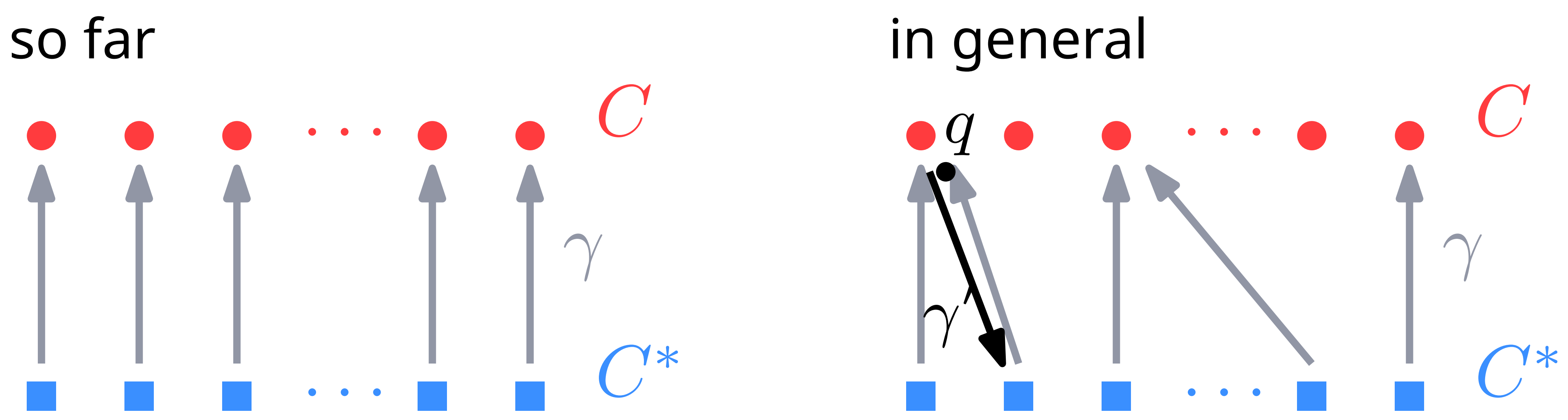

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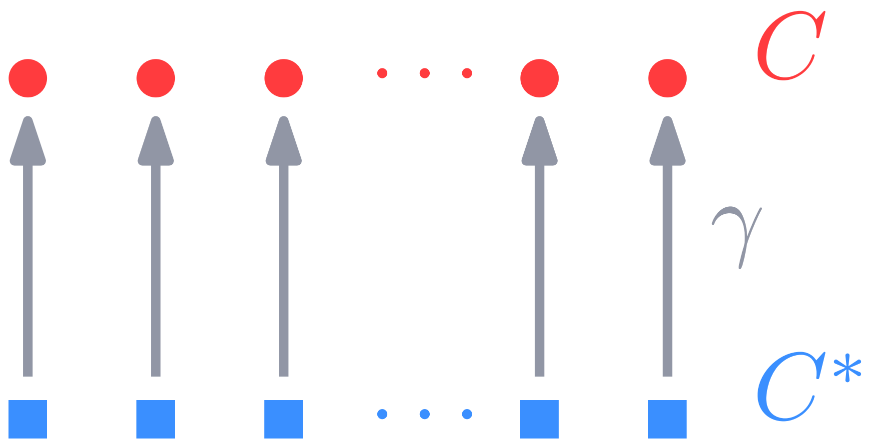

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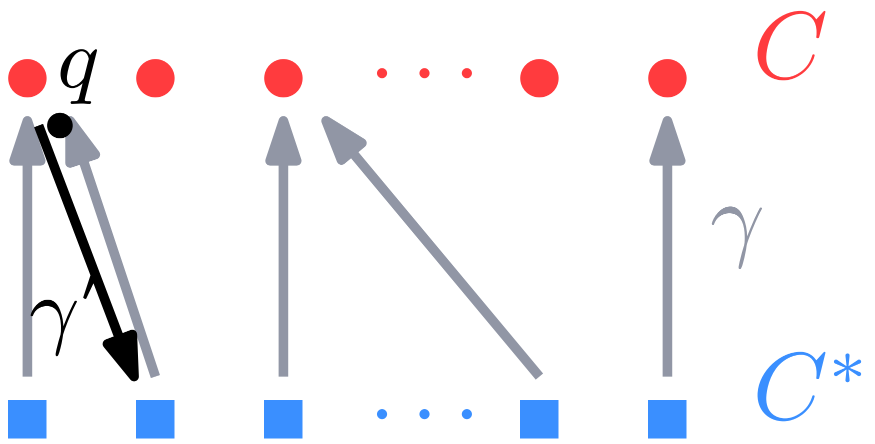

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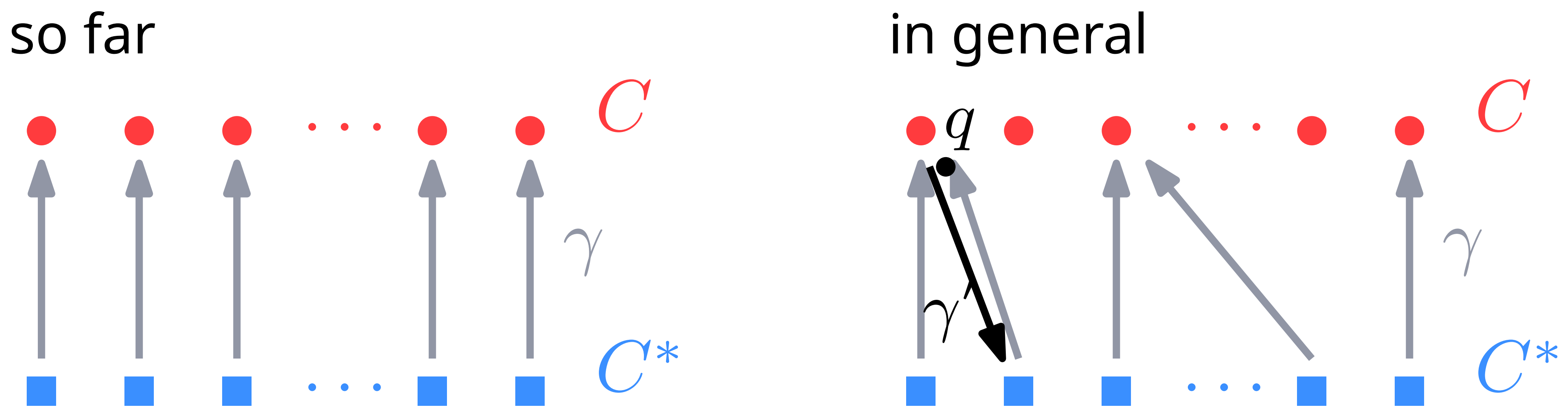

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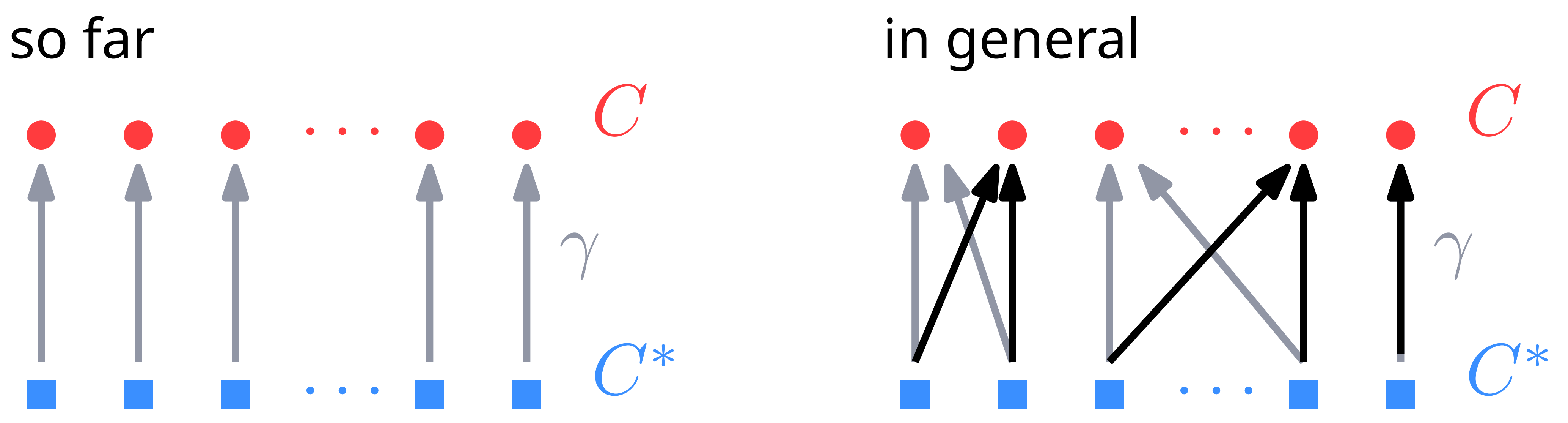

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Same argument works, but since we swap out each $c \in C$
up to 2 times, we get $\sum A_p \leq \sum O_p + 2 \cdot 2O_p$

summary + discrete k-means + open problems

k-center: 2-approximation by greedy algorithm

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in my research: geometric spaces beyond points, in particular, clustering curves