Fast Algorithms for a New Relaxation of OT

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“Non-Locality” of Geometric Problems makes them difficult.

Input:

- Specify two sets of vectors: $\{x_1, \dots, x_n\}, \{y_1, \dots, y_n\} \subset \mathbb{R}^d$
- “High-dimensional regime:” $\Omega(\log n) \leq d \leq n^{o(1)}$

Closest Pair	Chamfer (Sum of NNs)	EMD (min-cost matching)
$\min_{i,j \in [n]} \|x_i - y_j\|_2$	$\min \sum_{i=1}^{n} \min_{j \in [n]} \|x_i - y_j\|_2$	$\min_{\pi} \sum_{i=1}^{n} \|x_i - y_{\pi(i)}\|_2$

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$$\gamma \geq 0$$

$$\min \sum_{i=1}^{n} \sum_{j=1}^{n} \gamma_{ij} \|x_i - y_j\|_2$$

Closest Pair	Chamfer (Sum of NNs)	EMD (min-cost matching)
$\sum_{i,j} \gamma_{ij} = 1$	$\forall i : \sum_j \gamma_{ij} = 1$	$\forall i : \sum_j \gamma_{ij} = 1$ $\forall j : \sum_i \gamma_{ij} = 1$

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Closest Pair

$$\sum_{i,j} \gamma_{ij} = 1$$

Hard

Chamfer

(Sum of NNs)

$$\forall i : \sum_{j} \gamma_{ij} = 1$$

Hard and Easy

BIJSW'23

EMD

(min-cost matching)

$$\forall i : \sum_{j} \gamma_{ij} = 1$$

$$\forall j : \sum_{i} \gamma_{ij} = 1$$

Hard and ?

R'19

Talk Outline:

- “Spanner approach”
- Sinkhorn distances
- Main Result

The "Spanner Approach"

Theorem [Har-Peled, Indyk, Sidiropolous'13]:

c-approximate spanners in time $n^{1+O(1/c^2)}$

$$d_G(x,z) \overset{c}{\approx} \|x-z\|_2 \qquad \forall x,z \in X$$

Geometric Spanners ⟷ Approximate Nearest Neighbors

Time complexity $\approx$ $\tilde{O}(1)\,(n \cdot T(n) + S(n))$

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Conceptual Challenge:
"Accurate" approximations essentially take quadratic time.

Optimal transport,
Euclidean MST,
Closest Pair, …

except for kernel density estimation.

EMD ⟷ Sinkhorn

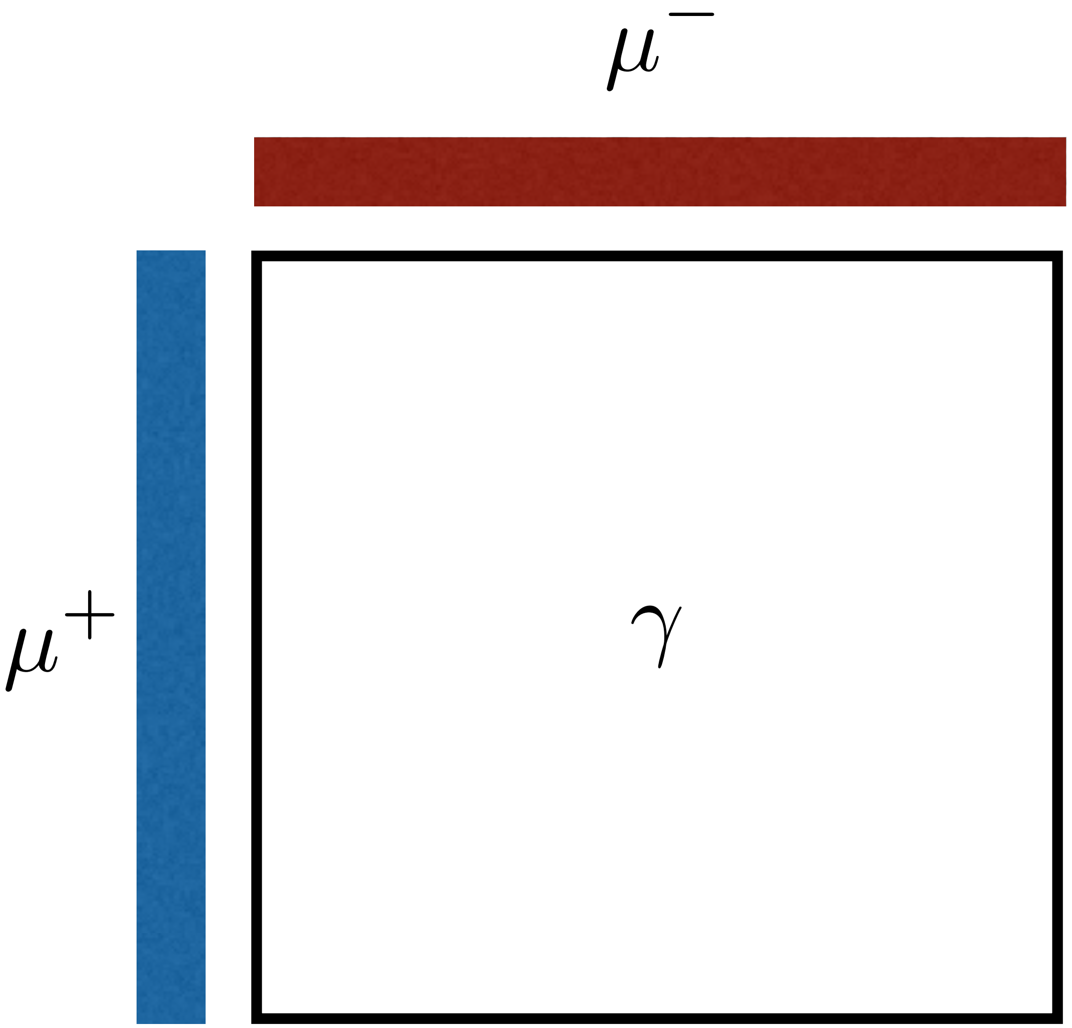
Fast algorithm
crude approx

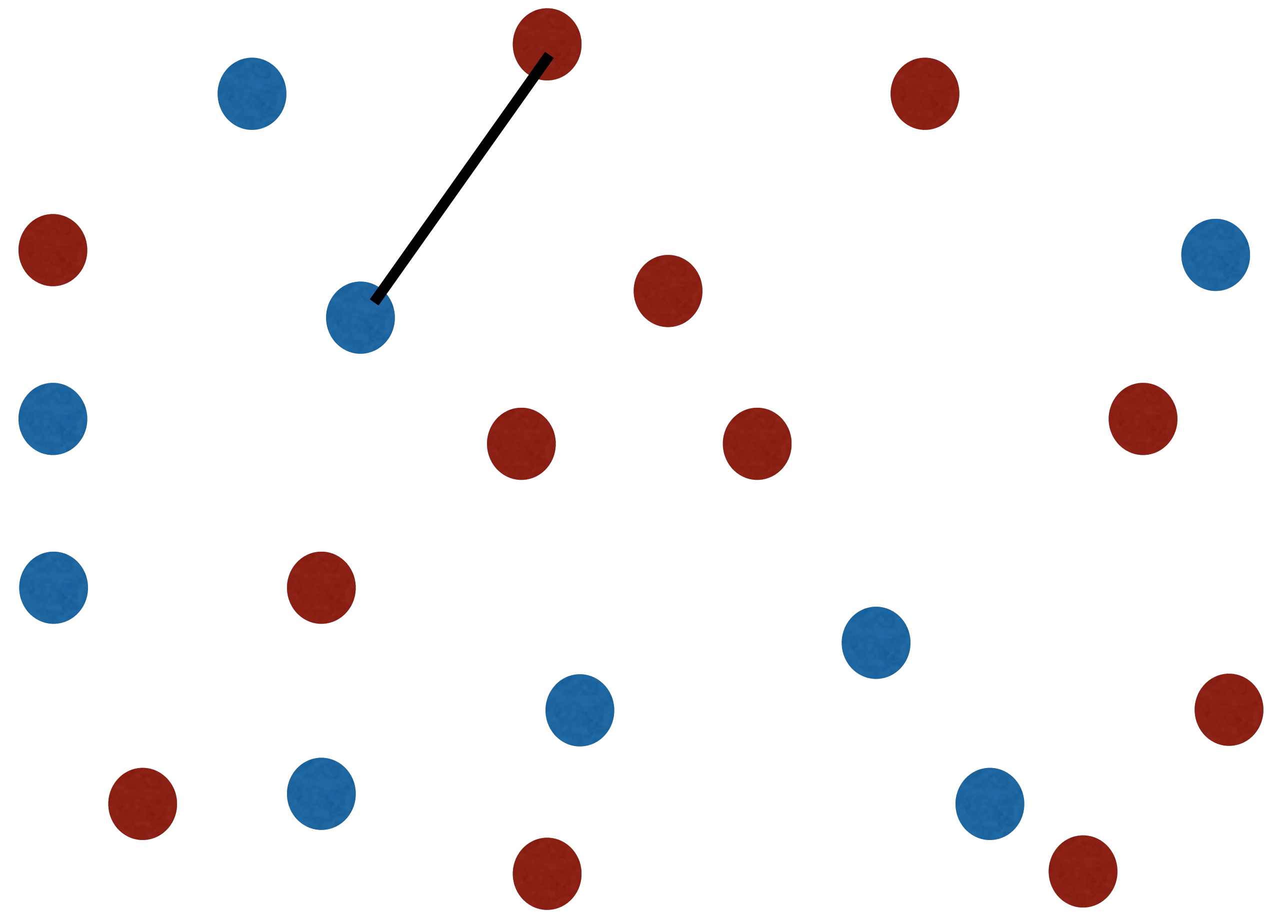
Slow algorithm
accurate additive
approx

Motivating Questions:

1. Can we break away from spanner approach?
2. Which transports approximate accurately?

Main Idea: Focus on a slight perturbation to EMD.





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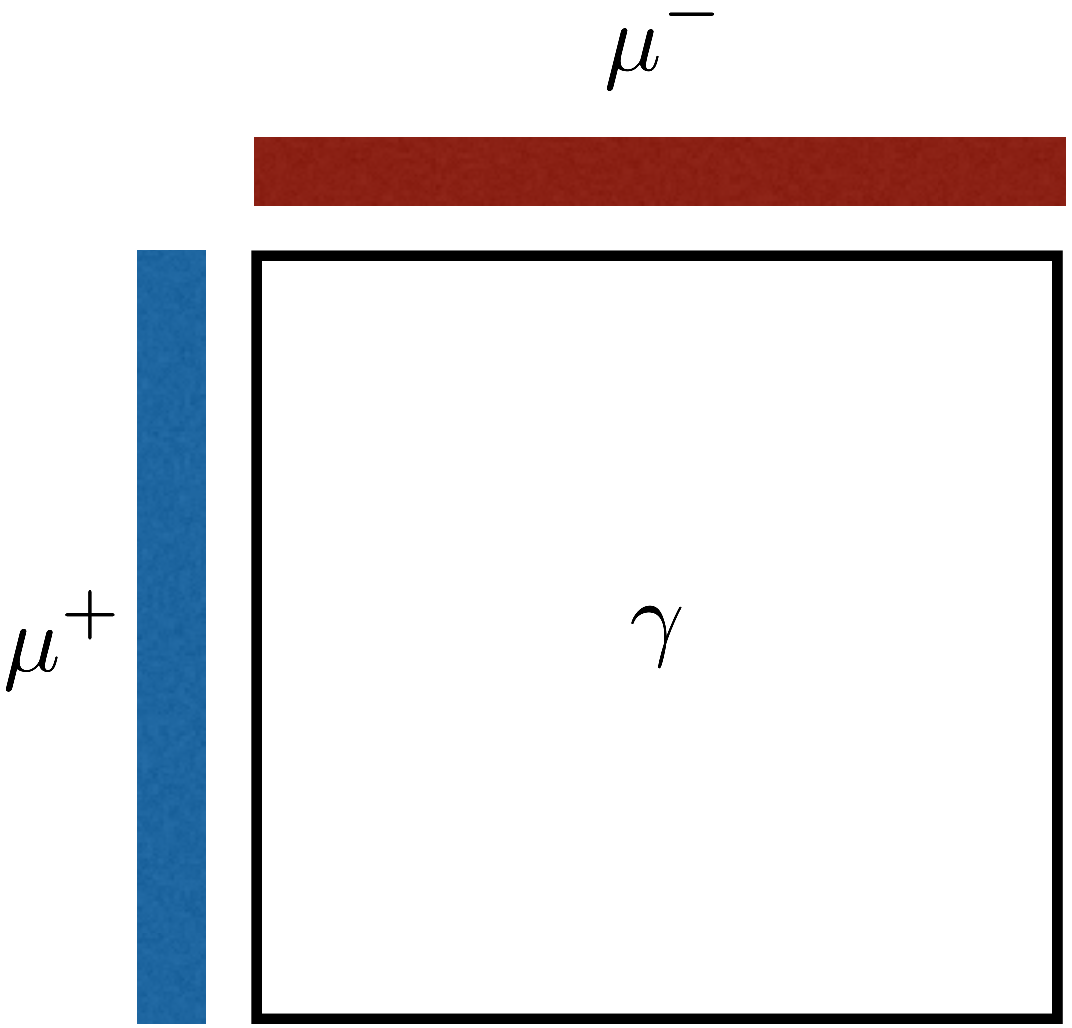

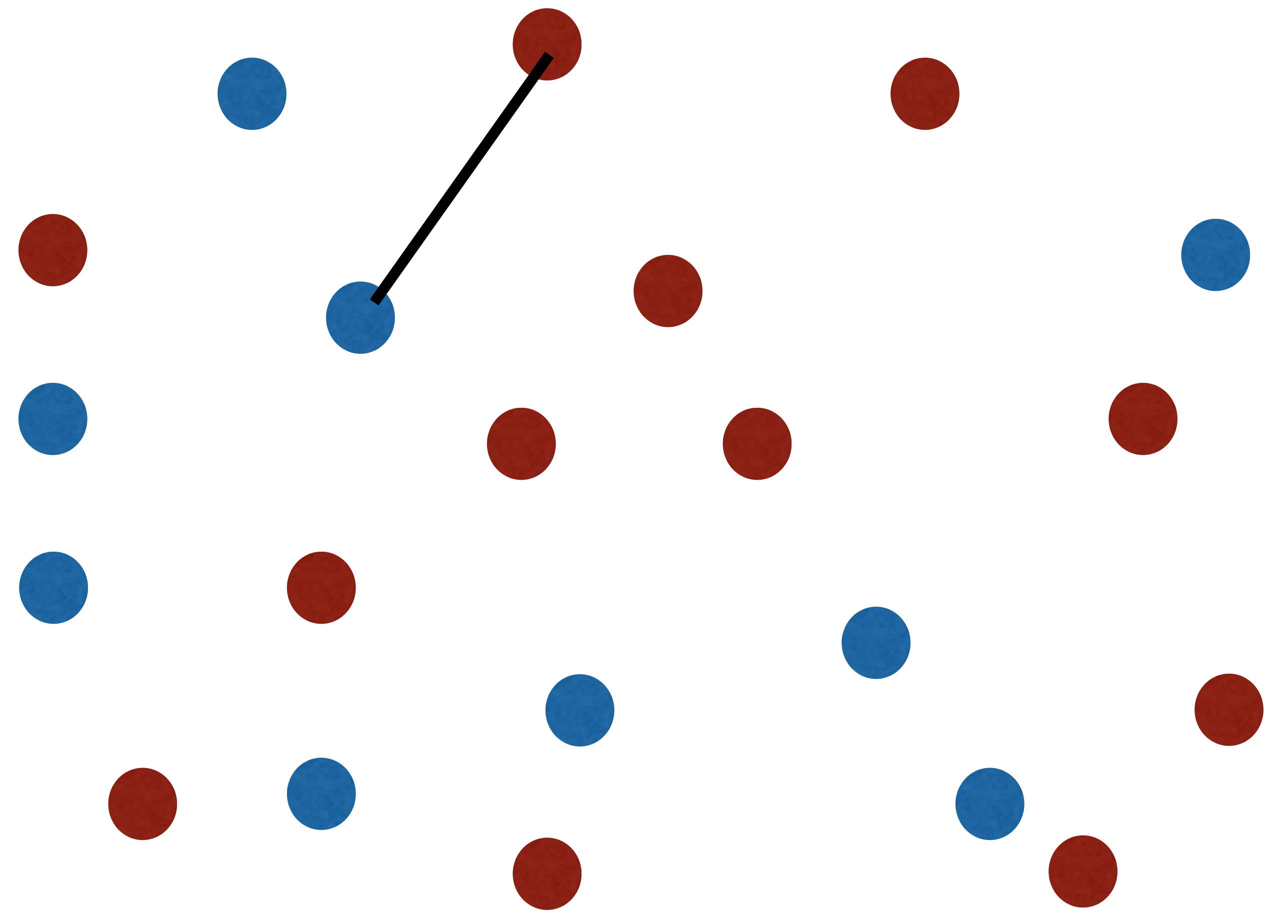

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Our perturbation:

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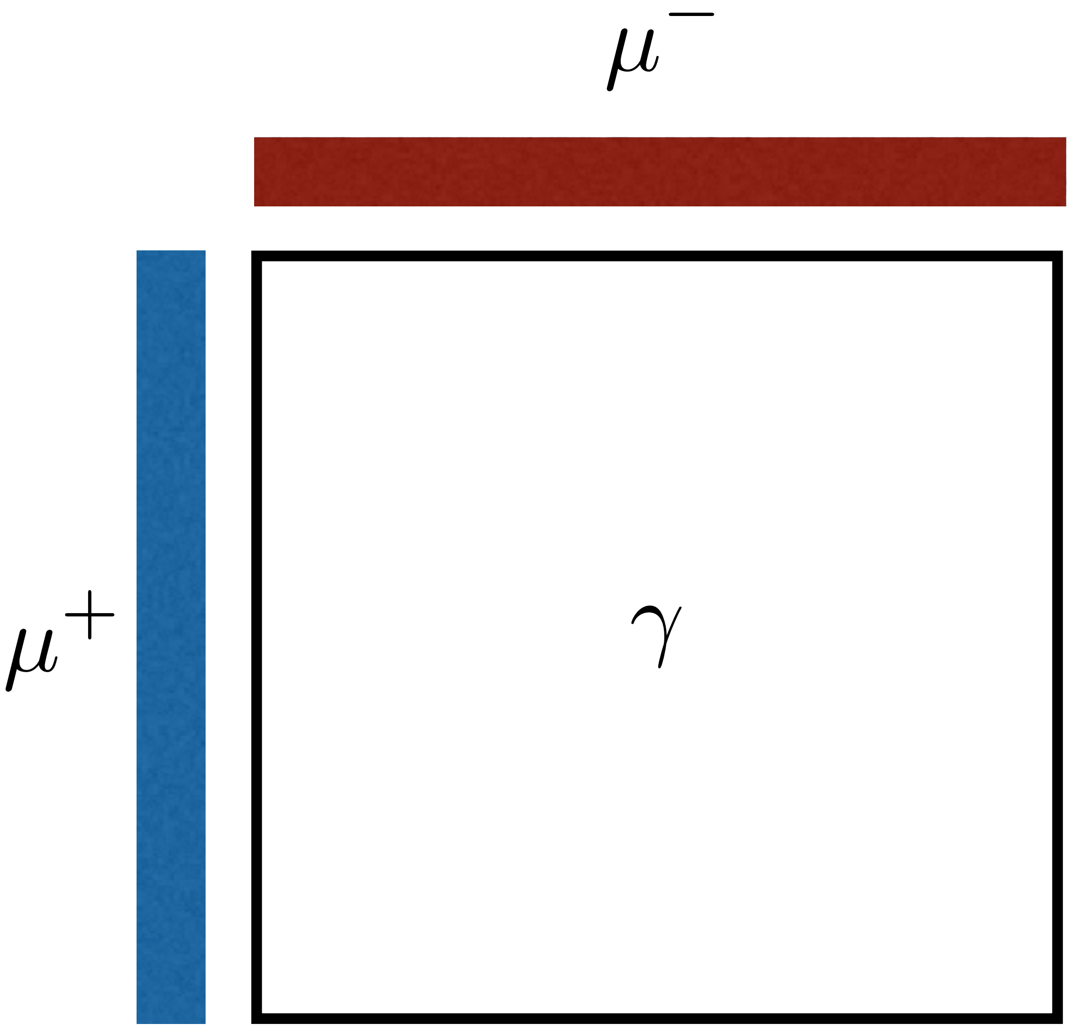

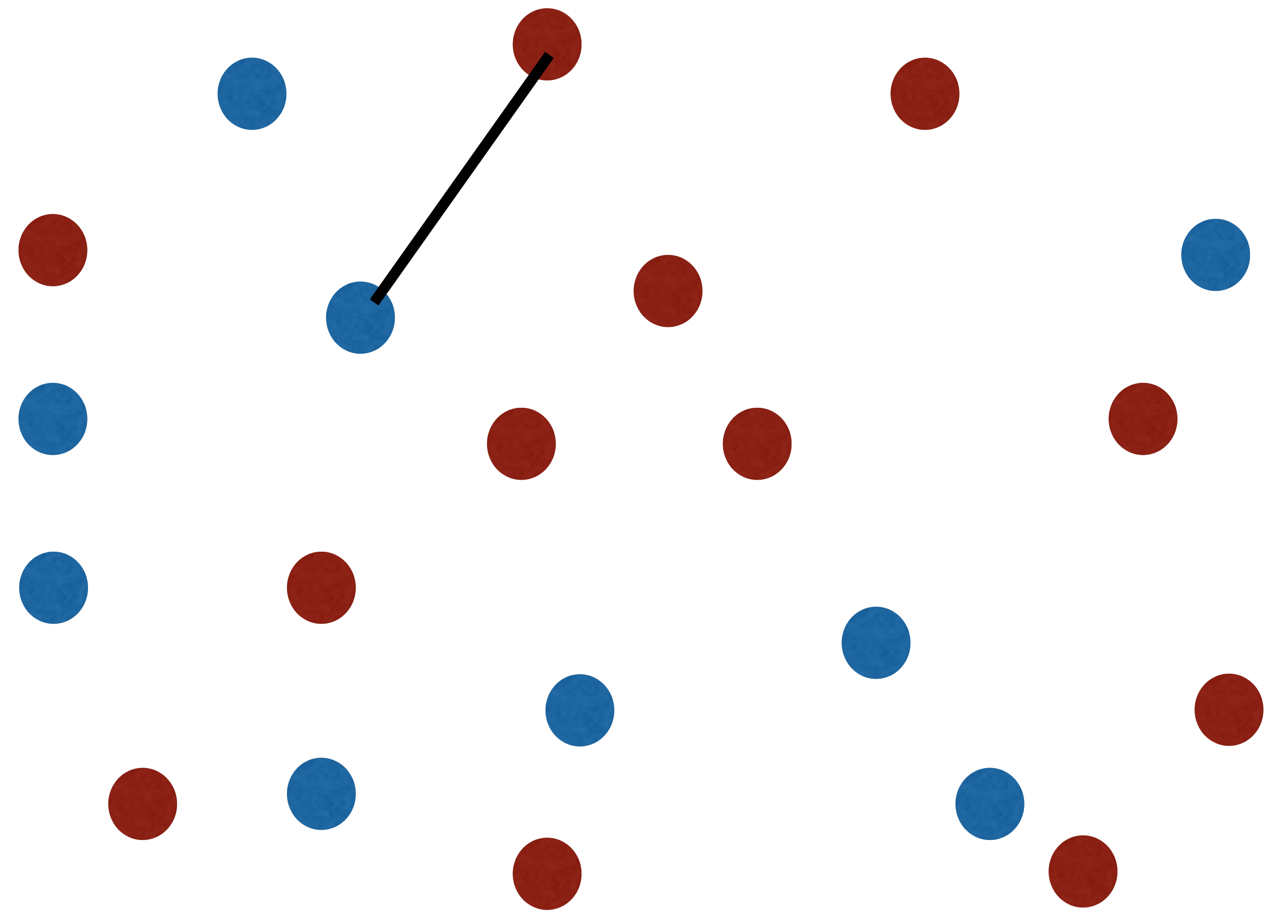

$\mathtt{EMD}(\mu)$

$$\min_{\gamma} \sum \sum \gamma_{ij} \|x_i - x_j\|_2$$

$\mathcal{R}_\rho(\mu)$

$$\min_{\gamma} \left(\sum \sum \gamma_{ij}^{\rho} \|x_i - x_j\|_2^{\rho} \right)^{1/\rho}$$

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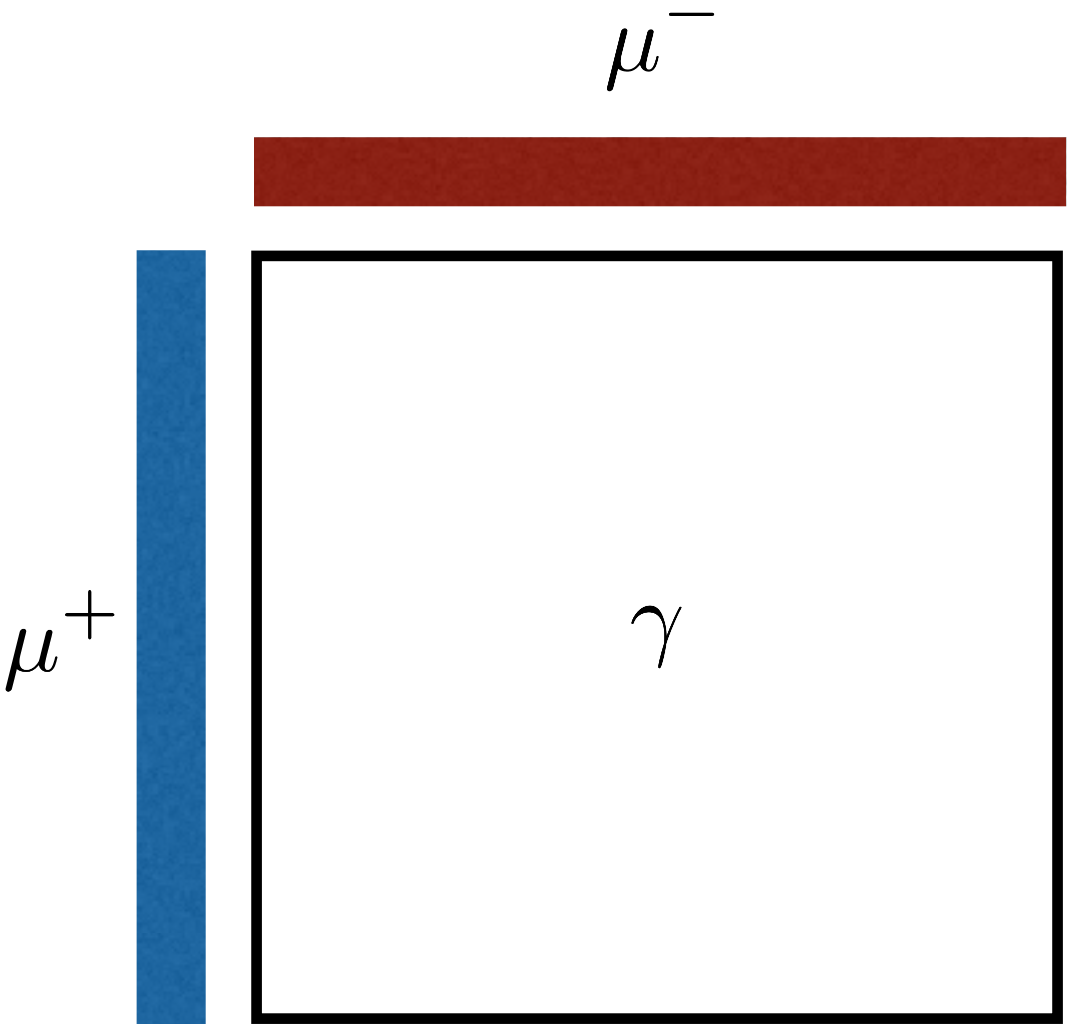

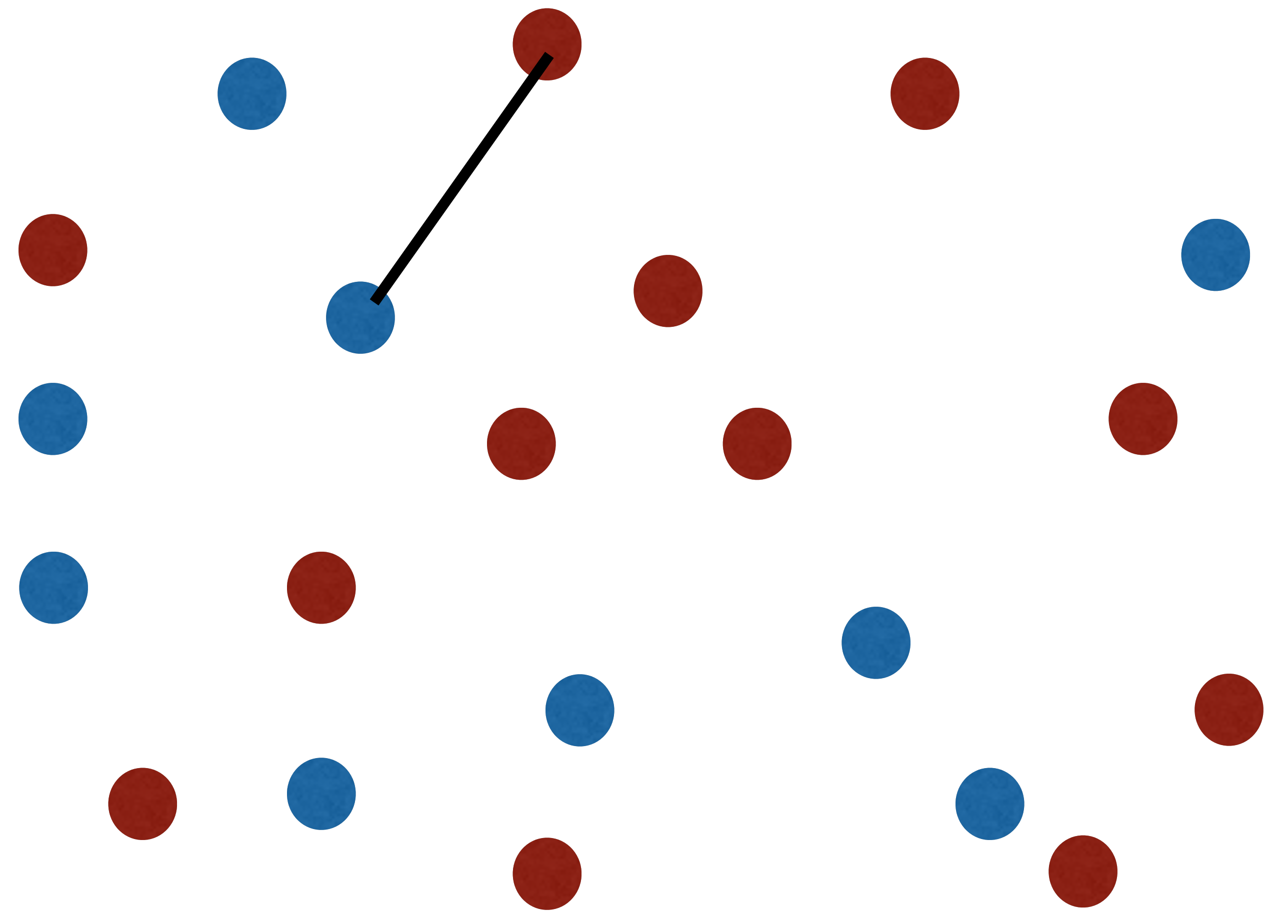

$$\mathtt{EMD}(\mu) \qquad 1 \longleftarrow \rho \qquad \mathcal{R}_\rho(\mu)$$

$$\min_\gamma \sum \sum \gamma_{ij} \|x_i - x_j\|_2 \qquad \min_\gamma \left(\sum \sum \gamma_{ij}^\rho \|x_i - x_j\|_2^\rho \right)^{1/\rho}$$

Main Theorem: An algorithm for $\mathcal{R}_\rho(\mu)$

New Theorem:

For any $\rho > 1$ and any $\epsilon > 0$, there is an algorithm which receives as input $\{x_1, \dots, x_n\}$ and $\{y_1, \dots, y_n\}$ and in time at most $n \cdot \mathrm{poly}^*(n^{(\rho-1)/\rho} \cdot 2^{\rho/(\rho-1)}/\epsilon)$, outputs an $\pm\epsilon r$ approx to $\mathcal{R}_\rho(\mu)$.

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Time: $n^{1+o(1)}/\mathrm{poly}(\epsilon)$

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EMD ⟷ Sinkhorn

Fast, crude approx — Slow, accurate approx

Talk Outline:

- “Spanner approach”
- Main Result
- **Kernel Density Estimation**
- Techniques

Kernel Density Estimation (KDE)

[Charikar, Siminelakis '17]

Preprocessing:

- A dataset $X = \{x_1, \ldots, x_n\} \subset \mathbb{R}^d$
- A kernel function $\mathsf{K}(x, y)$

Query:

- A point $y \in \mathbb{R}^d$
- Output approximation to $\tau = \frac{1}{n} \sum_{i=1}^{n} \mathsf{K}(x_i, y)$

e.g. $\mathsf{K}(x, y) = \frac{1}{\|x - y\|_2^2}$

Smoothness is very helpful in sketching.

[Backurs, Charikar, Indyk, Siminelakis '18]:

- Message: complexity governed by decay of $\mathsf{K}(x, y)$

Smooth Kernel:

$$\mathsf{K}(x, y) \text{ decays polynomially with } \|x - y\|_2$$

$$\text{e.g.: } \mathsf{K}(x, y) = \frac{1}{\|x - y\|_2^s}$$

Theorem: there exists a data structure for approximating KDE of smooth kernels running in time $\mathrm{poly}(d \log n \cdot 2^s / \epsilon)$.

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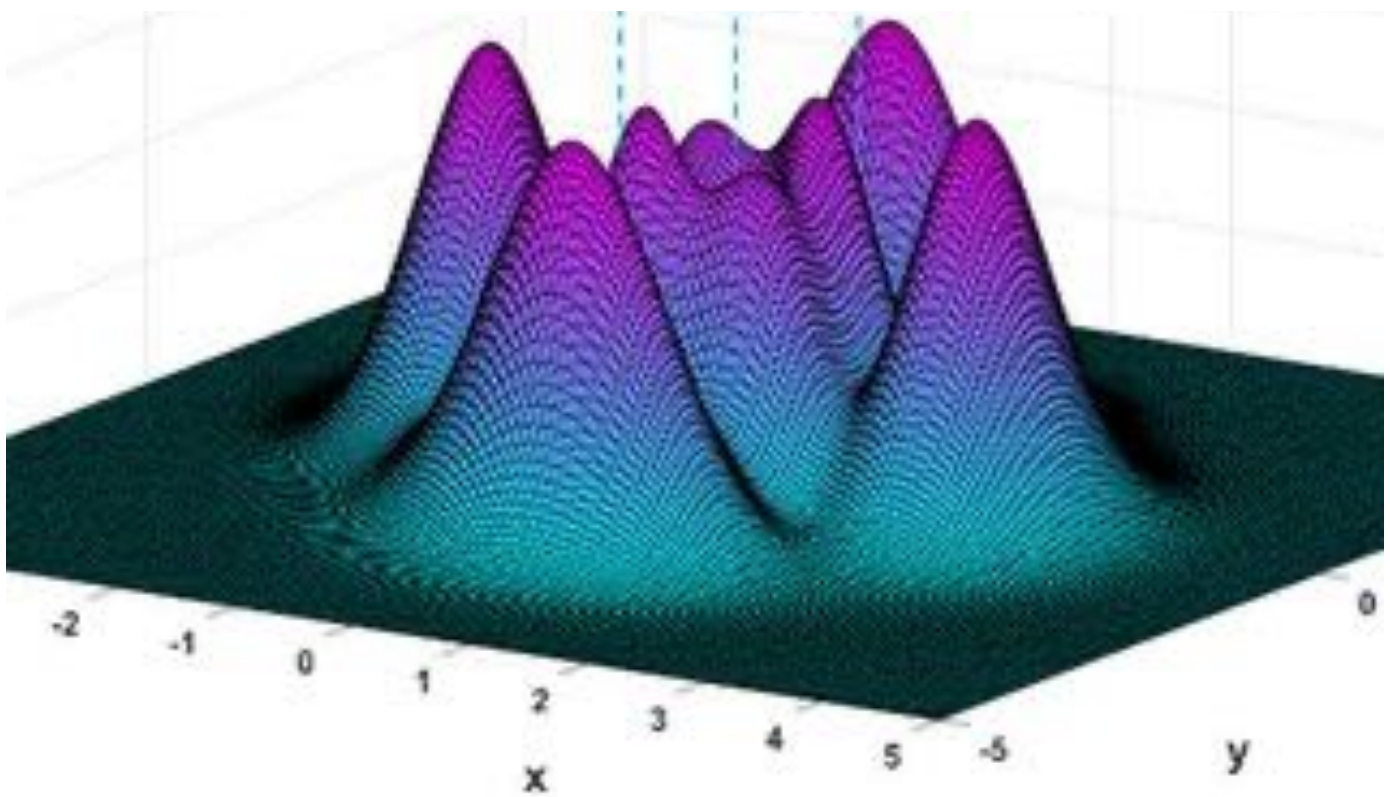

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time per query.

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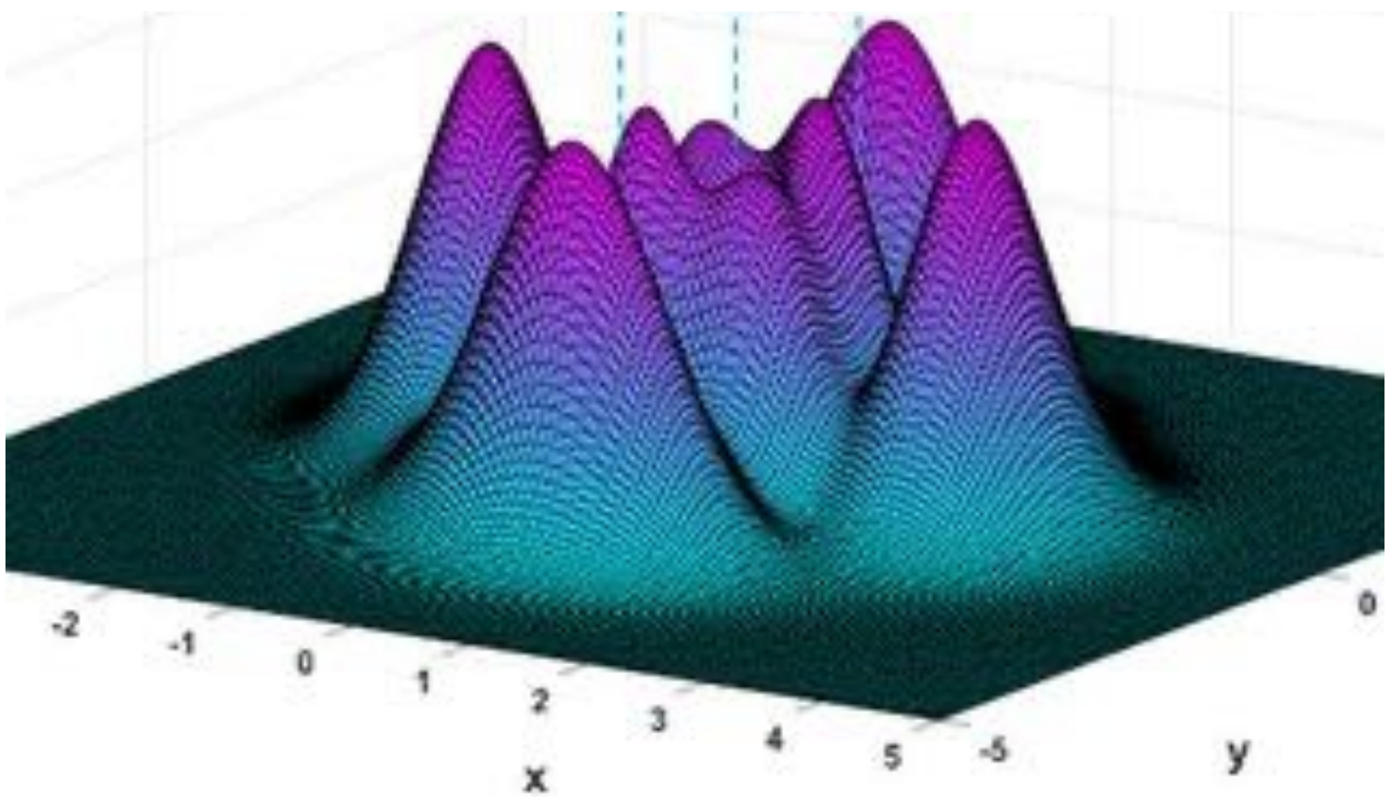

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Looking forward to… $\mathcal{R}_\rho(\mu) \longleftrightarrow s = \dfrac{\rho}{\rho-1}$

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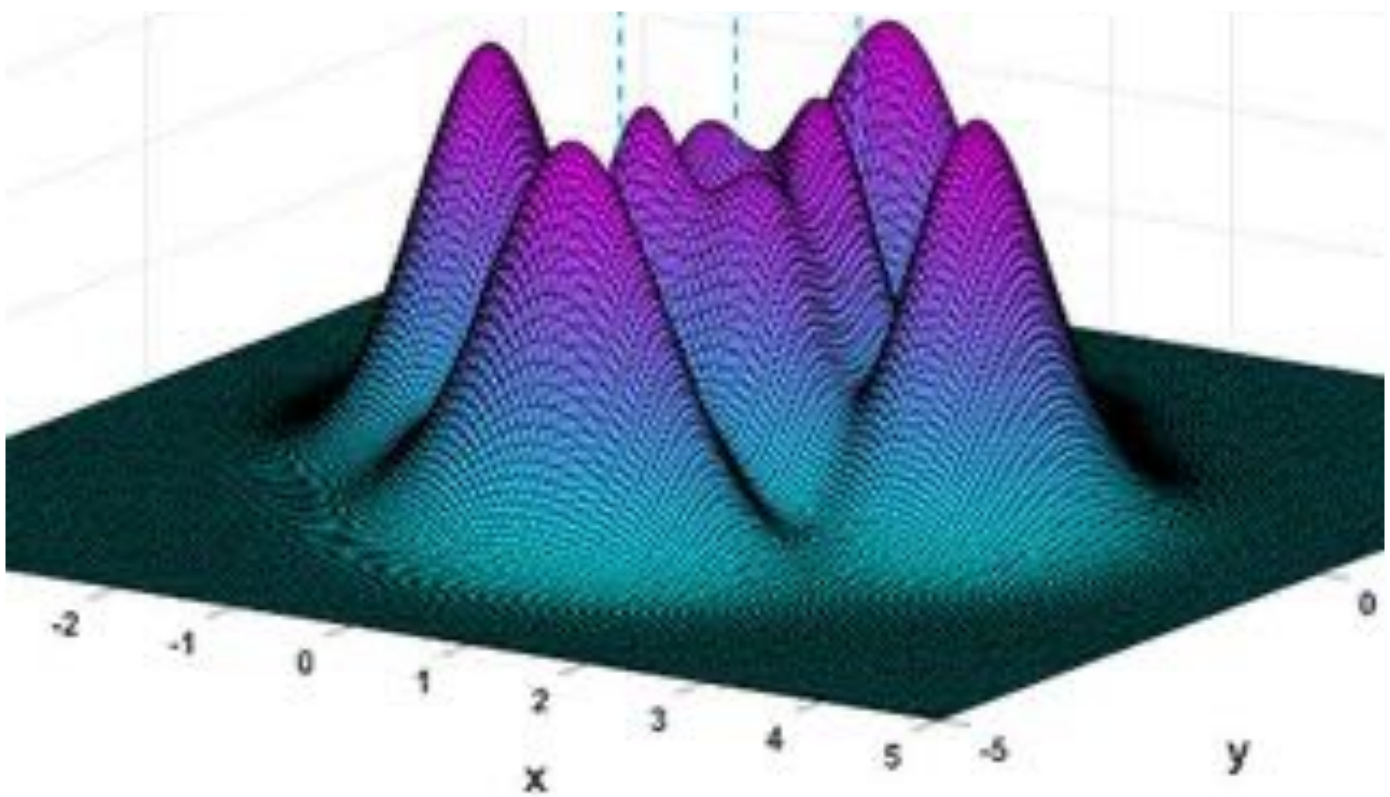

$\mathrm{poly}(d \log n \cdot 2^s/\epsilon)$

time per query.

Traditional sketching vectors ℓ_p : $\tilde{\Theta}(d^{1-2/p}/\epsilon^2)$

Techniques:
Using KDE for $\mathcal{R}_\rho(\mu)$.

The Linear Program for the Earth Mover's Distance

$$
\begin{aligned}
\texttt{EMD}(\mu) \quad &= \quad \min_{\gamma} \sum_{i=1}^{n} \sum_{j=1}^{n} \gamma_{ij} \|x_i - y_j\|_2 \\
\text{s.t} \quad & \sum_{i=1}^{n} \gamma_{ij} = \frac{1}{n} \text{ for all } i \in [n] \\
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Even representing γ is complicated!

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$$= \quad \max_{\alpha, \beta \in \mathbb{R}^n} \frac{1}{n} \sum_{i=1}^{n} \alpha_i - \frac{1}{n} \sum_{j=1}^{n} \beta_j$$

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The Perturbation $\mathcal{R}_\rho(\mu)$

$$\mathcal{R}_\rho(\mu)^\rho = \min_\gamma \sum_{i=1}^n \sum_{j=1}^n \gamma_{ij}^\rho \|x_i - y_j\|_2^\rho$$

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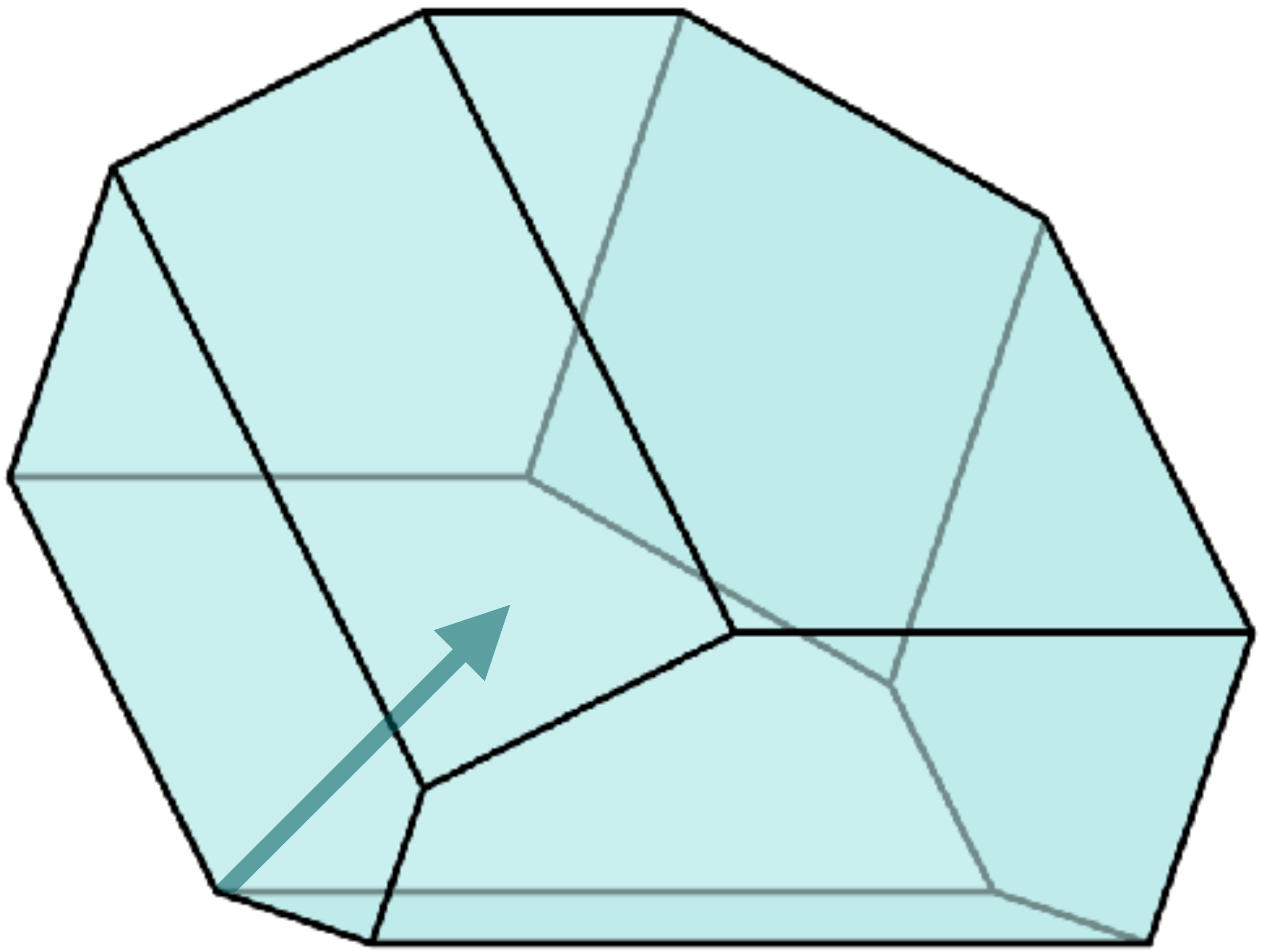
Picture: EMD vs $\mathcal{R}_\rho(\mu)$



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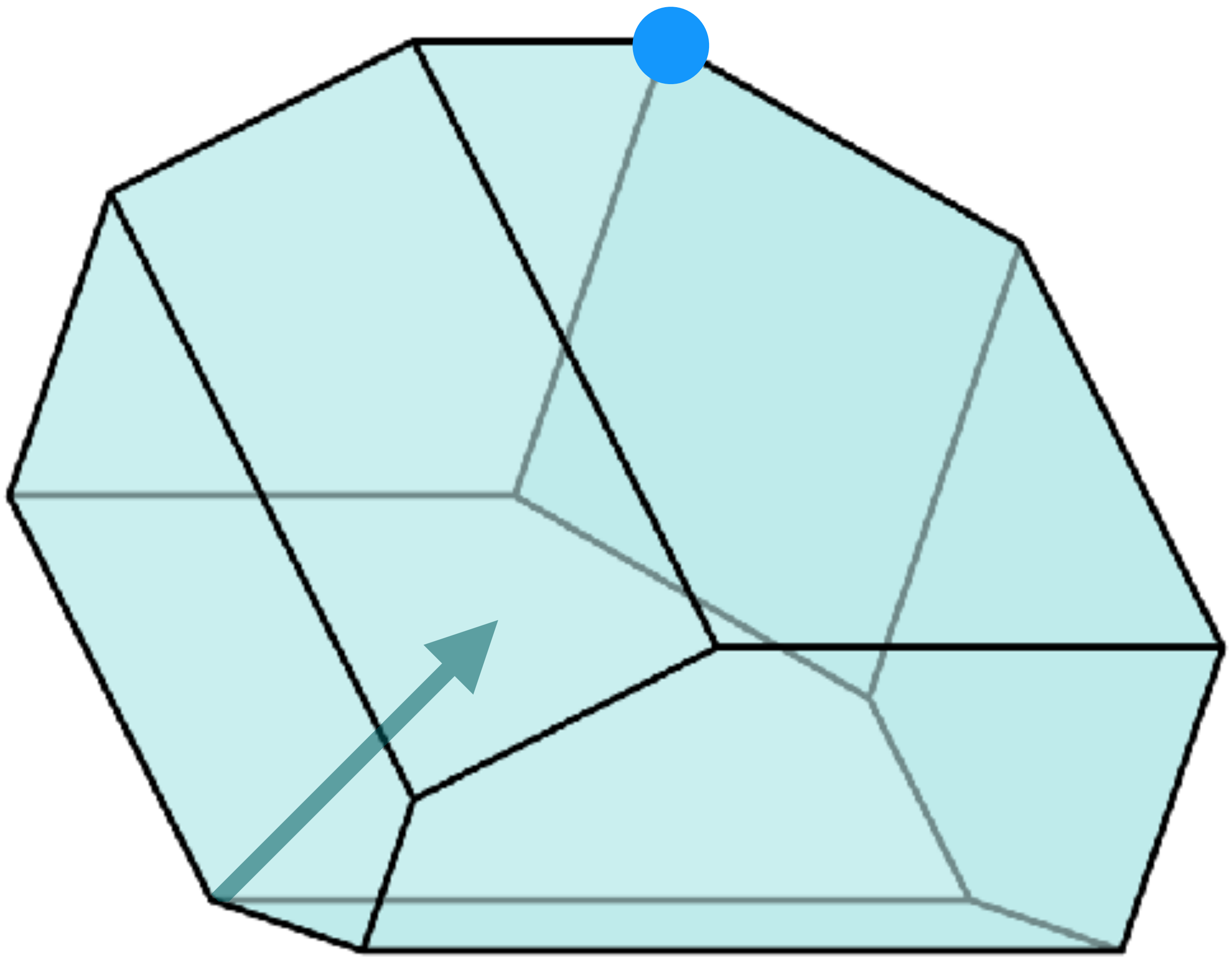

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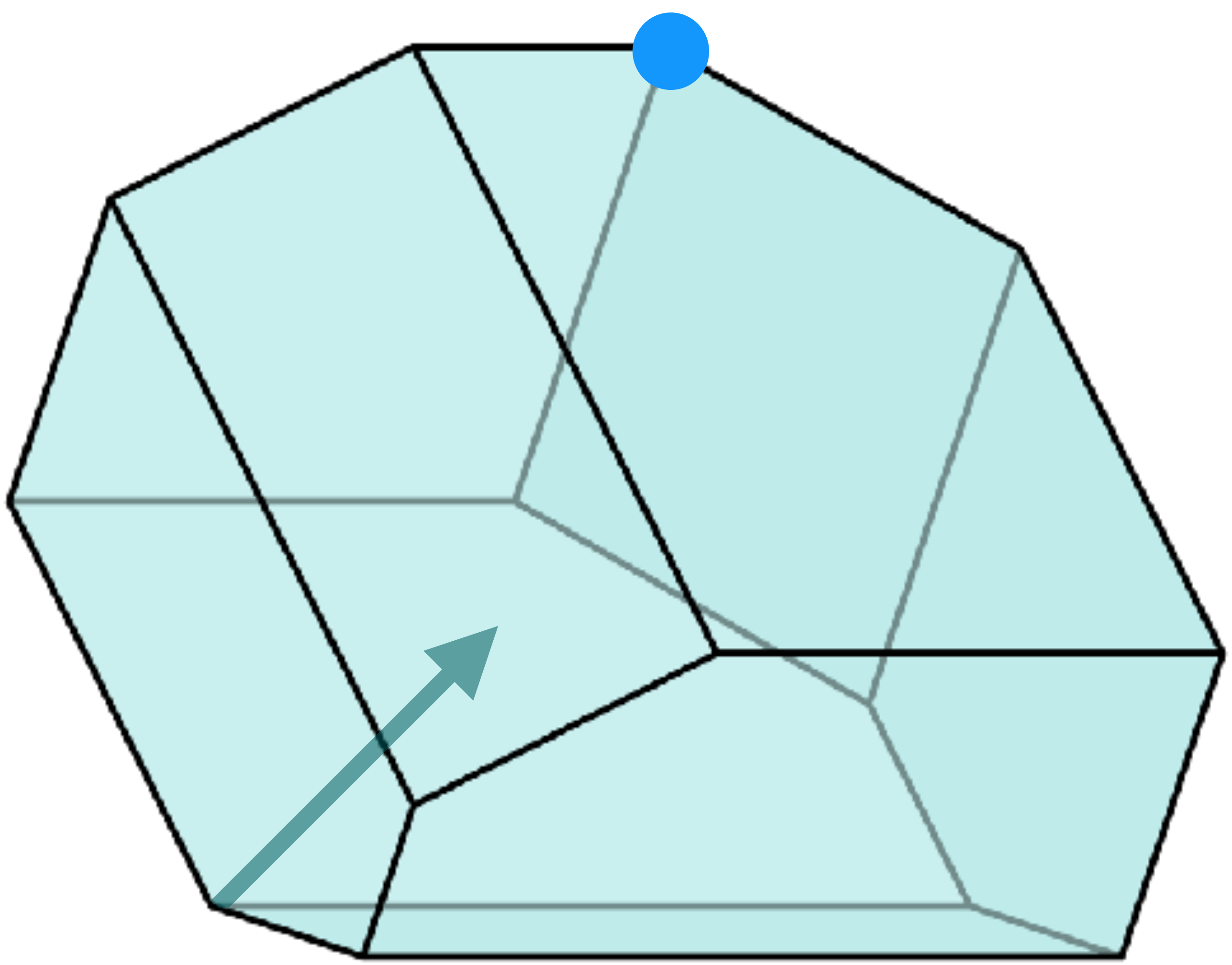

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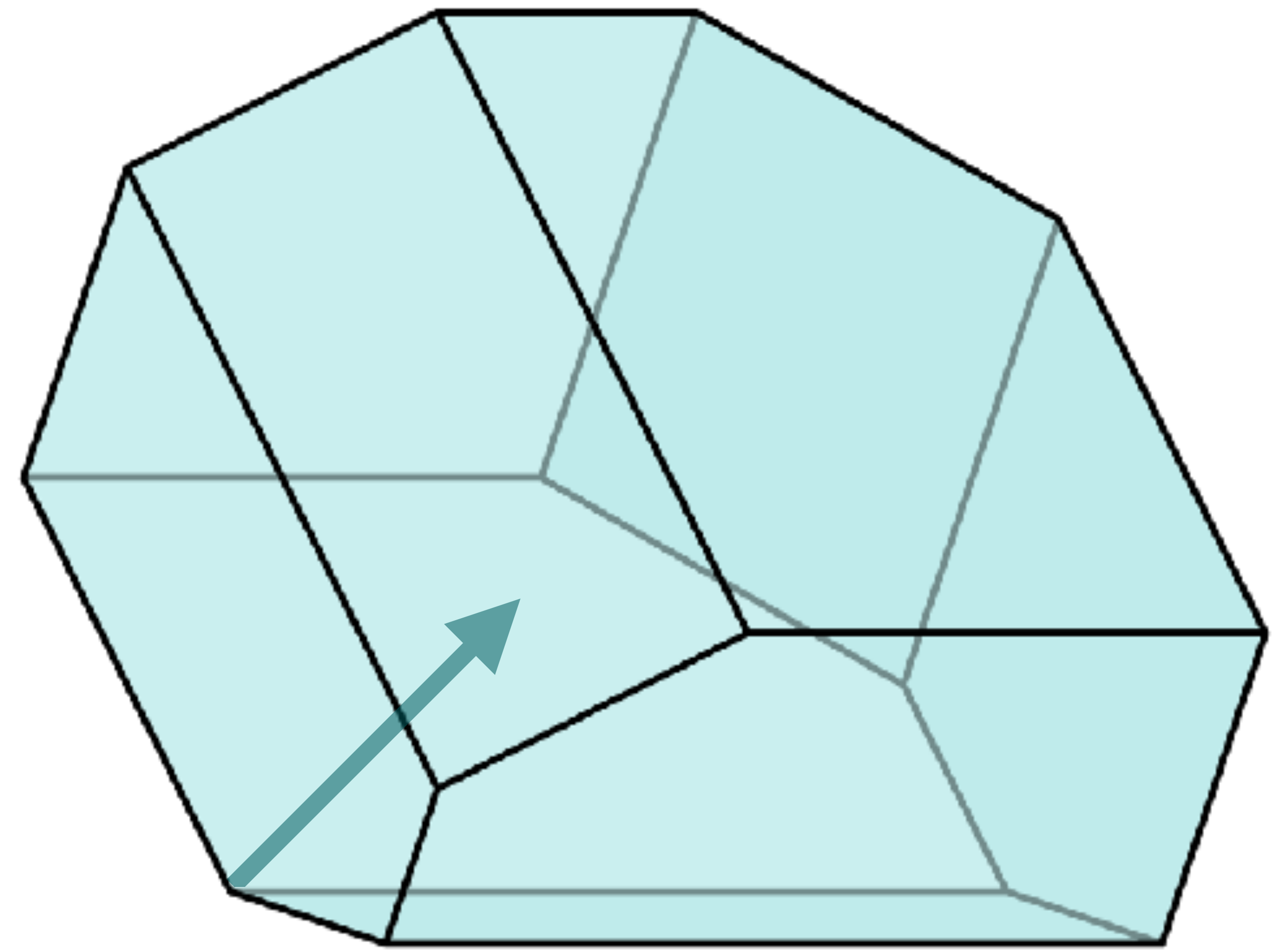

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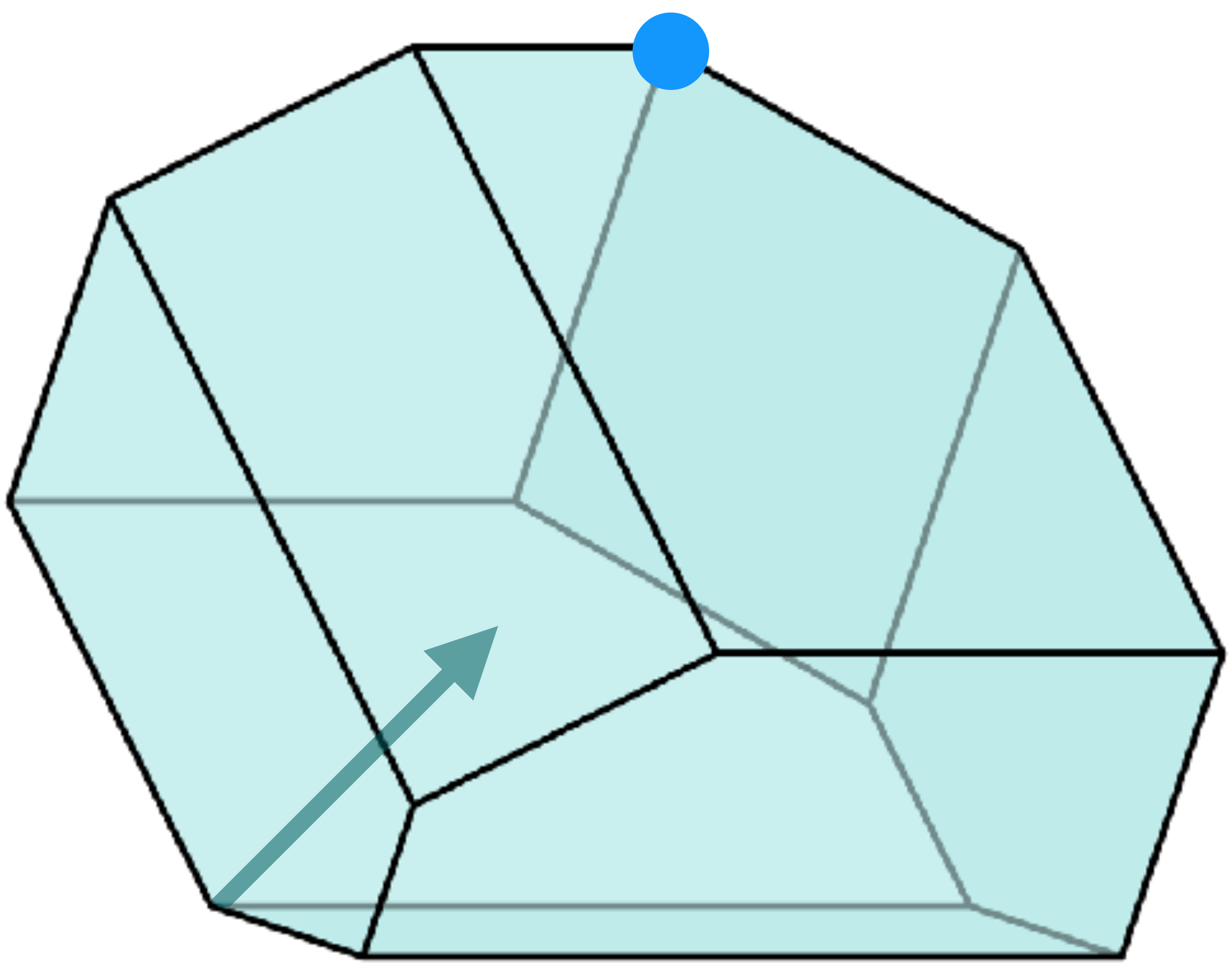

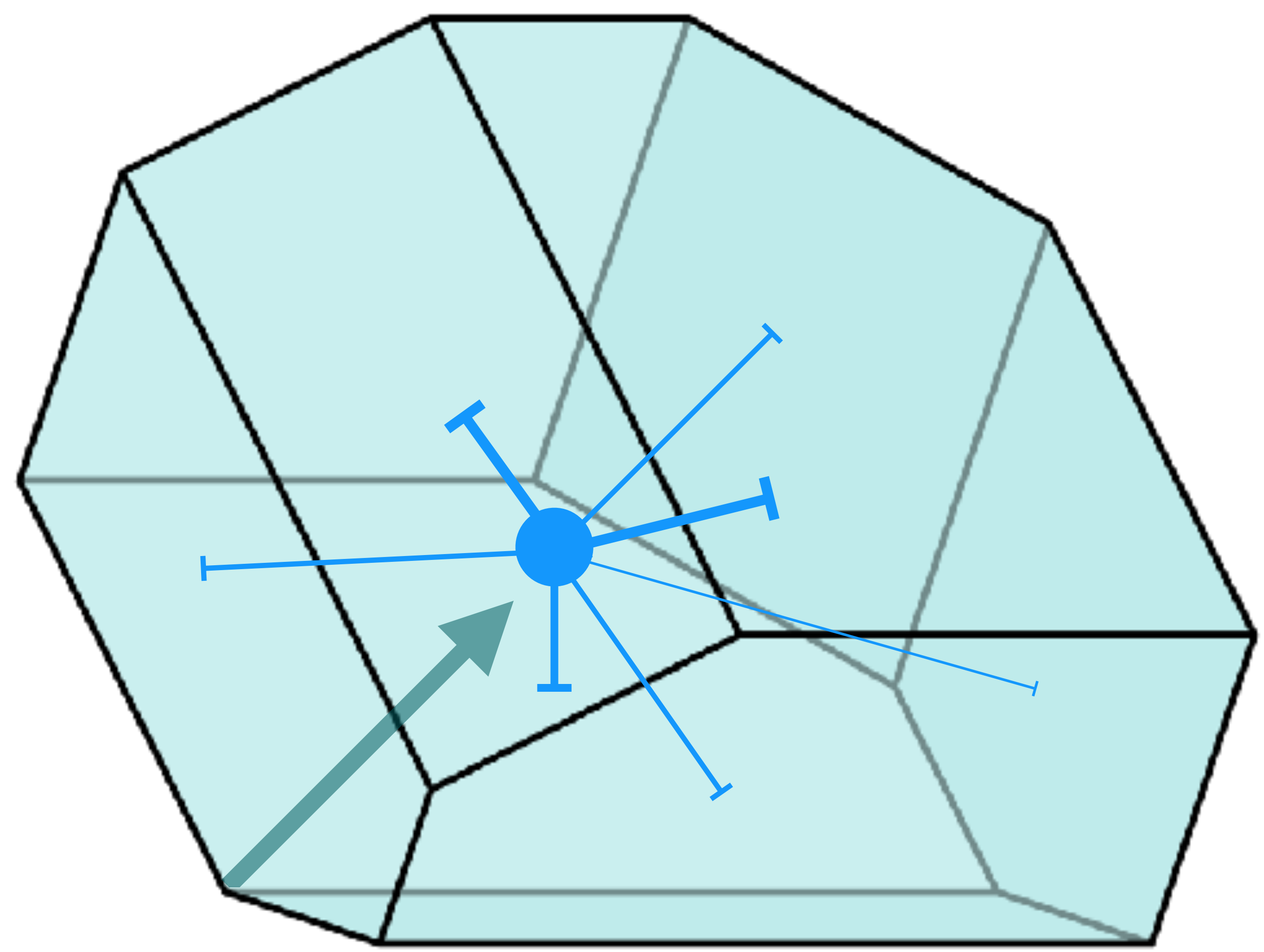

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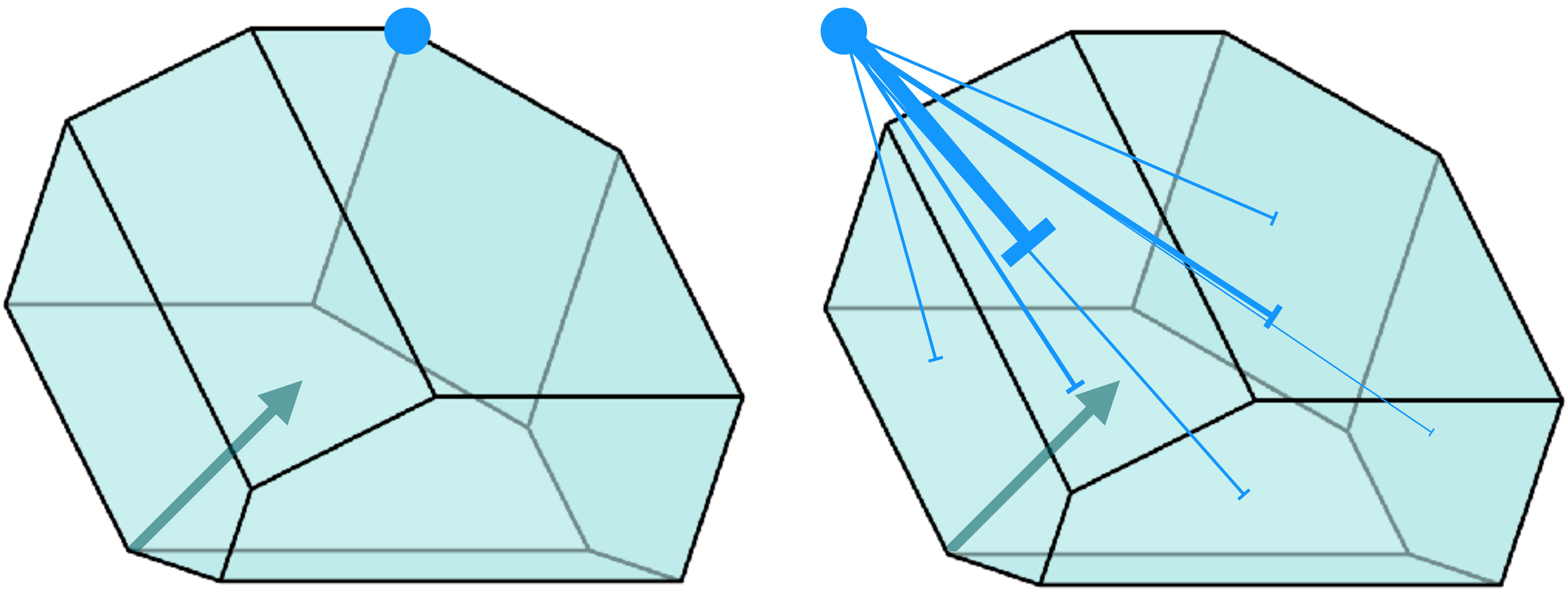

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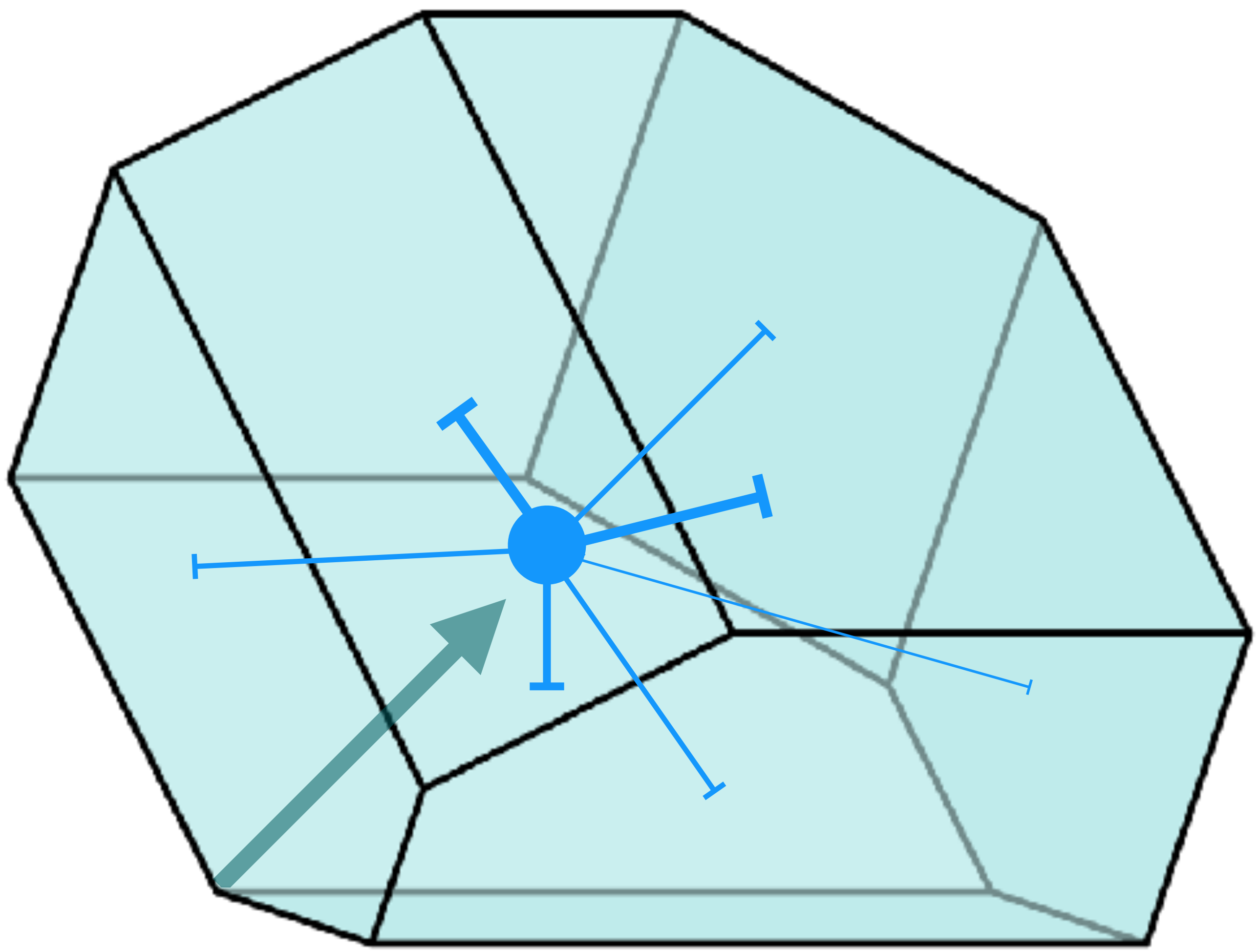
We can efficiently run first-order methods.



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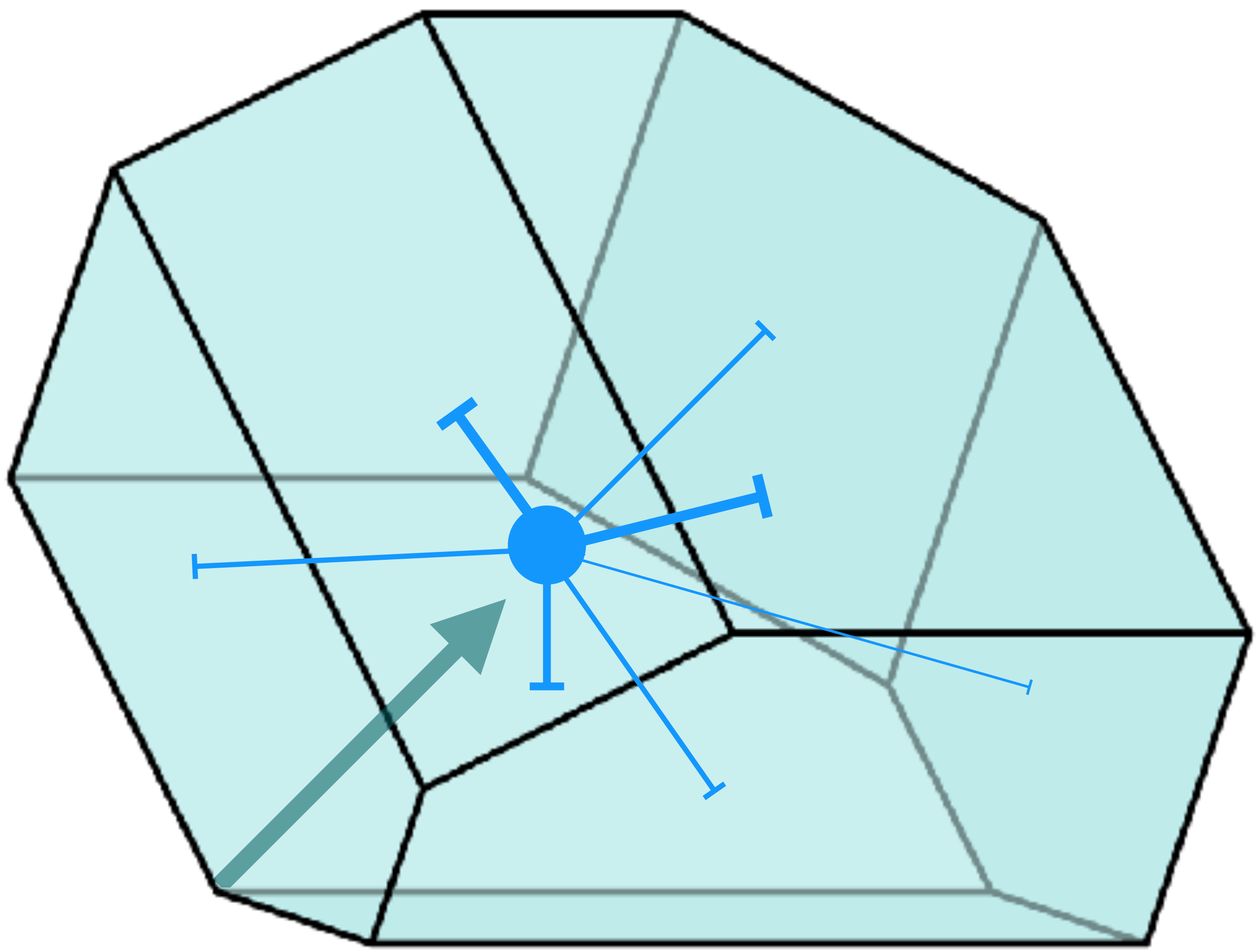

$$\frac{\partial}{\partial \alpha_i} = \frac{1}{n} - sC_\rho \sum_{j=1}^{n} \frac{((\alpha_i - \beta_j)^+)^{s-1}}{\|x_i - y_j\|_2^s}$$

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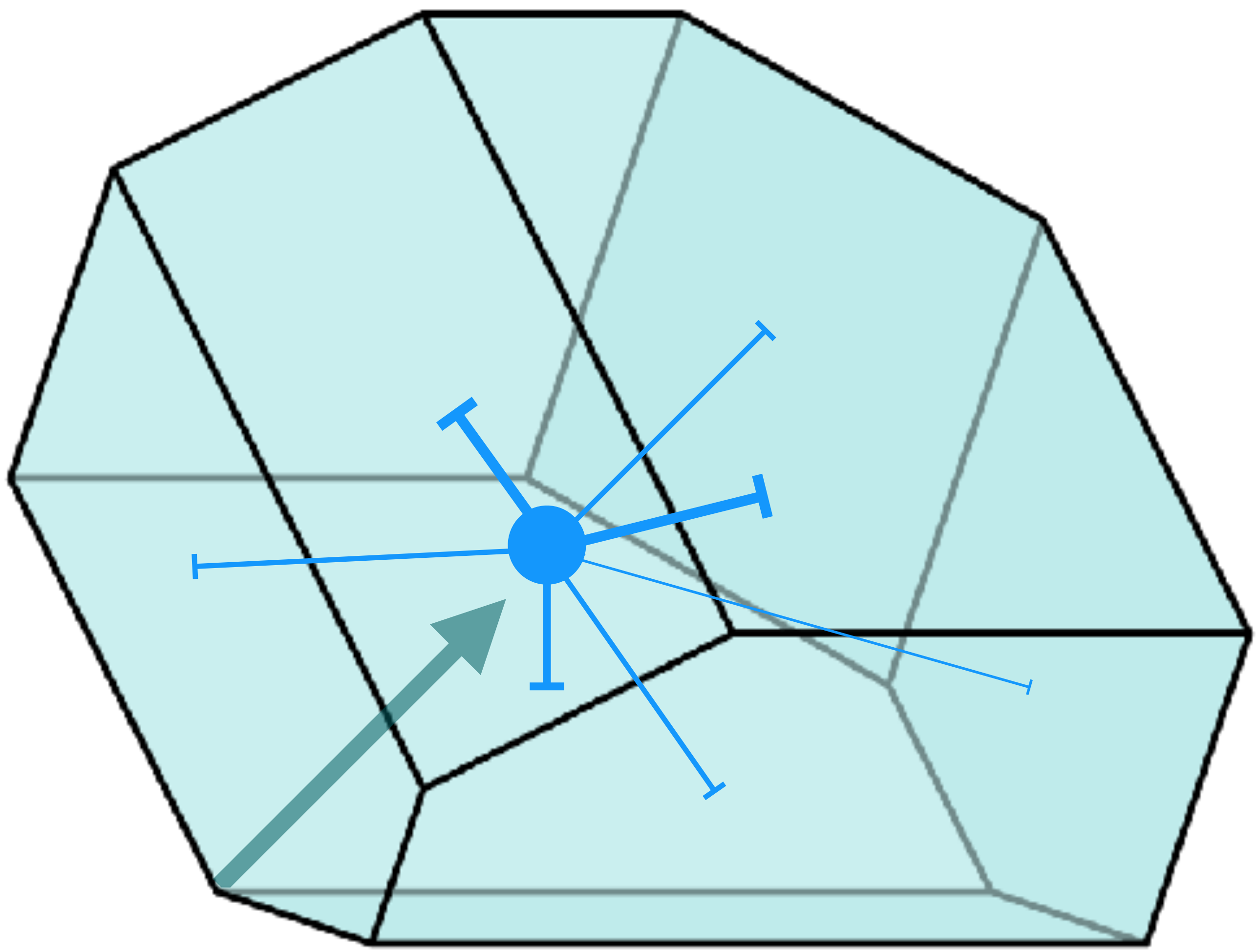

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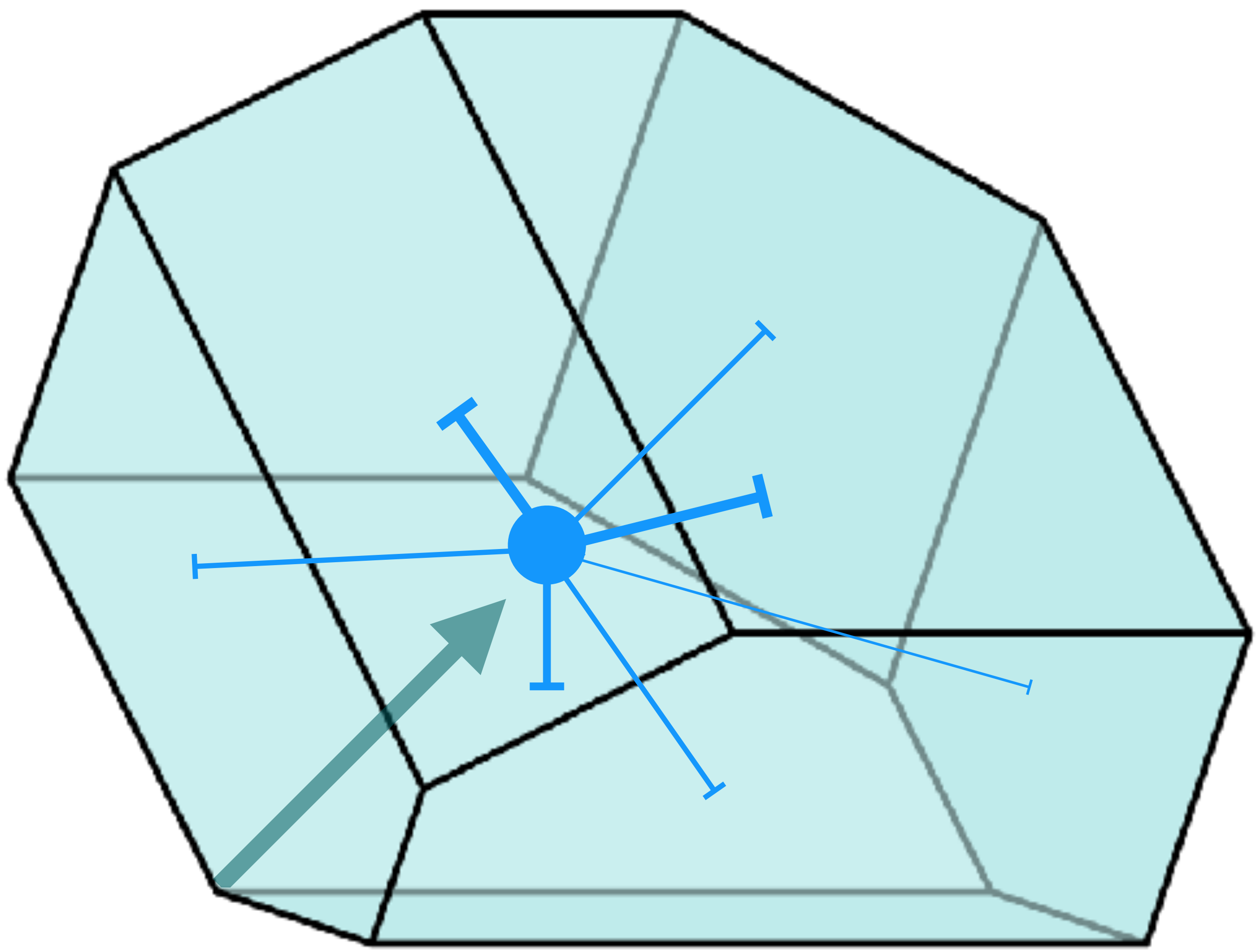

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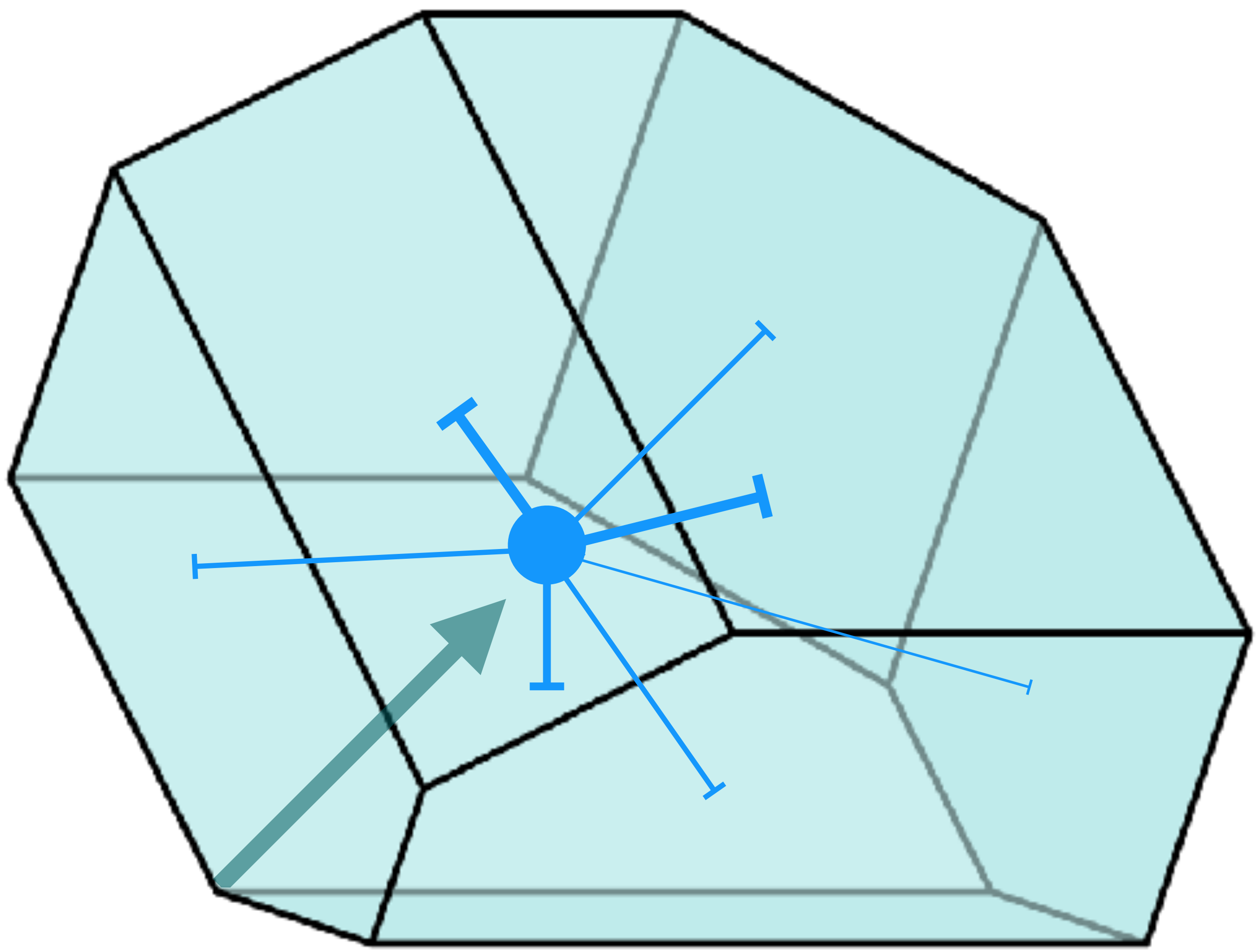
If can handle $((\alpha_i - \beta_j)^+)^{s-1}$,
rest is a smooth kernel.

$$\max_{\alpha,\beta \in \mathbb{R}^n} \frac{1}{n}\sum_{i=1}^{n} \alpha_i - \frac{1}{n}\sum_{j=1}^{n} \beta_j - C_\rho \sum_{i=1}^{n}\sum_{j=1}^{n} \left(\frac{(\alpha_i - \beta_j)^+}{\|x_i - y_j\|_2}\right)^s$$

We can efficiently run first-order methods.



$$\frac{\partial}{\partial \alpha_i} = \frac{1}{n} - sC_\rho \sum_{j=1}^{n} \frac{((\alpha_i - \beta_j)^+)^{s-1}}{\|x_i - y_j\|_2^s}$$

$$\frac{\partial}{\partial \beta_j} = -\frac{1}{n} + sC_\rho \sum_{i=1}^{n} \frac{((\alpha_i - \beta_j)^+)^{s-1}}{\|x_i - y_j\|_2^s}$$

If can handle $((\alpha_i - \beta_j)^+)^{s-1}$,
rest is a smooth kernel.

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In time $O(n) \cdot \text{poly}(d \log n \cdot 2^s/\epsilon)$
good approximations to gradient

Algorithm

1. Maintain α, β.
2. Estimate $\frac{\partial}{\partial\alpha}, \frac{\partial}{\partial\beta}$.
3. If $\partial/(\partial\alpha)$ far from 0, update α
4. If $\partial/(\partial\beta)$ far from 0, update β

$$\max_{\alpha,\beta\in\mathbb{R}^n} \frac{1}{n}\sum_{i=1}^{n}\alpha_i - \frac{1}{n}\sum_{j=1}^{n}\beta_j - C_\rho \sum_{i=1}^{n}\sum_{j=1}^{n}\left(\frac{(\alpha_i-\beta_j)^+}{\|x_i-y_j\|_2}\right)^s$$

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Thanks