Lifting to paraboloids Clustering — k-center, k-median

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Computaional Geometry Summer semester 2020

• Lifting to paraboloids: Delaunay, Voronoi Edelsbrunner–Seidel (1986)

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- k-median, local search 1

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(x, y) $\in \gamma \Rightarrow$

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x^2 + y^2 = r^2 + 2xx_0 + 2yy_0 - x_0^2 - y_0^2
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 $L(\gamma) \subset H_{\gamma} := \{(x, y, z) \mid -\alpha_1 x - \alpha_2 y + z = c\}$

$$
DT(P) = \text{proj}_{z=0}(\text{conv}^{\downarrow}(L(P)))
$$

Lifting many paraboloids: Voronoi Opaque hanging paraboloid B_p for each $p \in P$.

$$
dist(q, p') = dist(q, p)
$$

$$
\Leftrightarrow
$$

$$
q^* \in B_p \cap B_q
$$

 B_{p} \overline{p} Lifting many paraboloids: Voronoi p^{\prime} $B_{p'}$ Opaque hanging paraboloid B_p for each $p \in P$. \overline{q} \overline{q} ∗ $dist(q, p') = dist(q, p)$ ⇔ $q^* \in B_p \cap B_q$ upper envelope of $\bigcup_{p\in P}B_p$ looks like $\mathsf{Vor}(P)$ from $(0,0,\infty)$ Apply $L(.)$: polyhedron B with face $L(B_p)$ touching A at $L(p)$. L does not change view from $(0, 0, \infty)$ $\textsf{Vor}(P) = \text{proj}_{z=0}(B) = \text{proj}_{z=0}$ $\sqrt{ }$ $\overline{ }$ \bigcap touchplane $_A(L(p))^\uparrow$ \setminus $\overline{}$

 $p\!\in\!F$

Paraboloid lifting works in \mathbb{R}^d .

 $\mathsf{Vor}(P)$ and $DT(P)$ are projections of convex hulls in $\mathbb{R}^{d+1}.$

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Clustering variants in metric spaces

Metric spaces and clustering

Definition. $(X, dist)$ metric space with distance dist : $X \times X \to \mathbb{R}_{\geq 0}$ iff $\forall a, b, c \in X$:

- dist $(a, b) = \text{dist}(b, a)$ (symmetric)
- dist $(a, b) = 0 \Leftrightarrow a = b$
- dist $(a, b) + \text{dist}(b, c) \geq \text{dist}(a, c)$ (triangle ineq.)

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Given $P \subseteq X$, find a set of k centers $C \subseteq X$ s.t.

$$
vec_C := \Big(\text{dist}(p_1, C), \text{dist}(p_2, C), \dots, \text{dist}(p_n, C)\Big)
$$

"small"

 \bullet *k*-center:

$$
\min_{C \subset X, |C| = k} ||vec_C||_{\infty} = \min_{C \subset X, |C| = k} \max_{p \in P} \text{dist}(p, C)
$$

"minimize the max distance to nearest center"

• k -center:

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"minimize sum of distances to nearest center"

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"minimize sum of distances to nearest center"

 \bullet k-means:

$$
\min_{C \subset X, |C|=k} \lVert vec_C \rVert_2 = \min_{C \subset X, |C|=k} \sqrt{\sum_{p \in P} \left(\text{dist}(p, C)\right)^2}
$$

"minimize sum of squared distances to nearest center"

• k -center:

min $C\subset \mathbf{X}, |C|=k$ $\|vecC|_{\infty} = \min_{\alpha = \text{tr}\, \alpha}$ $C\subset X, |C|=k$ max $p\!\in\!F$ $\mathrm{dist}(p,C)$ "minimize the max distance to nearest center" a.k.a. cover X with $C \subseteq P$: discrete imizing r \bullet *k*-median: "minimize the max distance to nearest center"

a.k.a. cover X with $C \subseteq P$: discrete imizing r

k-median:
 $\lim_{C \in \mathcal{F}_r |C| = k} ||veC \subseteq X$: continuous $\lim_{C \in \mathcal{F}_r |C| = k} ||veC \subseteq X$: continuous $\lim_{C \in \mathcal{F}_r |C| = k} ||veC \subseteq X$: contin $C \subseteq P$: discrete clustering

$$
C\substack{\text{min}\\ \substack{C \subset \mathbf{X}, |C| = k}} \|v\epsilon C \subseteq X: \text{ continuous} \qquad \text{list}(p, C)
$$

"minimize sum of distances to nearest center"

 \bullet k-means:

$$
\min_{\substack{C \subset \mathbf{X}, |C| = k}} \|vec{vec}_C\|_2 = \min_{\substack{C \subset X, |C| = k}} \sqrt{\sum_{p \in P} (\text{dist}(p, C))^2}
$$

Facility location

Opening a center at $x \in X$ has cost $\gamma(x)$. Total cost is

$$
\sum_{x \in C} \gamma(x) + \|vec{v} \, e^c \, c\|_1
$$

"Hip" topic.

Scholar "k-means" Scholar "traveling salesman" About 1.300.000 results (0,15 sec) About 149.000 results (0,09 sec)

k -center via greedy

Theorem (Feder–Greene 1988). There is no polynomial time 1.8-approximation for *k*-center in \mathbb{R}^2 , unless $P = NP$.

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Reduction from planar vertex cover of max degree 3

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Reduction from planar vertex cover of max degree 3

Double subdivision:

Makes equivalent instance of VC with $k \to k+1$.

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Reduction from planar vertex cover of max degree 3

Double subdivision:

Subdivide, get length 2 edges and "smooth" turns only:

Hardness of k -center: disk radii

 $P :=$ edge midpoints of smooth drawing of G'

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Otherwise needs > 1 disk covering 2 non-neighbors u, v $dist(u, v) \geq 2 \cdot 1.8$ \Rightarrow $r \geq 1.8$

Greedy centers

Given $C \subseteq P$, the greedy next center is $q \in P$ where $dist(q, C)$ is maximized.

Greedy clustering: start with arbitrary $c_1 \in P$. For $i=2,\ldots,k$: Let $c_i = \textsf{GreedyNext}(c_1, \ldots, c_{i-1}).$ Return $\{c_1, \ldots, c_k\}$

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Let $r_i = \max_{p \in P} \text{dist}(p, \{c_1, \ldots, c_i\}).$ Balls of radius r_i with centers $\{c_1,\ldots,c_i\}$ cover P for any i . $\Rightarrow r_k, \{c_1, \ldots, c_k\}$ is valid k -center

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Store most distant center and update in each step \Rightarrow $O(nk)$ time

Theorem. Greedy k -center gives a 2-approximation.
Proof

 $r_1 \geq r_2 \geq \cdots \geq r_k$

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 $c_{k+1} :=$ point realizing r_k

If $i < j \leq k+1$, then

 $\mathop\mathrm{dist}(c_i, c_j) \geq \mathop\mathrm{dist}(c_j, \{c_1, \ldots, c_{j-1}\}) = r_{j-1} \geq r_k$

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 $r_{opt} :=$ is optimal k -cover radius, suppose $2r_{opt} < r_k$ each ball in opt has ≤ 1 pt from c_1, \ldots, c_{k+1}

r -packing from greedy

Definition. $S \subset X$ is an r-packing if

- *r*-balls cover $X: dist(x, S) \leq r$ for each $x \in X$
- S is sparse: $\mathop\mathrm{dist}(s,s') \geq r$ for each $s,s' \in S$

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Theorem. For any i , $\{c_1, \ldots, c_i\}$ is an r_i -packing.

Exact k -center in \mathbb{R}^d , approximating k Trivial: $O(n^{k+1})$

Exact *k*-center in
$$
\mathbb{R}^d
$$
, approximating *k*

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\n
$$
\mathbb{R}^2
$$
\n
$$
n^{O(\sqrt{k})}
$$
\nor $2^{O(\sqrt{n})}$

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\nno $n^{o(k)}$ known

\n
$$
2^{O(n^{1-1/d})}
$$

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Exact k -center in \mathbb{R}^d , approximating k $n^{O(}$ √ $k)$ Trivial: $O(n^{k+1})$ $\overline{\mathbb{R}^2}$ or $2^{O(\lambda)}$ √ $\overline{n})$ no $n^{o(k)}$ known \quad 2 $O(n^{1-1/d})$ "optimal" $d^d, d = \mathrm{const.}$

Fix r , approximate k instead: poly $(1 + \varepsilon)$ -approximation for any fixed d, ε (PTAS)

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 $\frac{1}{2}$ poly $(1 + \varepsilon)$ -approximation for any fixed d, ε (PTAS)

 $O(n^{1-1/d})$

Later lectures!

no $n^{o(k)}$ known \quad 2

k -median

k -median via local search

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• Compute $C = \{c_1, \ldots, c_k\}$ and $r_k : k$ -center 2-approx. Gives $2n$ -approx for k-median as

 $\|vecC\|_1 \leq n\|vecCC}\|_{\infty}$

so $\text{OPT}(k\text{-med}) \leq n\text{OPT}(k\text{-cent}) \leq 2nr_k$

• Iteratively replace $c \in C$ with c' if it improves $\|vec_C\|_1$ (by at least factor $1 - \tau$, $\tau = \frac{1}{10}$ $\frac{1}{10k}$ \Rightarrow Results in local opt center set L

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Running time: $O(nk)$ possible swaps, $O(nk)$ to compute new distances. At most $\log_{\frac{1}{2}}$ $1-\tau$ $2n$ swaps.

$$
O((nk)^{2} \log_{\frac{1}{1-\tau}} 2n) = O((nk)^{2} \log_{1+\tau} n)
$$

=
$$
O((nk)^{2} \cdot 10k \log n) = O(k^{3} n^{2} \log n)
$$

 k -median: quality of approximation

Theorem. The local optimum L gives a 5-approximation for k -median.

Challange: L and OPT may be very different. Idea: use "intermediate" clustering Π to relate them

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assign cluster of center $o \in OPT$ to $nn(o, L)$

 k -median: quality of approximation

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Cost of moving from L to Π $\Pi(p), L(p), OPT(p)$ be the center (= nearest neighbor) of p in each clustering.

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 $-\|vec\|_1 \leq 2\|vec{vec}_{OPT}\|_1.$

 $dist(p, \Pi(p)) \leq dist(p, OPT(p)) + dist(OPT(p), \Pi(p))$ \leq dist $(p, OPT(p)) +$ dist $(OPT(p), L(p))$ \leq dist $(p, OPT(p)) +$ dist $(OPT(p), p)$ $+\operatorname{dist}(p, L(p))$ **Claim.** $||vec{p} - ||vec{p}||_1 \le 2||vec{p} - \frac{1}{2}||\frac{1}{2}||\frac{1}{2}||\frac{1}{2}||\frac{1}{2}||\frac{1}{2}||\frac{1}{2}||\frac{1}{2}||\frac{1}{2}||\frac{1}{2}||\frac{1}{2}||\frac{1}{2}||\frac{1}{2}||\frac{1}{2}||\frac{1}{2}||\frac{1}{2}||\frac{1}{2}||\frac{1}{2}||\frac{1}{2}||\frac{1}{2}||\frac{1}{2}||\frac{1}{2}||\frac{1}{2}||\frac{$

Cost of moving from L to Π $\Pi(p), L(p), OPT(p)$ be the center (= nearest neighbor) of p in each clustering.

Claim. $||vec_{1} - ||vec_{L}||_1 \le 2||vec_{OPT}||_1$.

 $dist(p, \Pi(p)) \leq dist(p, OPT(p)) + dist(OPT(p), \Pi(p))$ \langle dist(p, OPT(p)) + dist(OPT(p), $L(p)$) \leq dist(p, OPT(p)) + dist(OPT(p), p) $+\operatorname{dist}(p, L(p))$ $= 2 \text{dist}(p, OPT(p)) + \text{dist}(p, L(p))$ For $c \in L$, the cost of reassigning its cluster to Π is $ran(c) := \sum_{p \in Cl(L,c) \setminus Cl(\Pi,c)}$ $\Big(\text{dist}(p,\Pi(p))-\text{dist}(p,L(p))\Big)$ $\textsf{claim} \Rightarrow \sum_{c \in L} \textit{ran}(c) \leq 2\|\textit{vec}_{OPT}\|_1$

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Lemma. For $c \in L_0$ and $o \in OPT$ we have $localcost(o) \leq ran(c) + cost(o).$

Proof. Removing c and adding o to L does not improve:

$$
0 \leq ran(c) - localcost(o) + cost(o).
$$

Bounding the contribution of $OPT_{\geq 2}$ Since $|L_1| = |OPT_1|$ (mathcing) and $|L_0| + |L_1| + |L_{\geq 2}| = |OPT_1| + |OPT_{\geq 2}| = k$

$$
|L_0| = |OPT_{\geq 2}| - |L_{\geq 2}| \geq |OPT_{\geq 2}|/2
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Bounding the contribution of $OPT_{>2}$ Since $|L_1| = |OPT_1|$ (mathcing) and $|L_0| + |L_1| + |L_{\geq 2}| = |OPT_1| + |OPT_{\geq 2}| = k$

$$
|L_0| = |OPT_{\geq 2}| - |L_{\geq 2}| \geq |OPT_{\geq 2}|/2
$$

Proof. Let $c^* \in L_0$ minimize $ran(c)$. Earlier lemma: $local cost(o) \leq ran(c^*) + cost(o)$ Summing over $o \in OPT_{\geq 2}$:

 \sum $o \in OPT_{\geq 2}$ $local cost(o) \leq |OPT_{\geq 2}|ran(c^*) + \sum$ $o \in OPT_{\geq 2}$ $cost(o)$

Bounding the contribution of OPT_1

Lemma. \sum localcost(o) \leq \sum $o \in OPT_1$ $o \in OPT_1$ $ran(L(o)) + \sum$ $o \in OPT_1$ $cost(o)$

Bounding the contribution of OPT_1

Proof. $o \in OPT_1$ is assigned to $L(o) = \Pi(o)$. Claim: $localcost(o) \leq ran(L(o)) + cost(o)$. Replacing $L(o)$ with o in L doesn't improve.

Potential increased prices in $Cl(L, L(o)) \cup Cl(OPT, o)$. Replace cost in $\sqrt{ }$ $Cl(L, L(o)) \setminus Cl(OPT, o)$ \setminus is $ran(L(o))$. Replace cost in $Cl(OPT, o)$ is $\leq -local cost(o) + cost(o)$. $\Rightarrow 0 \leq ran(L(o)) - localcost(o) + cost(o).$
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$$
||vec_{L1}| = \sum_{o \in OPT_1} localcost(o) + \sum_{o \in OPT_{\geq 2}} localcost(o)
$$

\n
$$
\leq \sum_{c \in L_0} ran(c) + \sum_{o \in OPT_{\geq 2}} cost(o)
$$

\n
$$
+ \sum_{o \in OPT_1} ran(L(o)) + \sum_{o \in OPT_1} cost(o)
$$

\n
$$
\leq 2 \sum_{c \in L} ran(c) + \sum_{o \in OPT} cost(o)
$$

\n
$$
\leq 4||vec_{CPT}||_1 + ||vec_{CPT}||_1
$$

k -median, k -means with local search

Theorem. For any $\varepsilon > 0$ the local optimum L wrp. 1 – τ -improvements ($\tau := \varepsilon/10k$) gives a $5 + \varepsilon$ -approximation for *k*-median in $O(n^2k^3 \frac{\log n}{\varepsilon})$ $\frac{g\,n}{\varepsilon})$ time.

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 \rightarrow Can get $3 + 2/p$ -approx with p-swaps (tight)

k -median, k -means with local search

Theorem. For any $\varepsilon > 0$ the local optimum L wrp. 1 – τ -improvements ($\tau := \varepsilon/10k$) gives a $5 + \varepsilon$ -approximation for *k*-median in $O(n^2k^3 \frac{\log n}{\varepsilon})$ $\frac{g\,n}{\varepsilon})$ time.

 \rightarrow Can get $3 + 2/p$ -approx with p-swaps (tight)

Theorem. For any $\varepsilon > 0$ local search gives a $25+\varepsilon$ -approximation for k-means in $O(n^2k^3\frac{\log n}{\varepsilon})$ $\frac{g\,n}{\varepsilon})$ time.

$$
\rightarrow
$$
 Can get $(3 + 2/p)^2$ -approx with p-swaps (tight)

k -median, k -means in \mathbb{R}^d

k -median, k -means in \mathbb{R}^d

k-median is NP-hard if k, d both in input. (Guruswami–Indyk 2003), but if at least one is cosntant, there is a PTAS.

For k-means with constant d , local search with $(1/\varepsilon)^{\Theta(1)}$ -swaps gives PTAS. (e.g. Cohen-Addad et al. 2019)

Next week: SoCG 2020! Check it out.