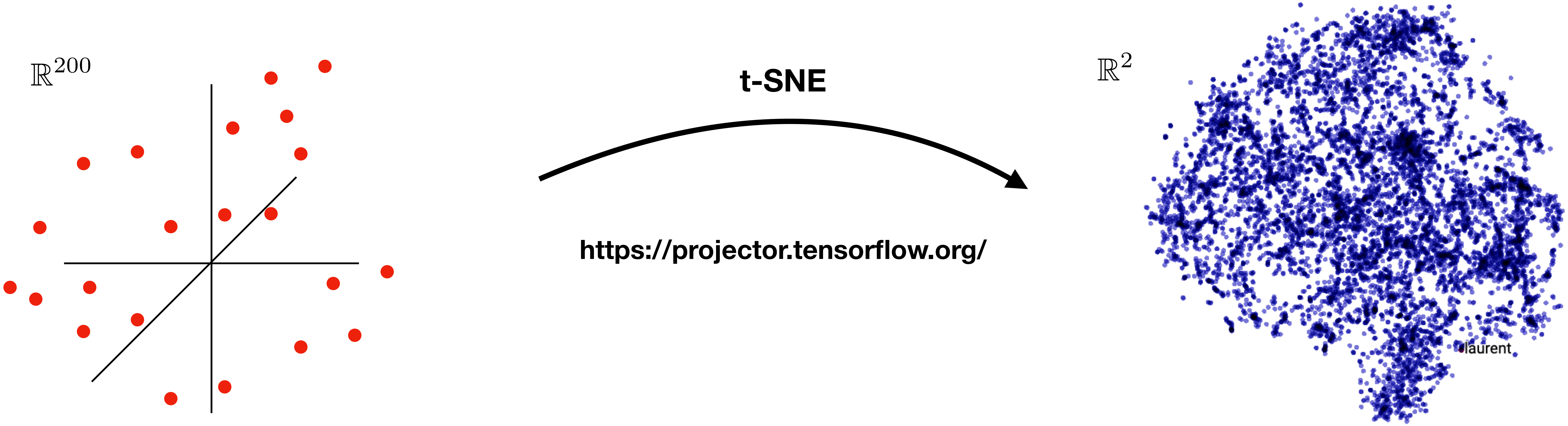
A Quasi-Monte Carlo Data Structure for Smooth Kernel Evaluation

Moses Charikar (Stanford)
Michael Kapralov (EPFL)
Erik Waingarten (Penn)

t-SNE: Visualization technique via "matching" geometric graphs.



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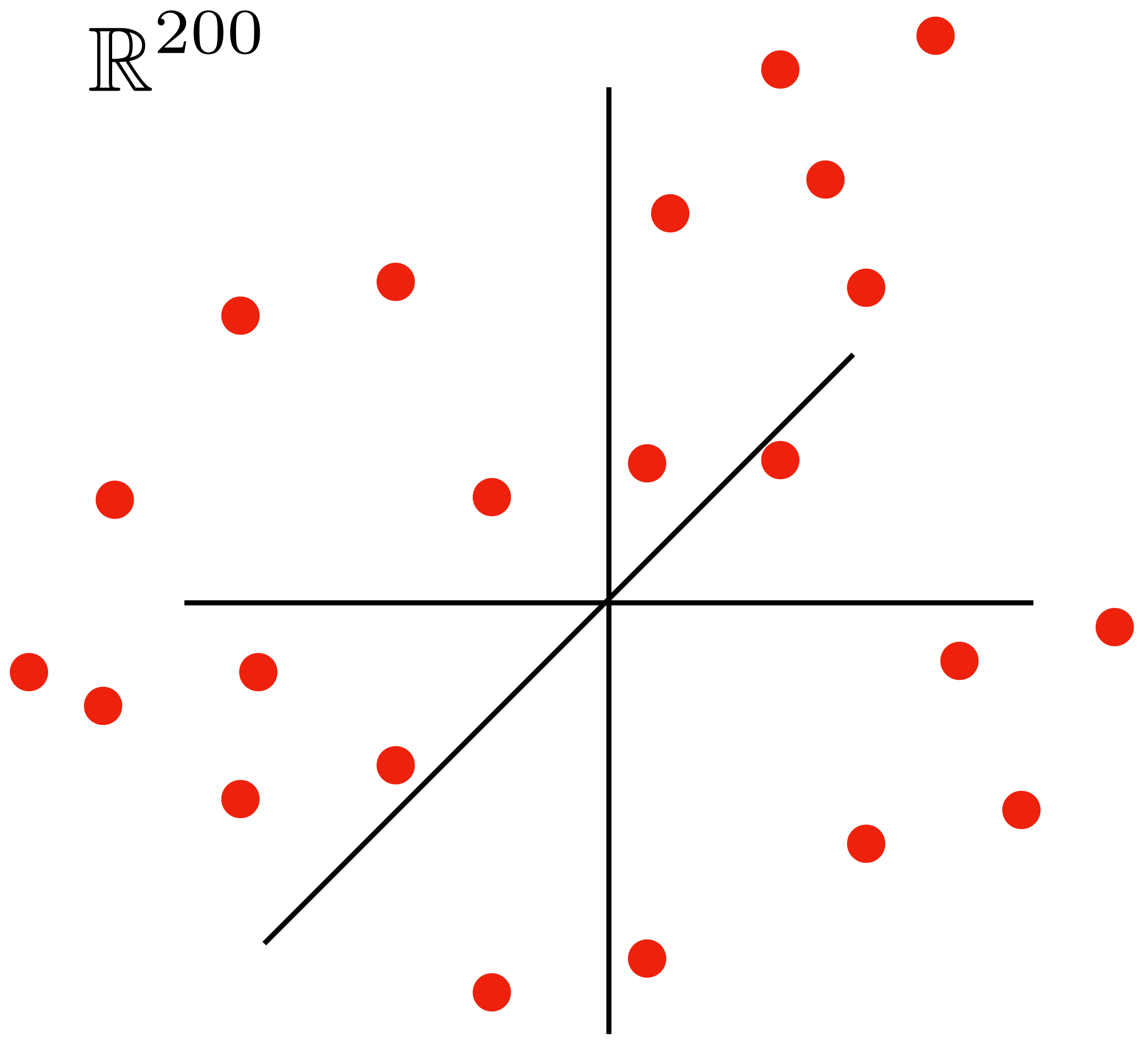
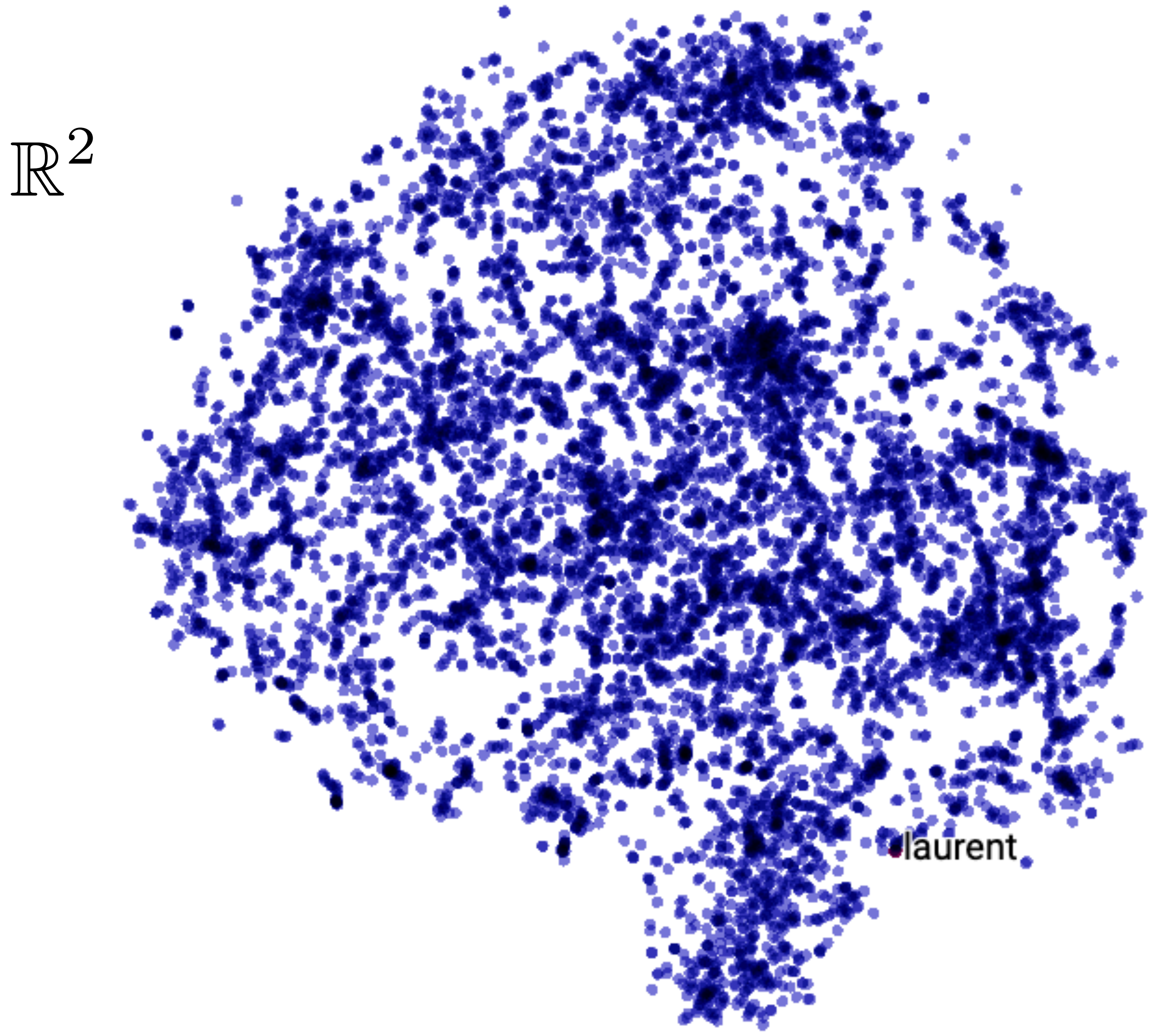
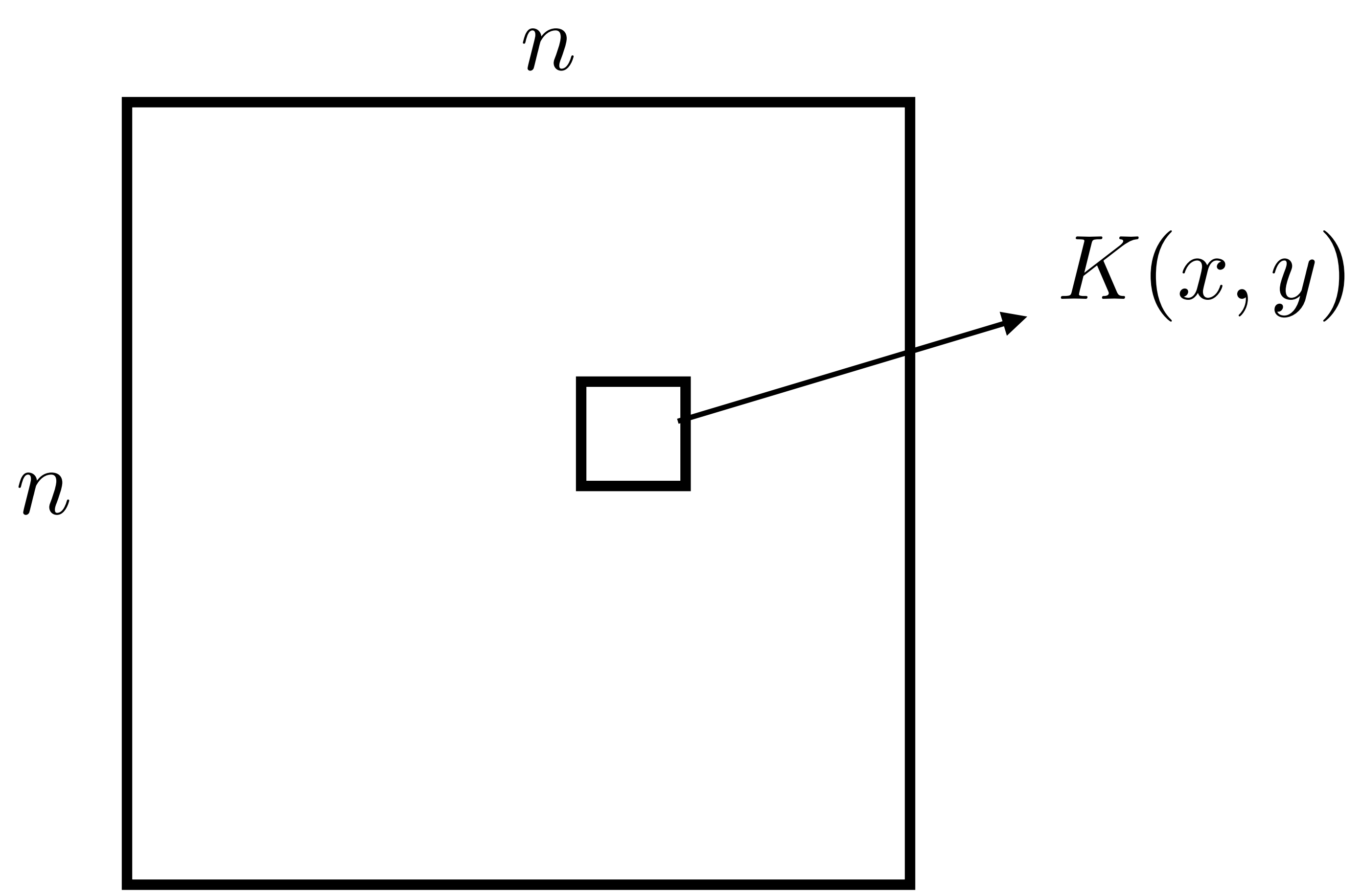


t-SNE

https://projector.tensorflow.org/

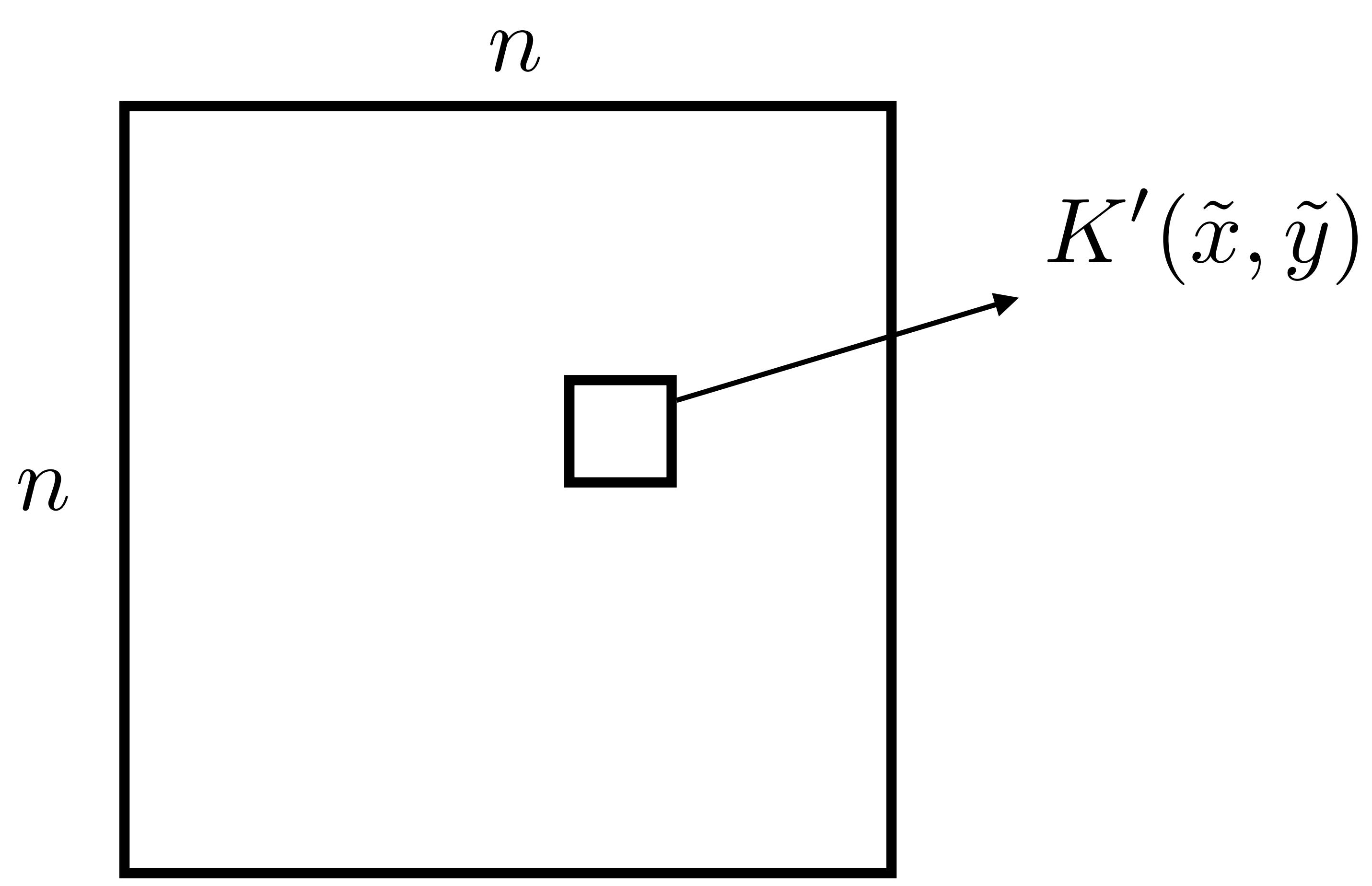




Kernel Function

$$K(x, y) \in [0, 1]$$

$$K(x, y) \to 0 \text{ as } \|x - y\|_2 \to \infty$$



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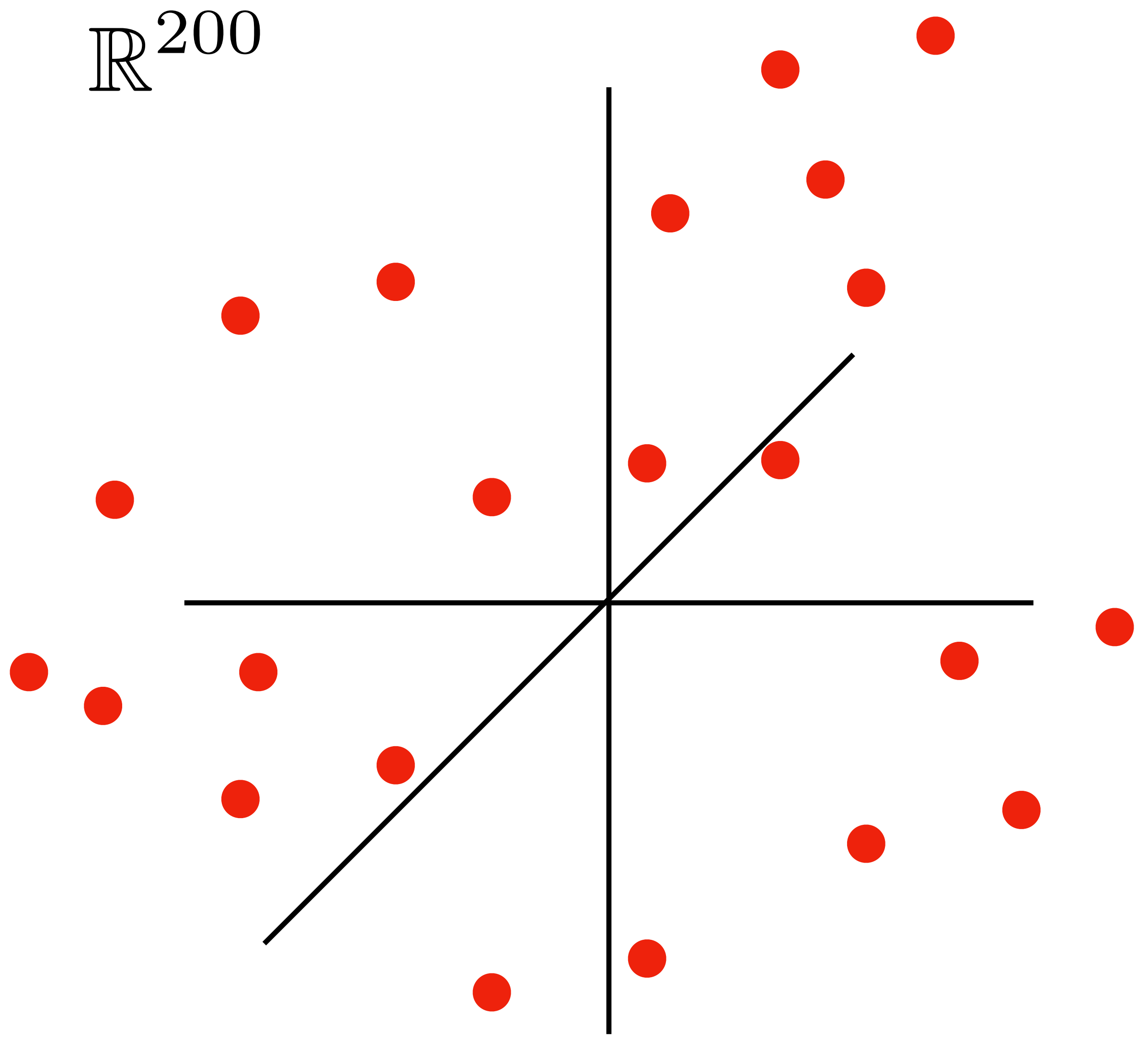

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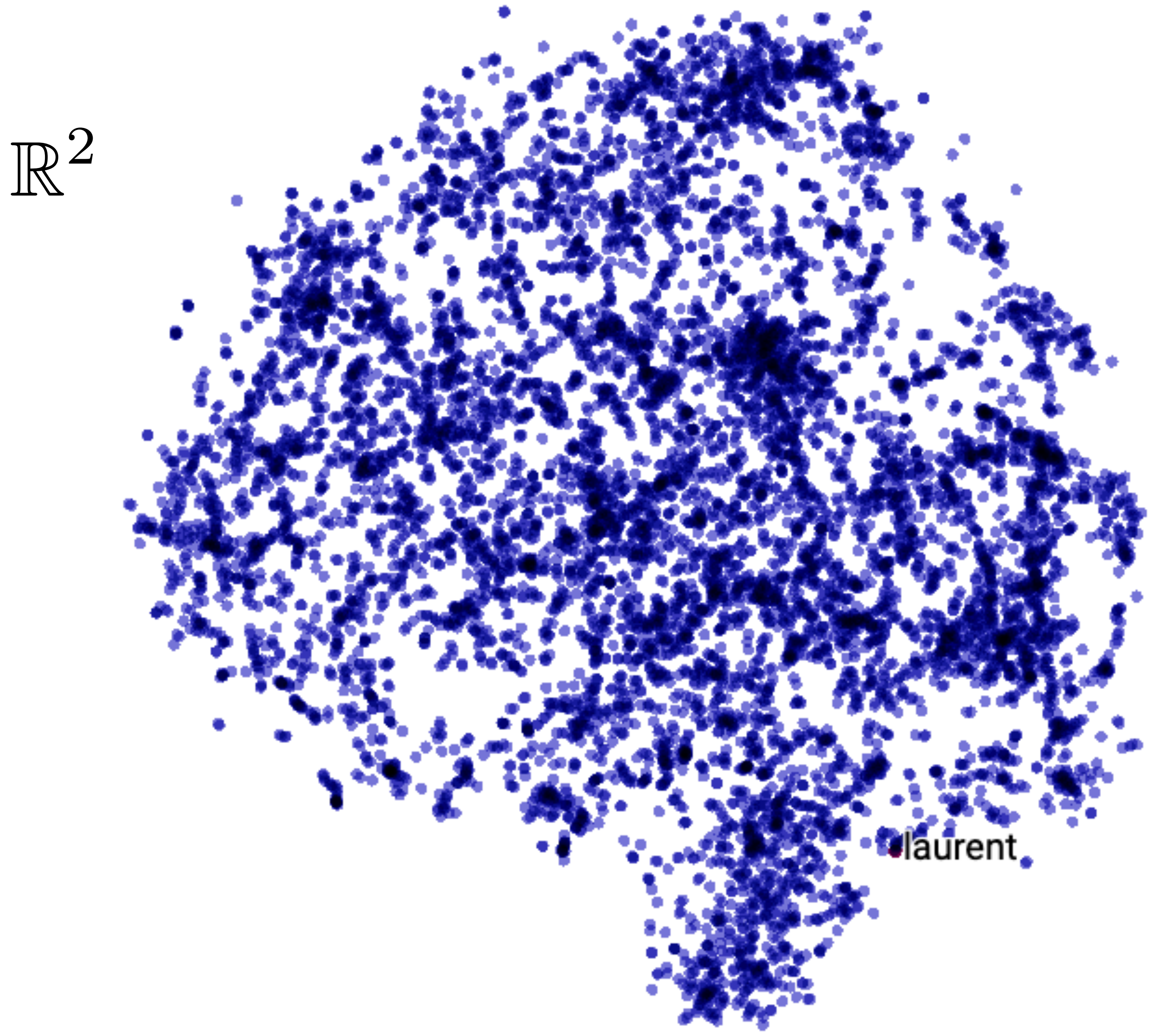

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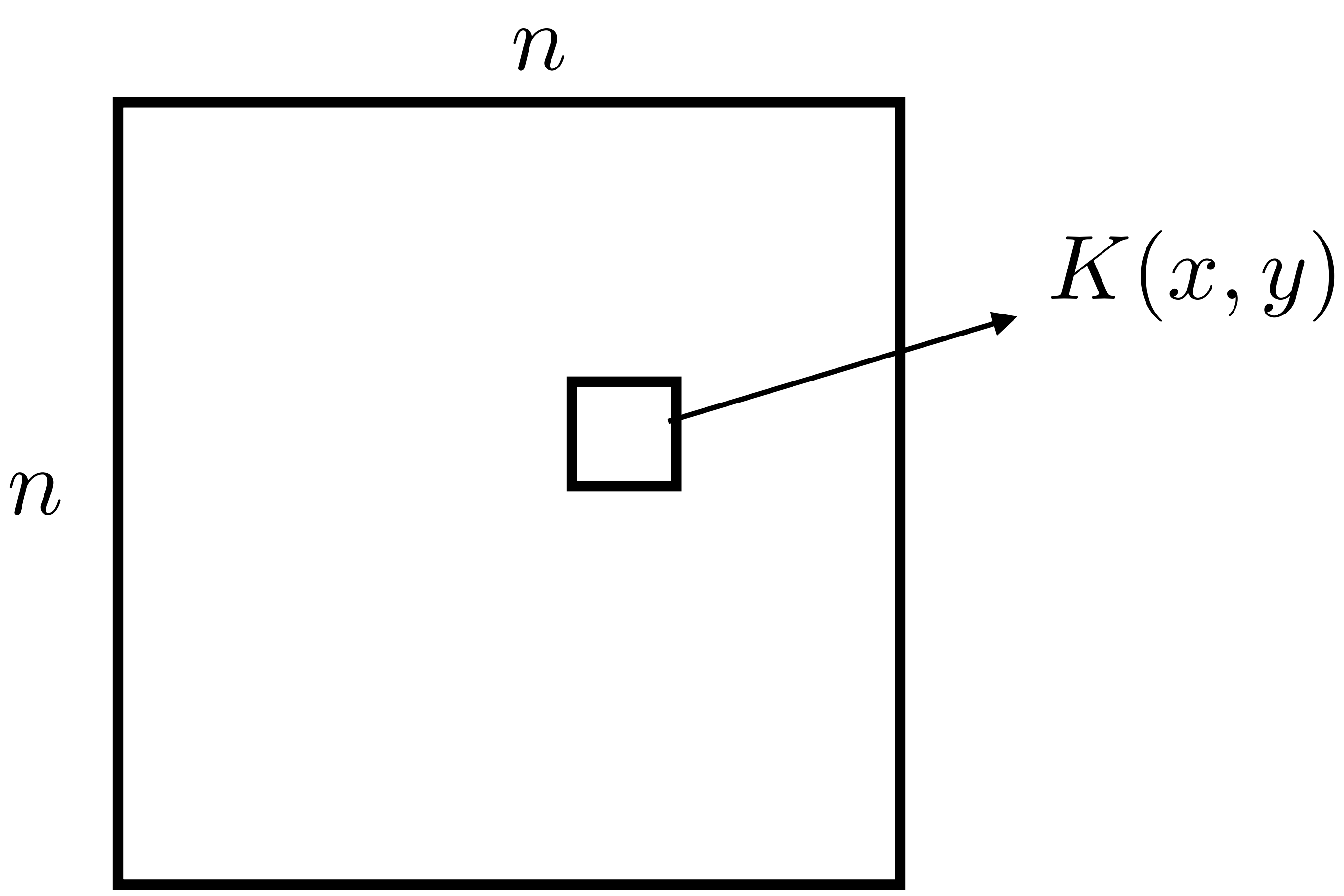
Ex: $K(x,y) = \exp\left(-\frac{\|x-y\|_2^2}{2\sigma^2}\right)$

$$K(x,y) = \left(1 + \|x-y\|_2^2\right)^{-1}$$



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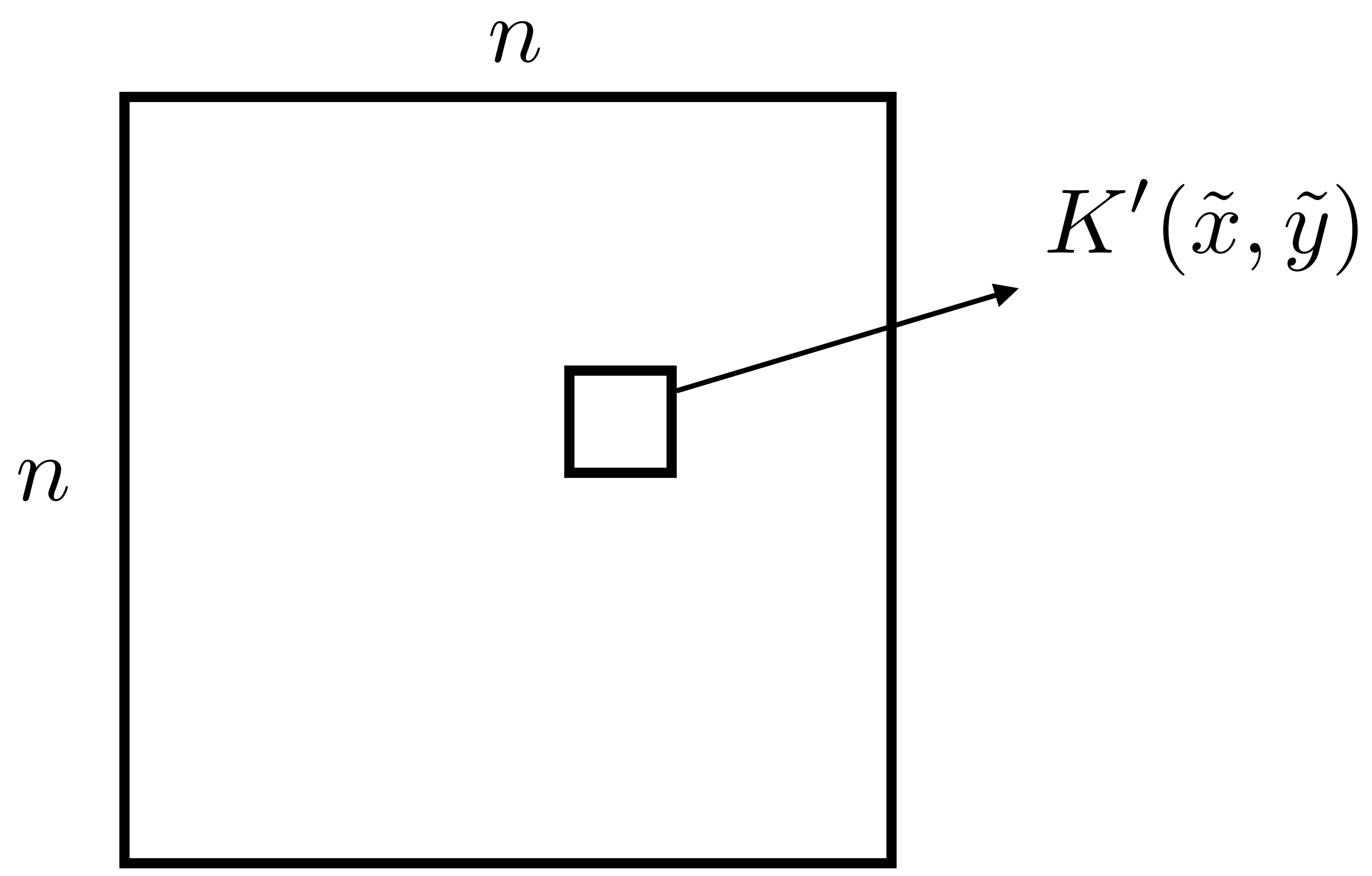
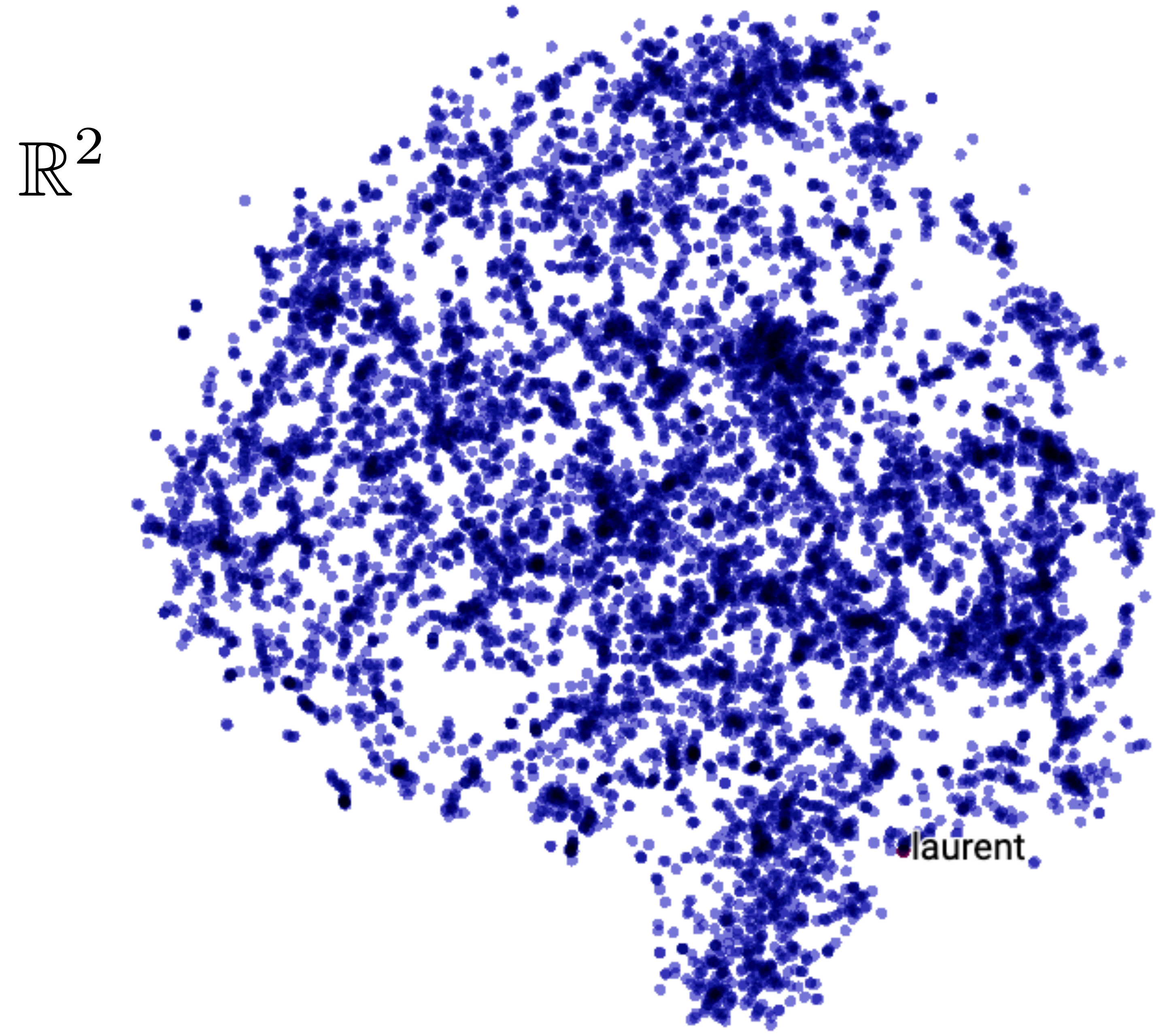
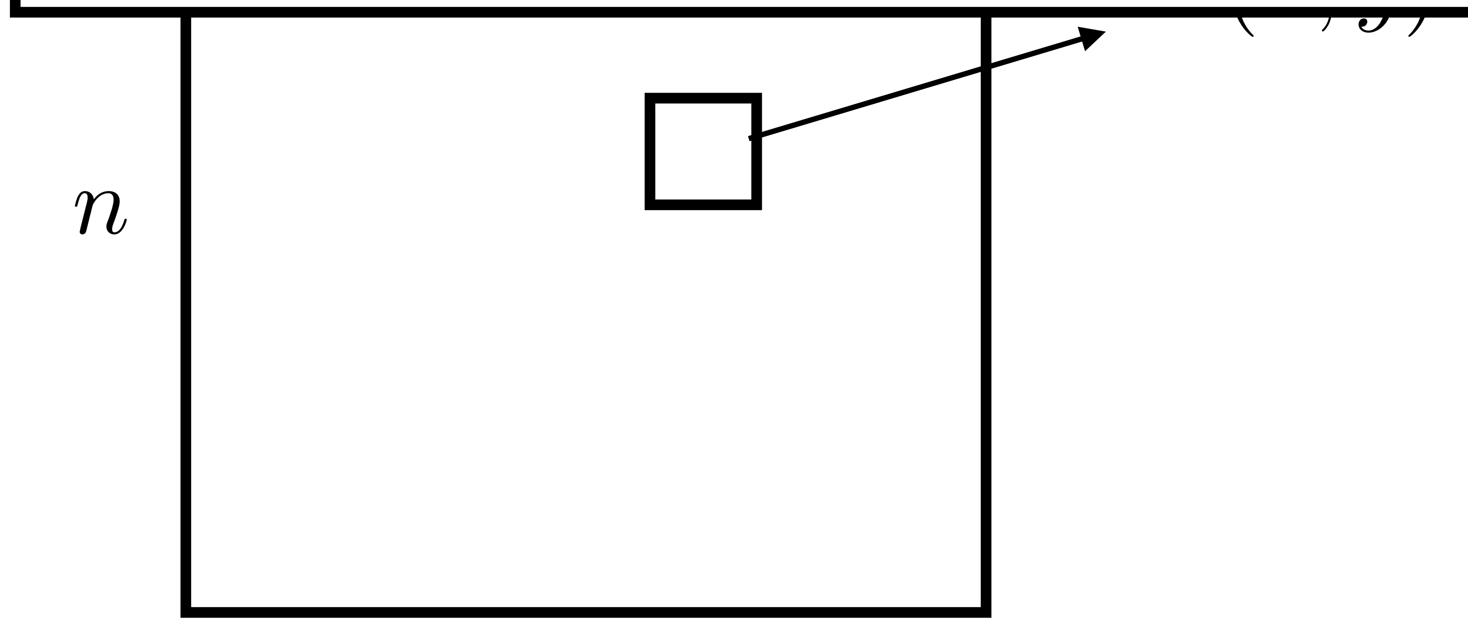


t-SNE: Visualization technique via "matching" geometric graphs.

- In low-dimensional space:
  - Computational geometry — kd-trees, ball-trees, vantage point trees, …, etc.
  - Scientific computing — fast multipole methods, n-body simulations, …, etc.





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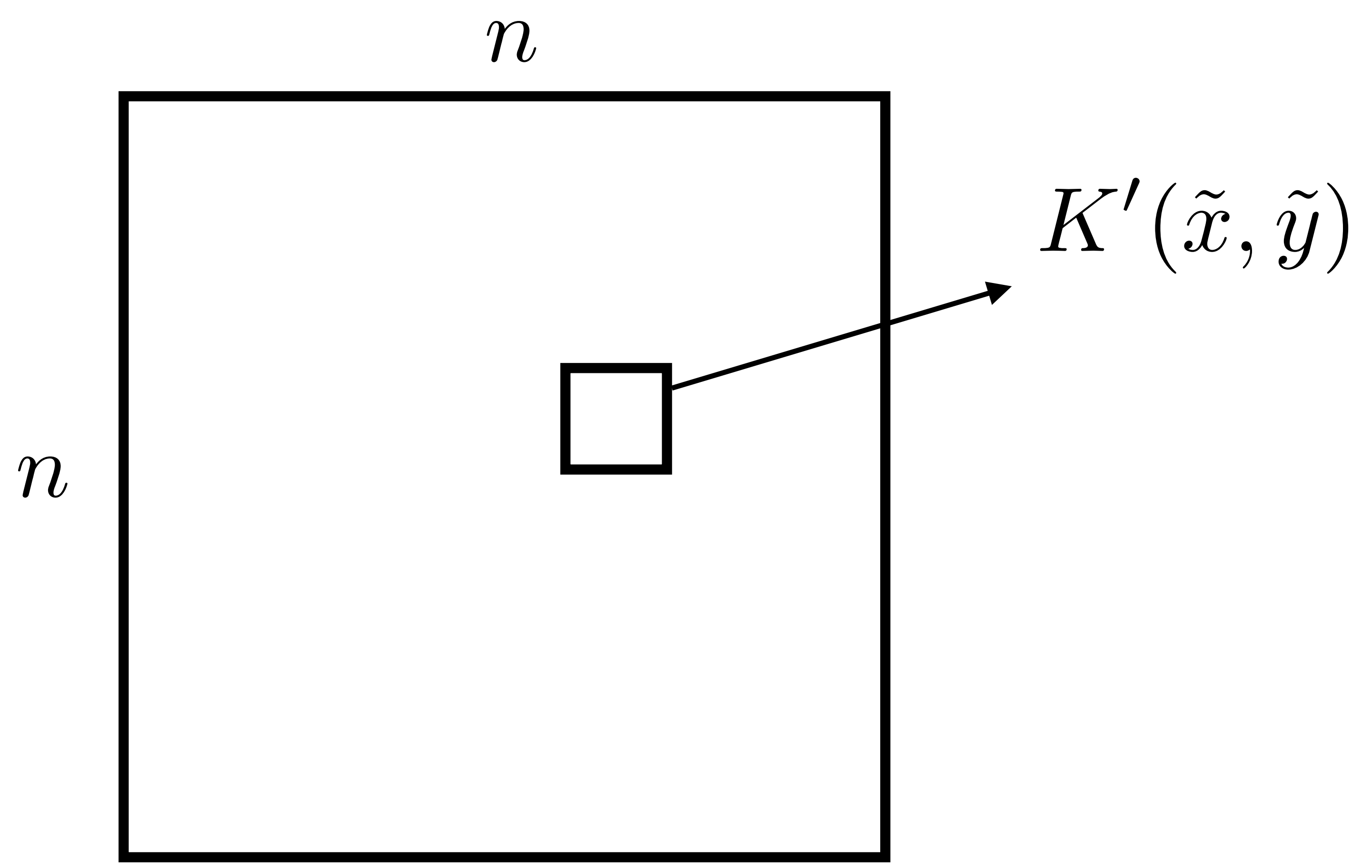

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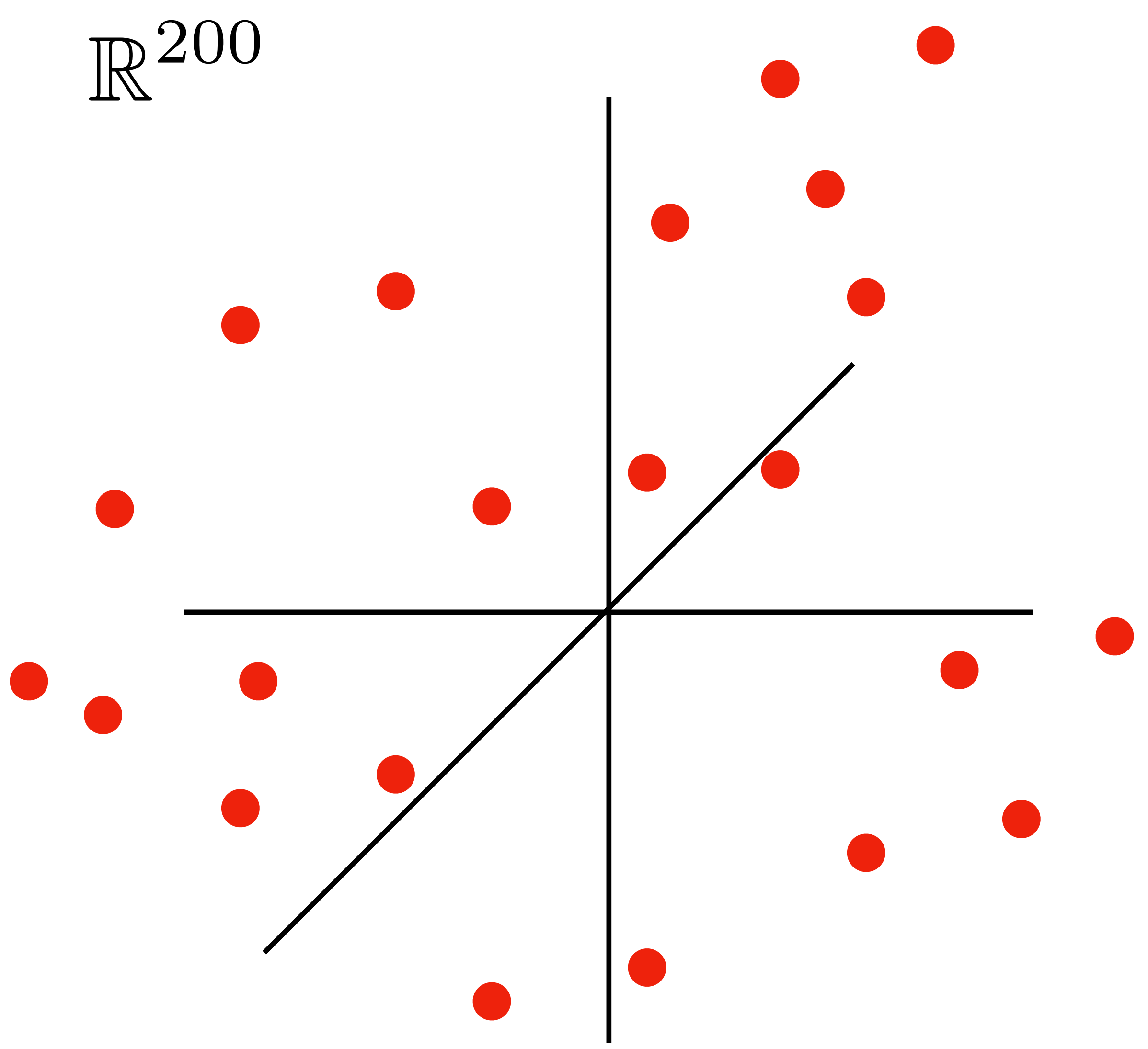
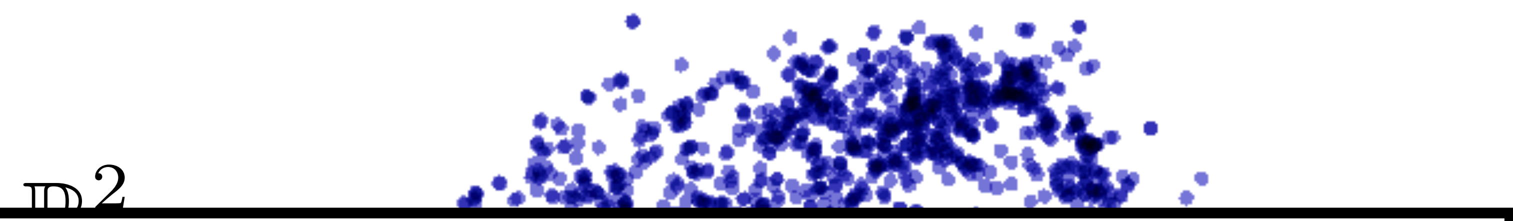
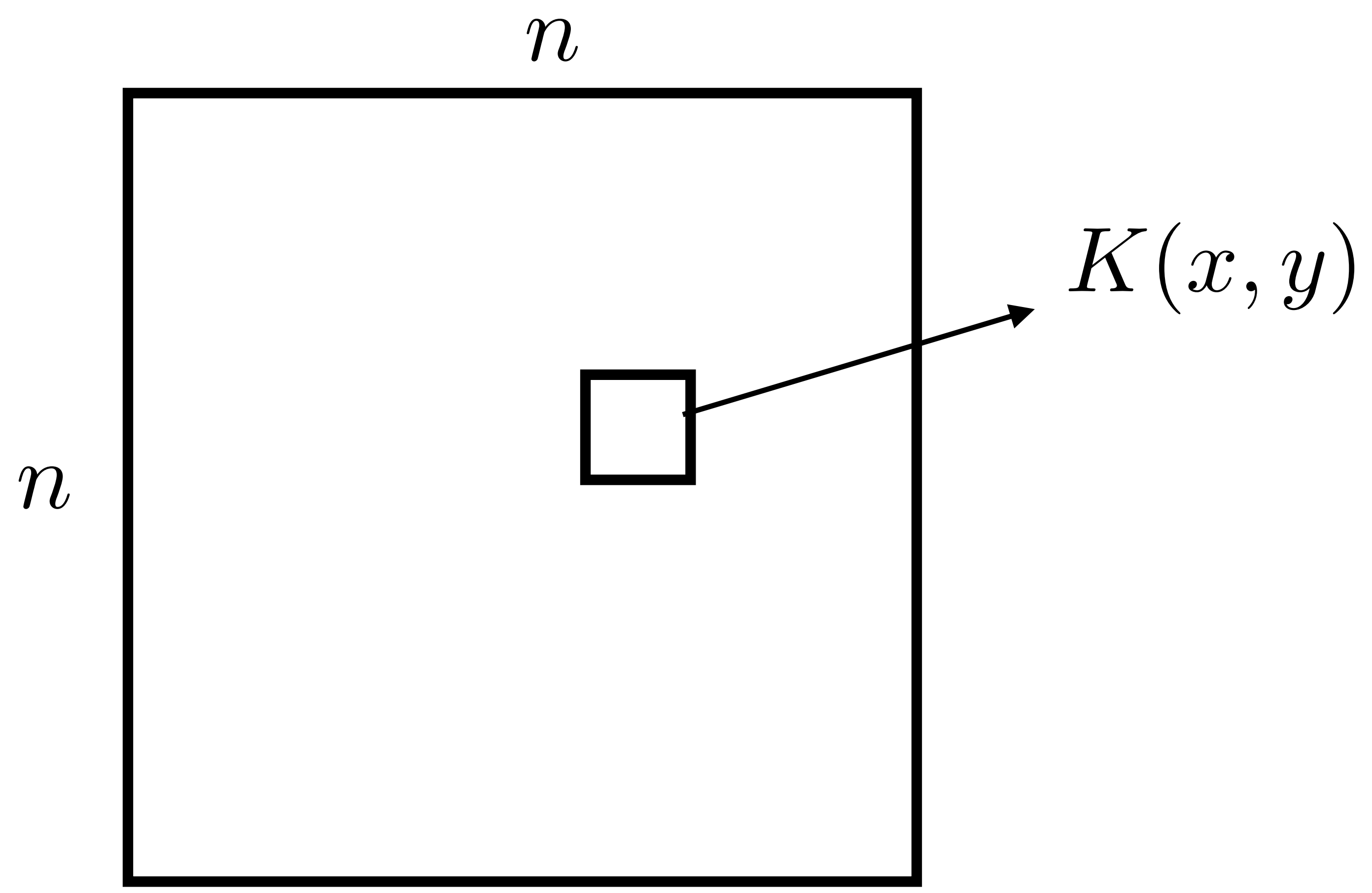




- In high-dimensional space:

  - Currently, explicitly working with nxn matrix
  - Incorporate tools from TCS:
    - LSH, sketching, random projections, coresets, …, etc.



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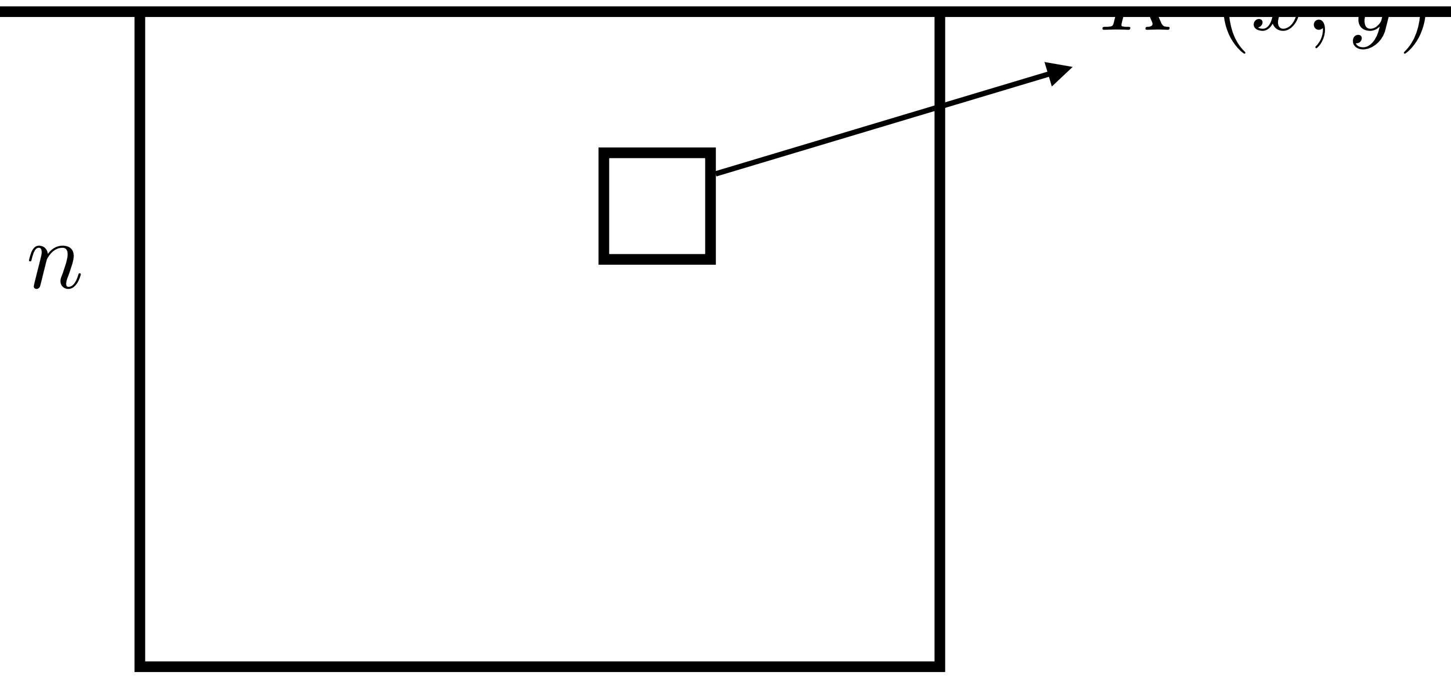
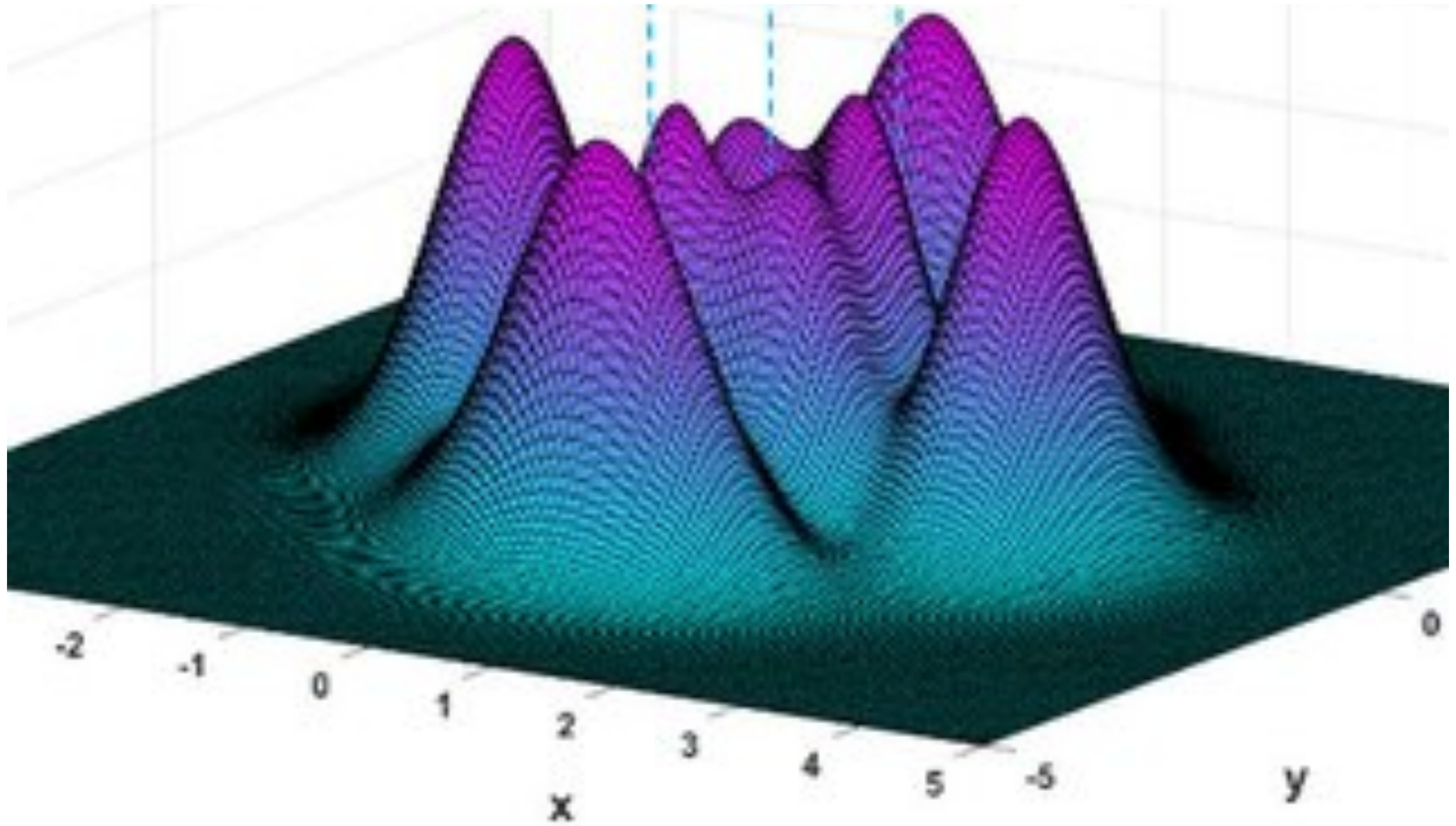


Kernel Density Evaluation: Estimating "Degree" in Geometric Graph



$$K(P,q) = \frac{1}{|P|}\sum_{p \in P} K(p,q) \stackrel{\text{def}}{=} \mu$$

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Kernel Density Estimation (KDE)

Preprocess: a dataset $P \subset \mathbb{R}^d$

Query: a point $q \in \mathbb{R}^d$

Compute $K(P,q)$ (approximately)

Time-Space Tradeoffs
for $(1+\epsilon)$-approx w.h.p

[Charikar-Siminelakis '17,
Backurs-Charikar-Indyk-Siminelakis '18,
Alman, Chu, Schild, Song '20, …, etc]

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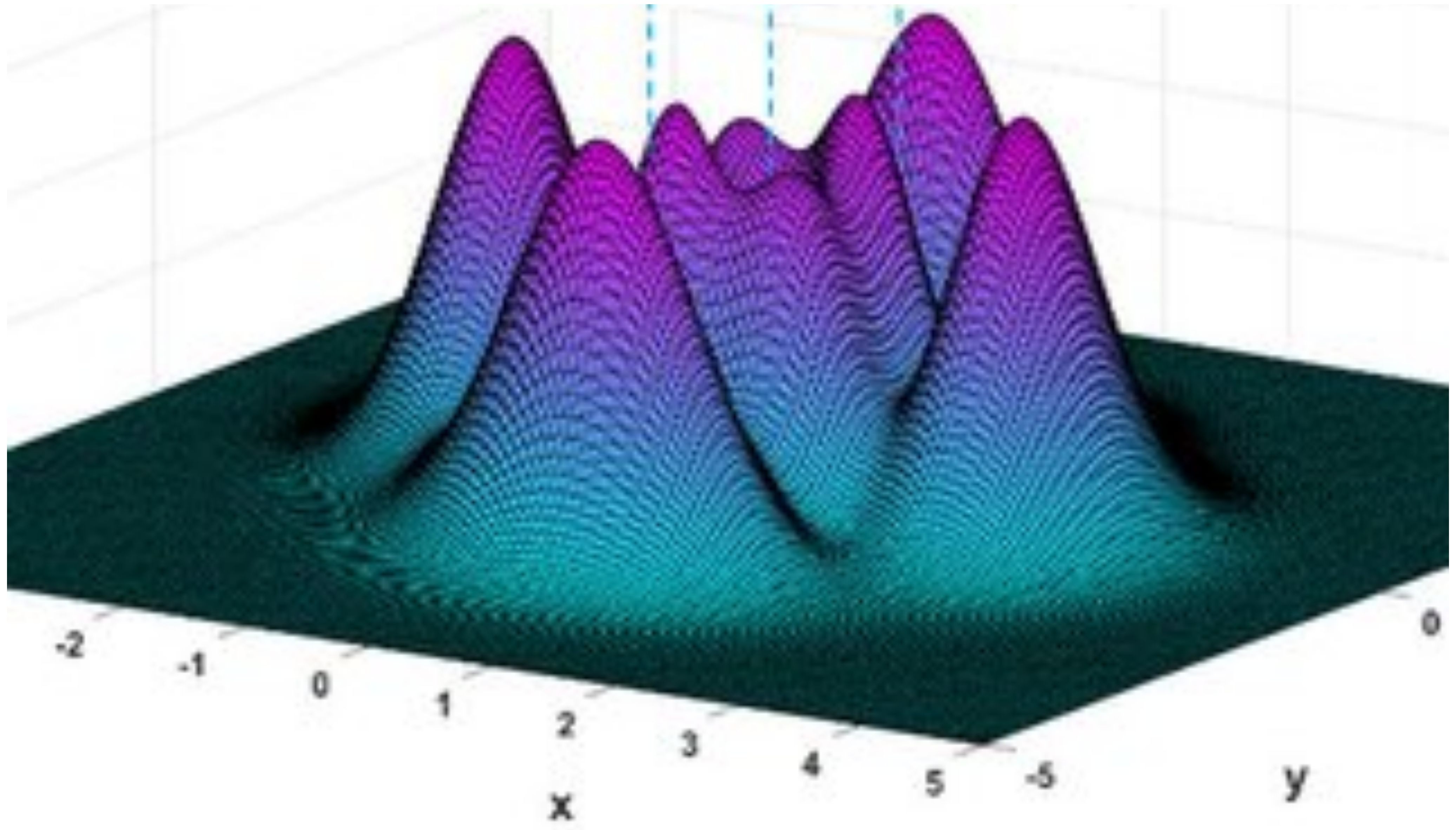

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Trivial: $O(nd)$ query time.

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Two approaches for "beating $O(nd)$ query time"

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$$O\left(\frac{1}{\mu\epsilon^2}\right)$$

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Our work:

$$\frac{\text{polylog}(1/\mu)}{\epsilon}$$

(smooth)

LSH Sampling
[Charikar, Siminelakis '17]

$O\left(\frac{1}{\sqrt{\mu}\epsilon^2}\right)$, $\frac{\text{polylog}(1/\mu)}{\epsilon^2}$ (smooth)

[Backurs, Charikar, Indyk, Siminelakis '18]

Coresets via Discrepancy
[Phillips-Tai '20]

$$O\left(\frac{1}{\mu\epsilon}\right)$$

Random/LSH Sampling

Store $\boldsymbol{p}_1, \ldots, \boldsymbol{p}_t \sim P \subset \mathbb{R}^d$

Query: $\frac{1}{t}\sum_{i=1}^{t} K(\boldsymbol{p}_i, q)$

Random

$$\mathbf{E}\left[\frac{1}{t}\sum_{i=1}^{t} K(\boldsymbol{p}_i, q)\right] = \mu$$

Chebyshev:

$$\mathbf{Pr}\left[\begin{array}{c}\text{accurate}\\ \text{estimate}\end{array}\right] \leq \frac{1}{(\epsilon\mu)^2} \cdot \boxed{\mathbf{Var}}$$

LSH

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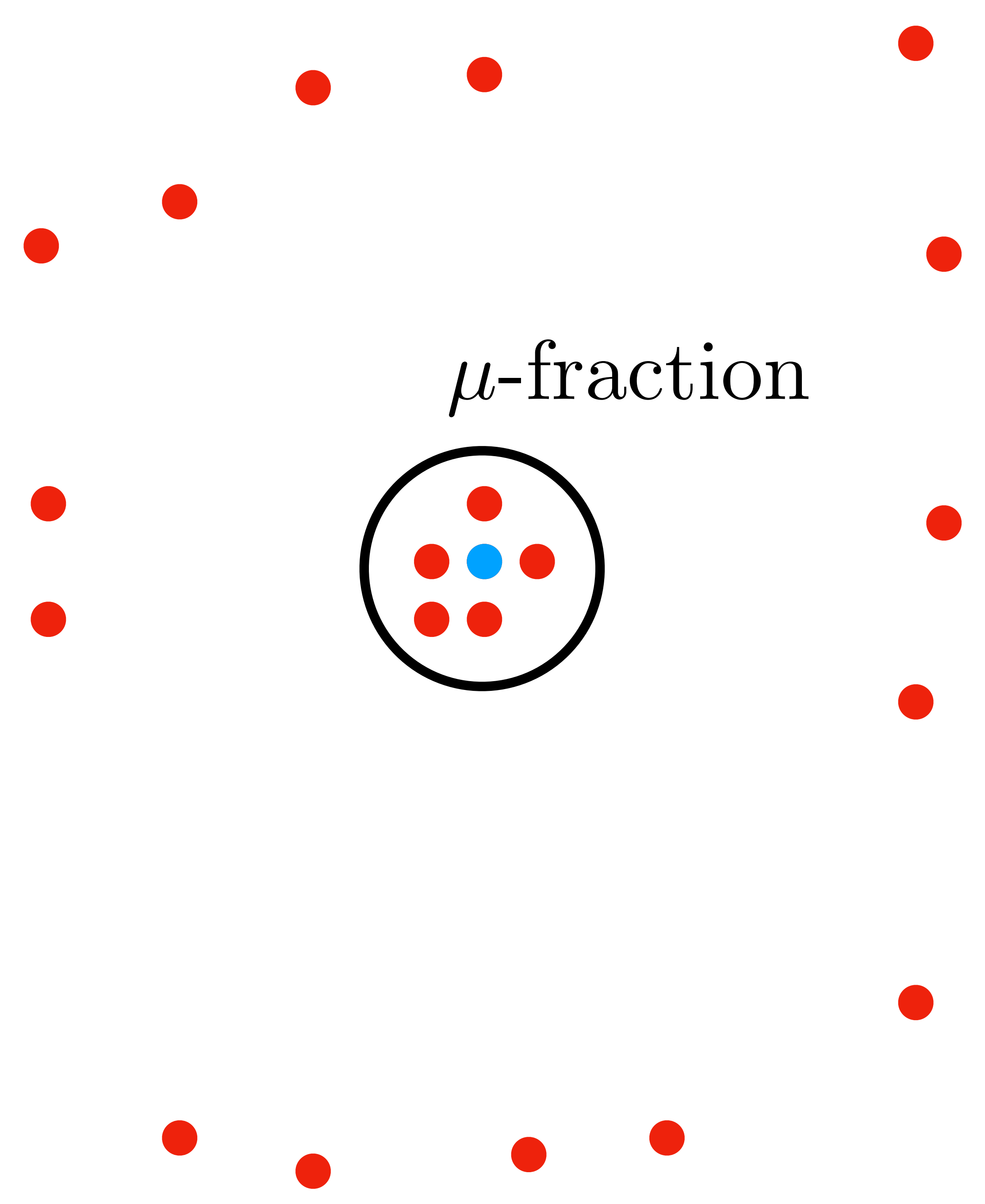

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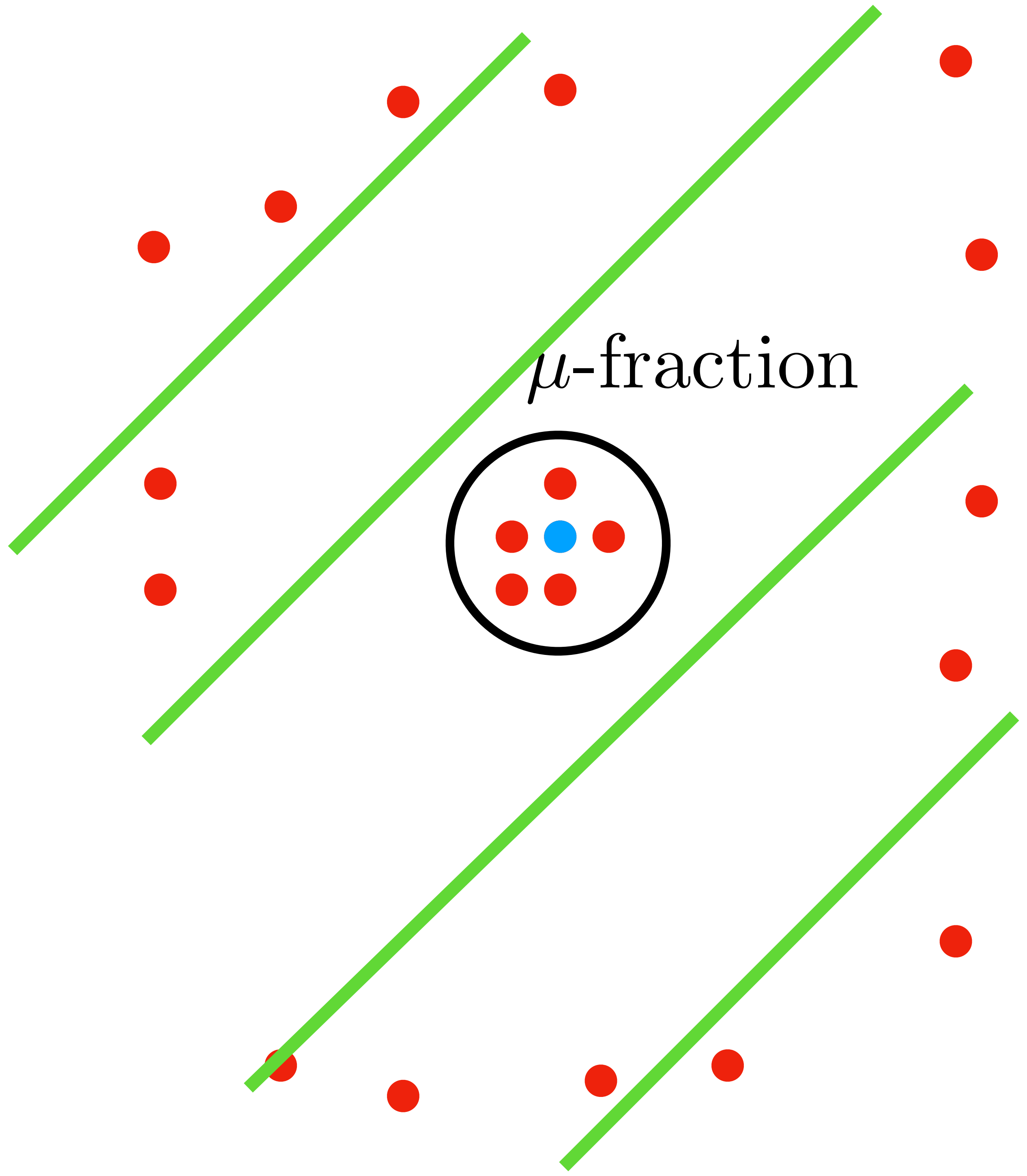

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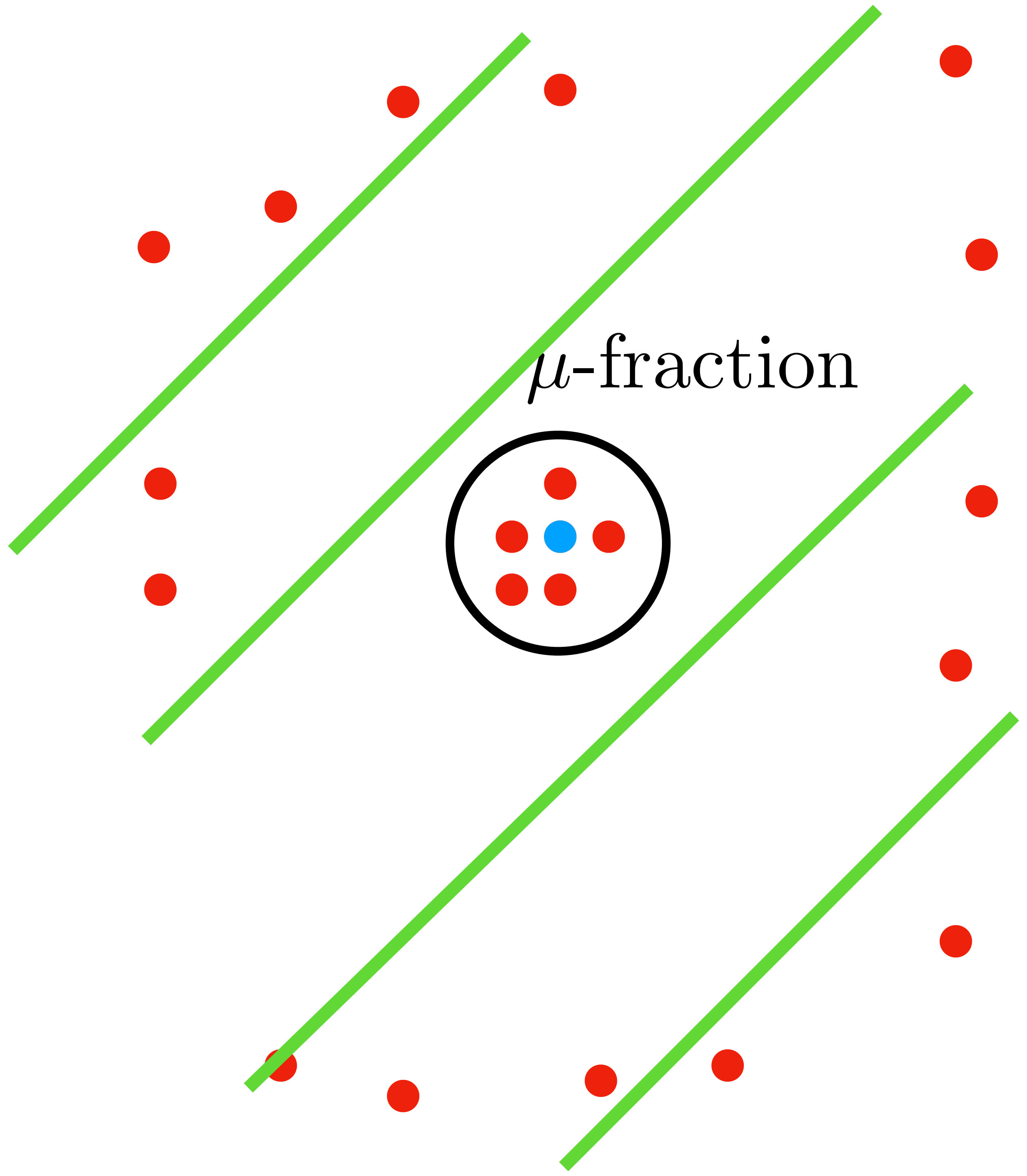

LSH

[Charikar, Siminelakis '17]

$$O\left(\frac{1}{\sqrt{\mu}\epsilon^2}\right)$$

[Backurs, Charikar Indyk, Siminelakis '18] (smooth)

$$\frac{\text{polylog}(1/\mu)}{\epsilon^2}$$

<u>Coresets via Discrepancy</u> (PSD)

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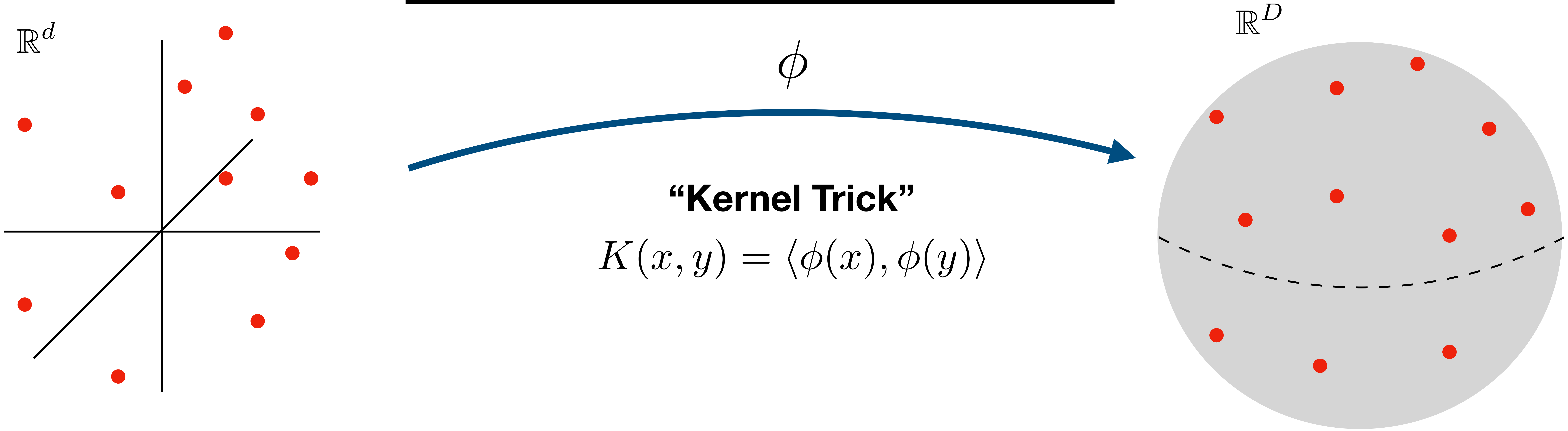

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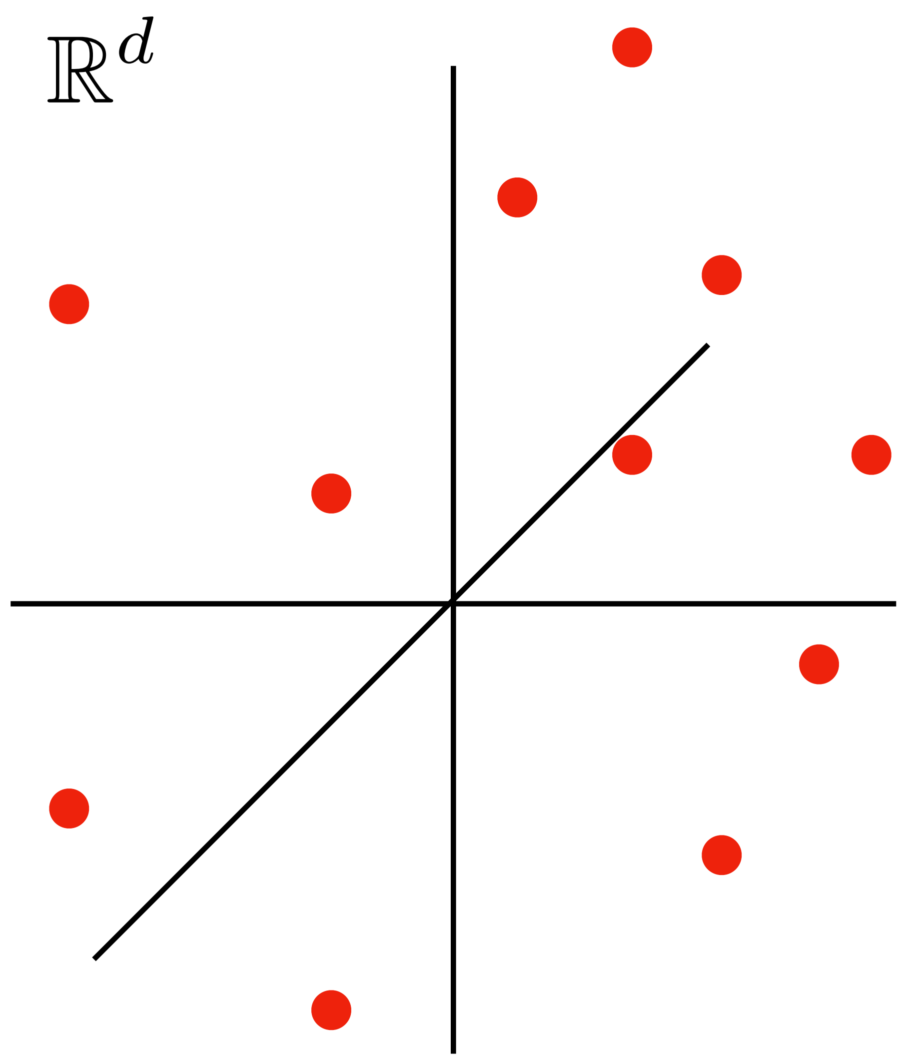

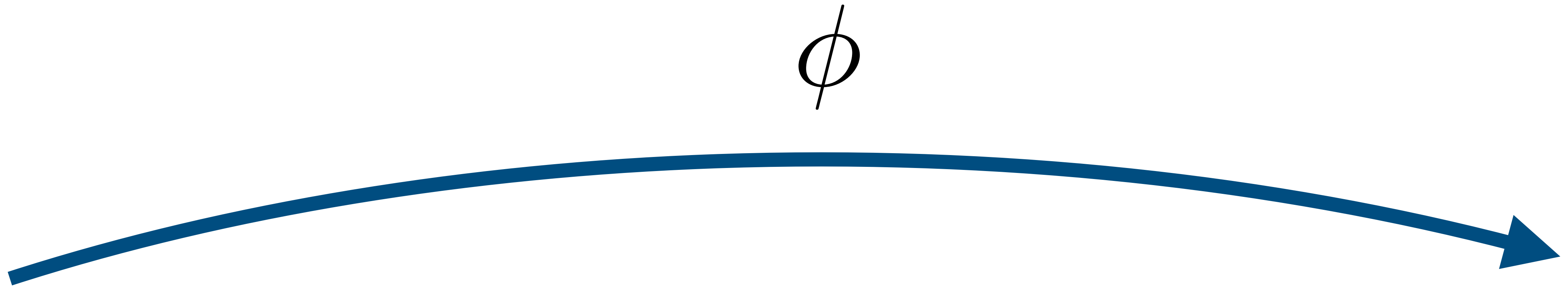

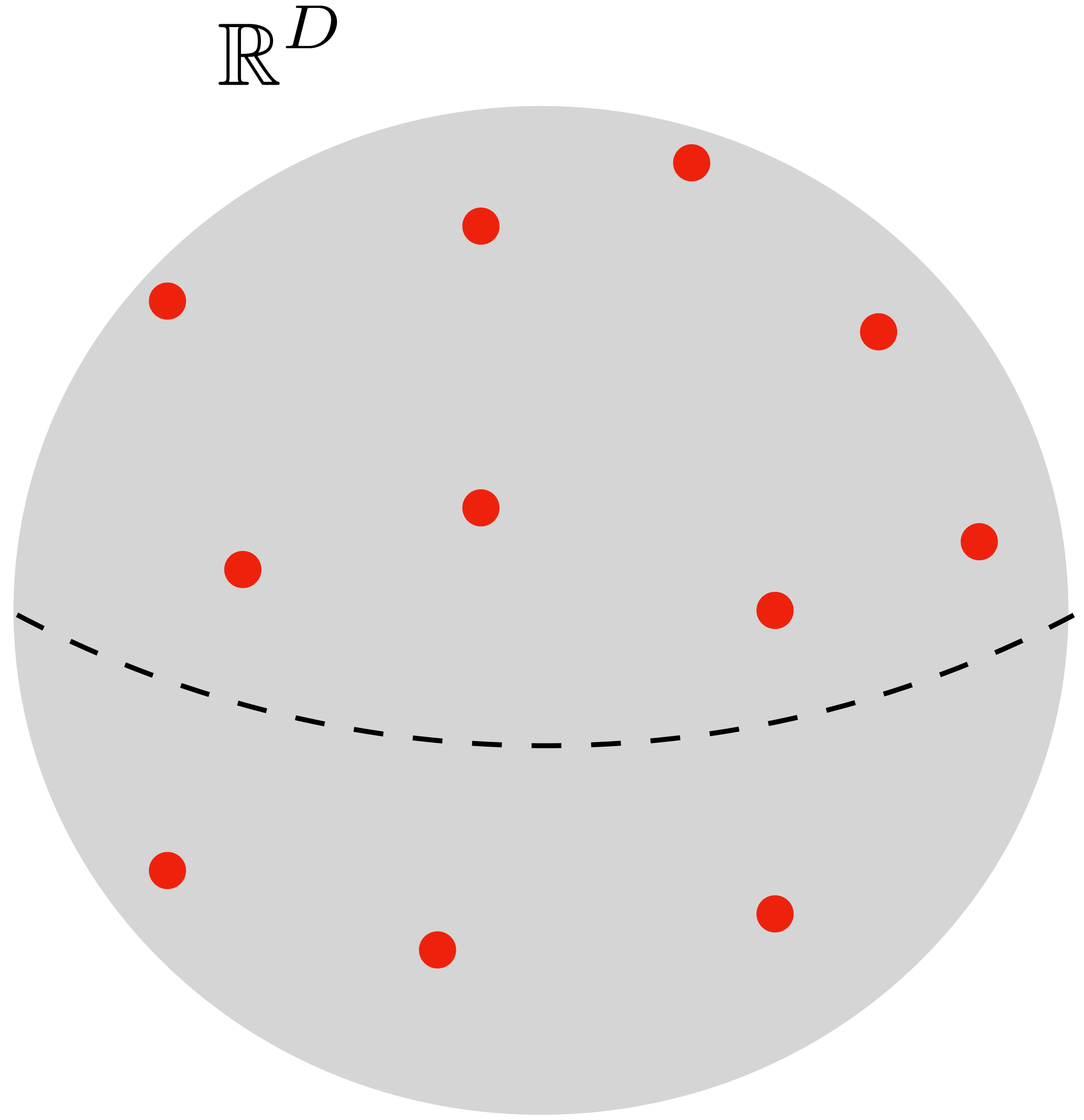

“Kernel Trick”

$$K(x, y) = \langle \phi(x), \phi(y) \rangle$$

“Halving Technique”

How to decrease your dataset by a factor of 2?

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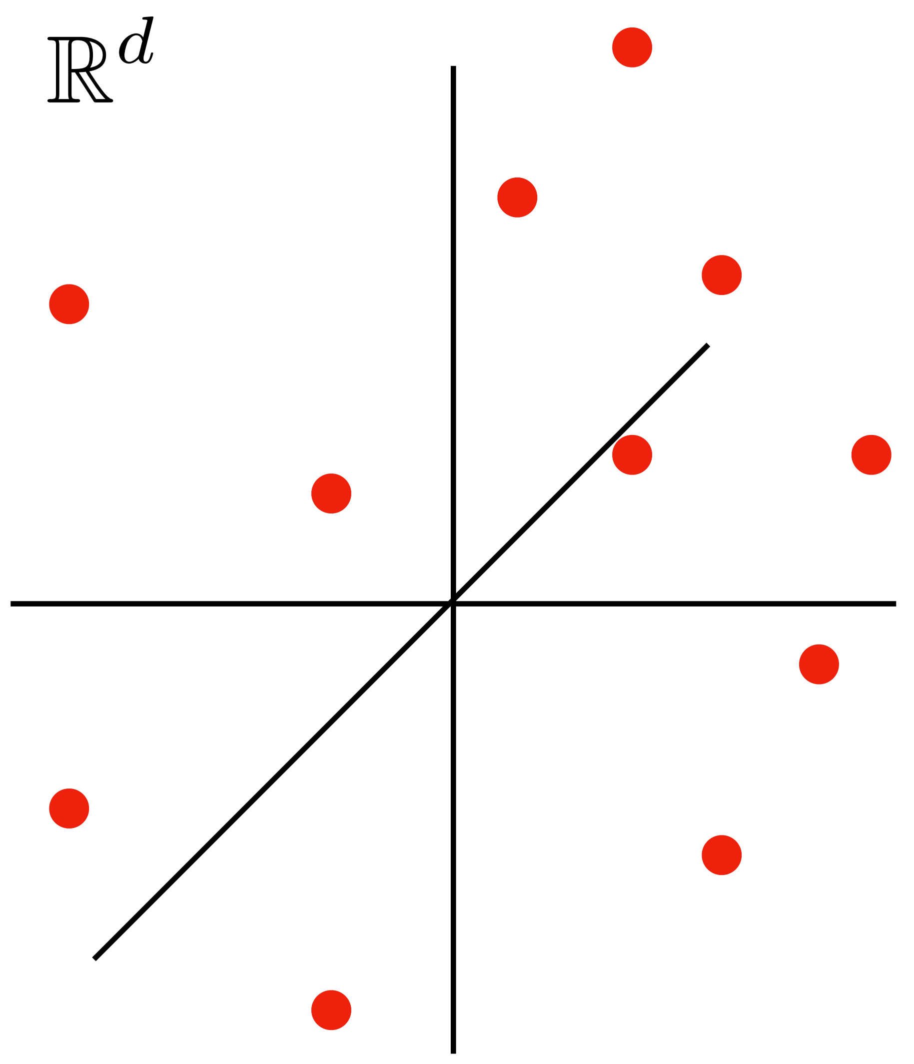

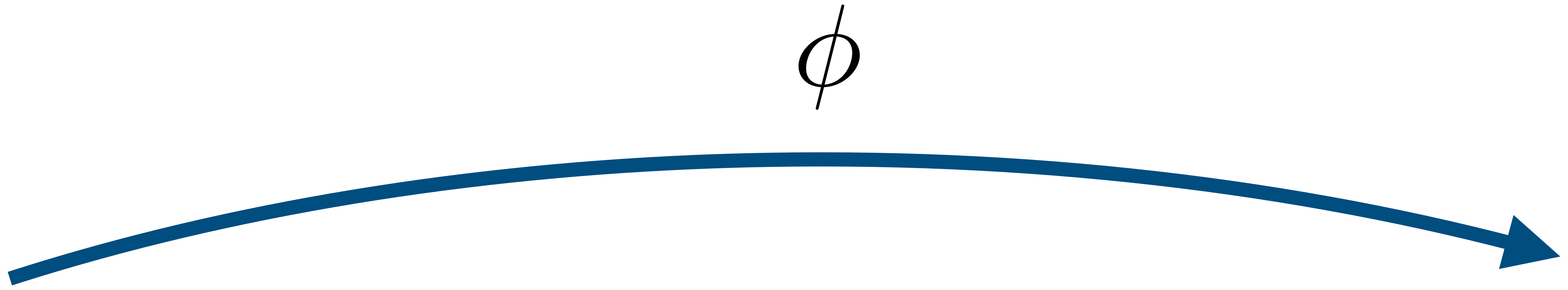

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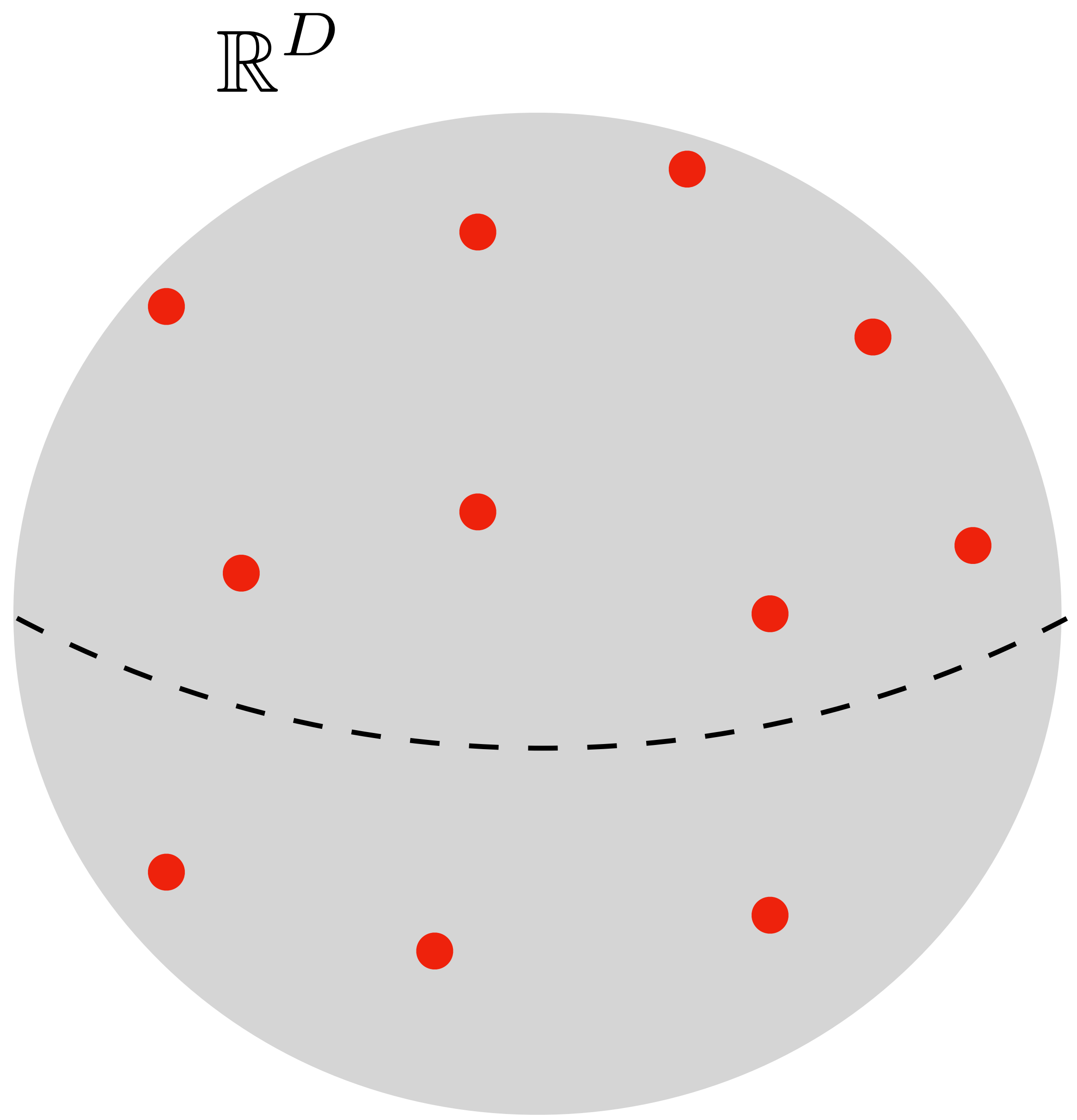

Vector Balancing:

Find a setting of signs $a_1, \dots, a_n \in \{-1, 1\}$ such that for (unknown) query q we minimize

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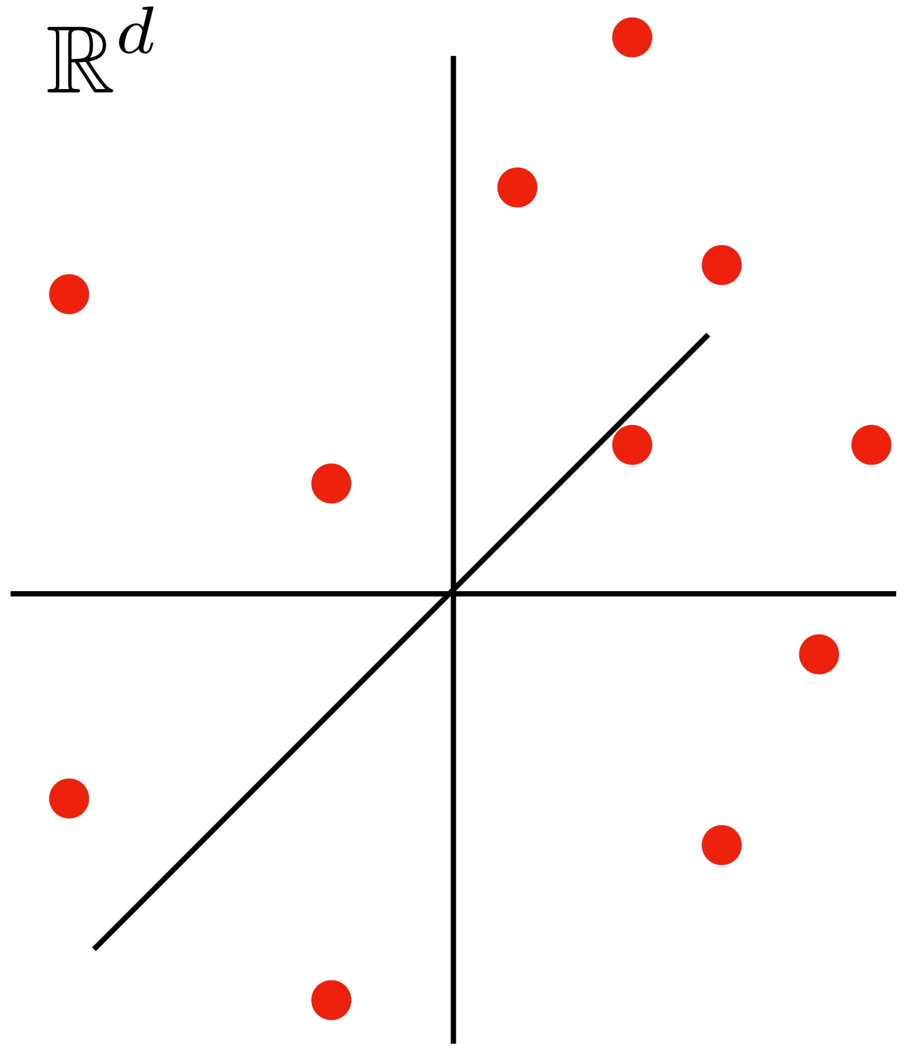

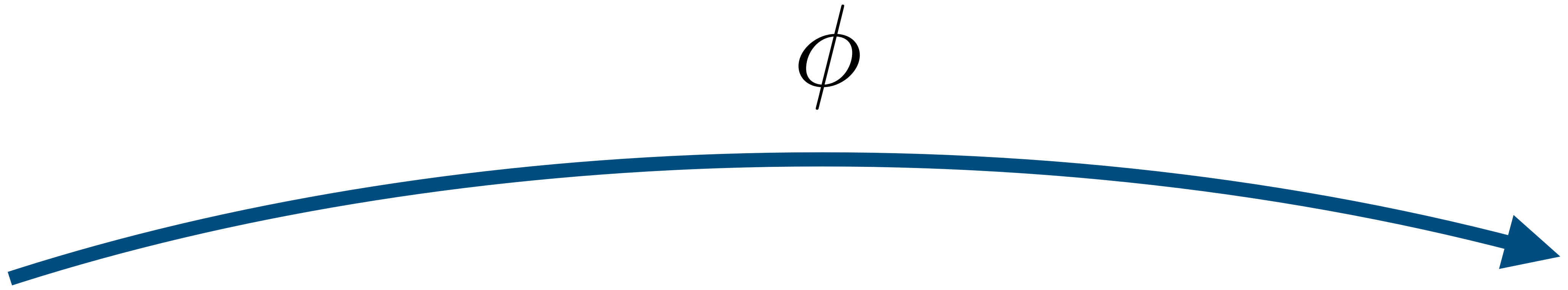

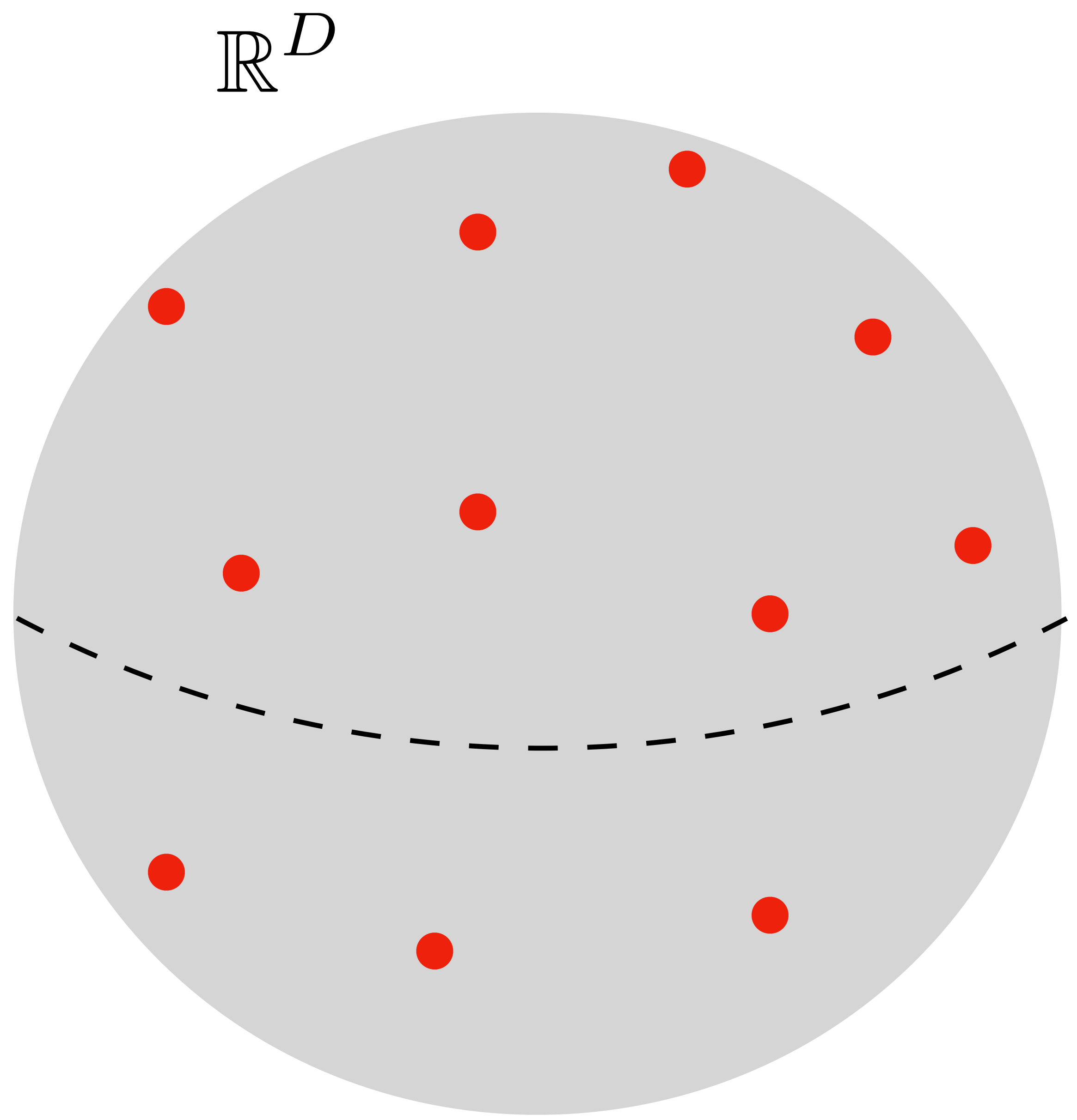

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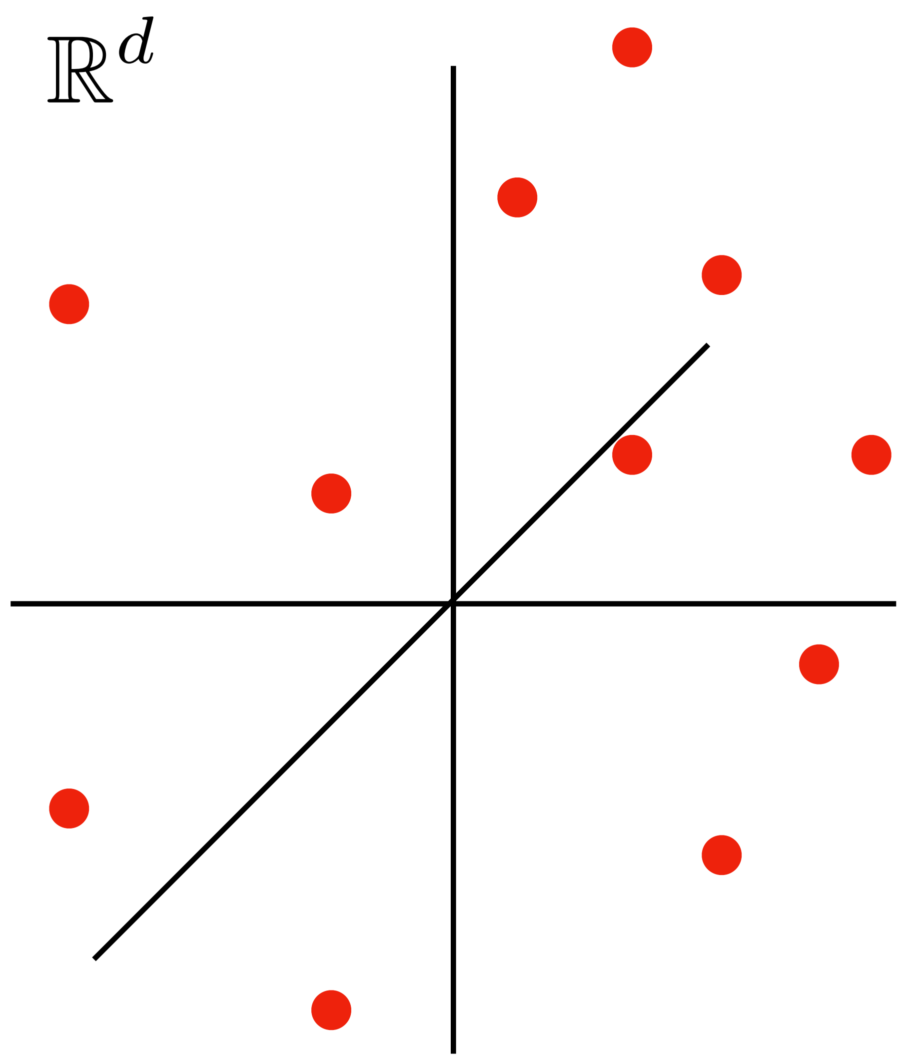

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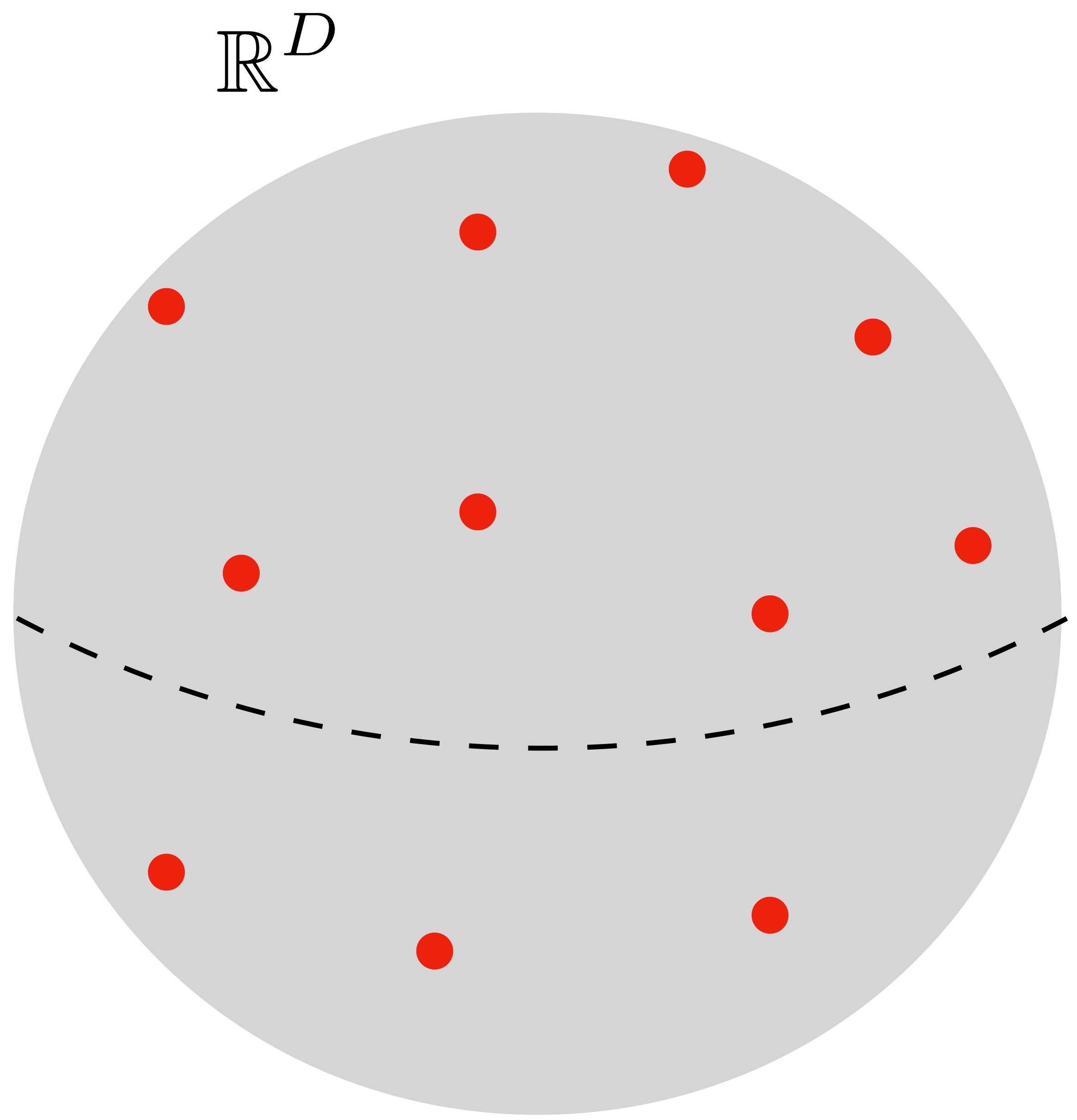

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As long as dataset is large, error incurred is at most $1/|P|$

$\longrightarrow \tilde{O}\left(\frac{1}{\mu \epsilon}\right)$

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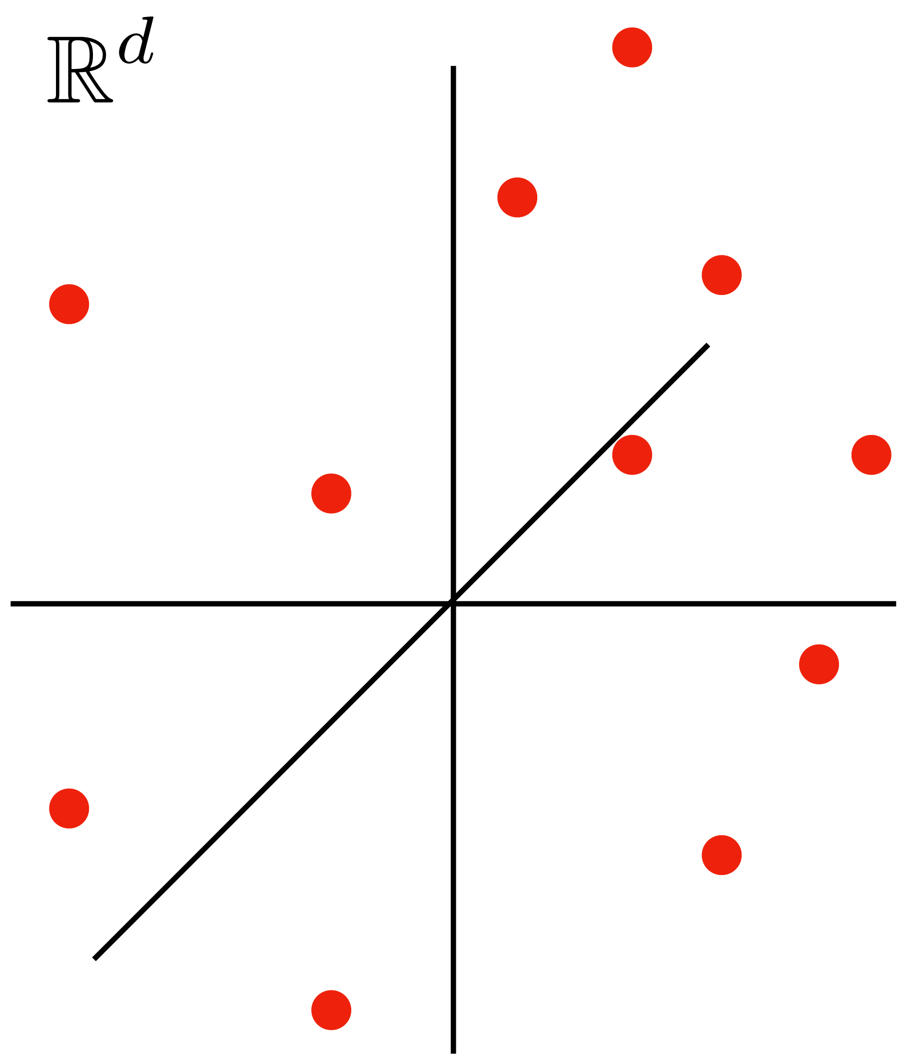

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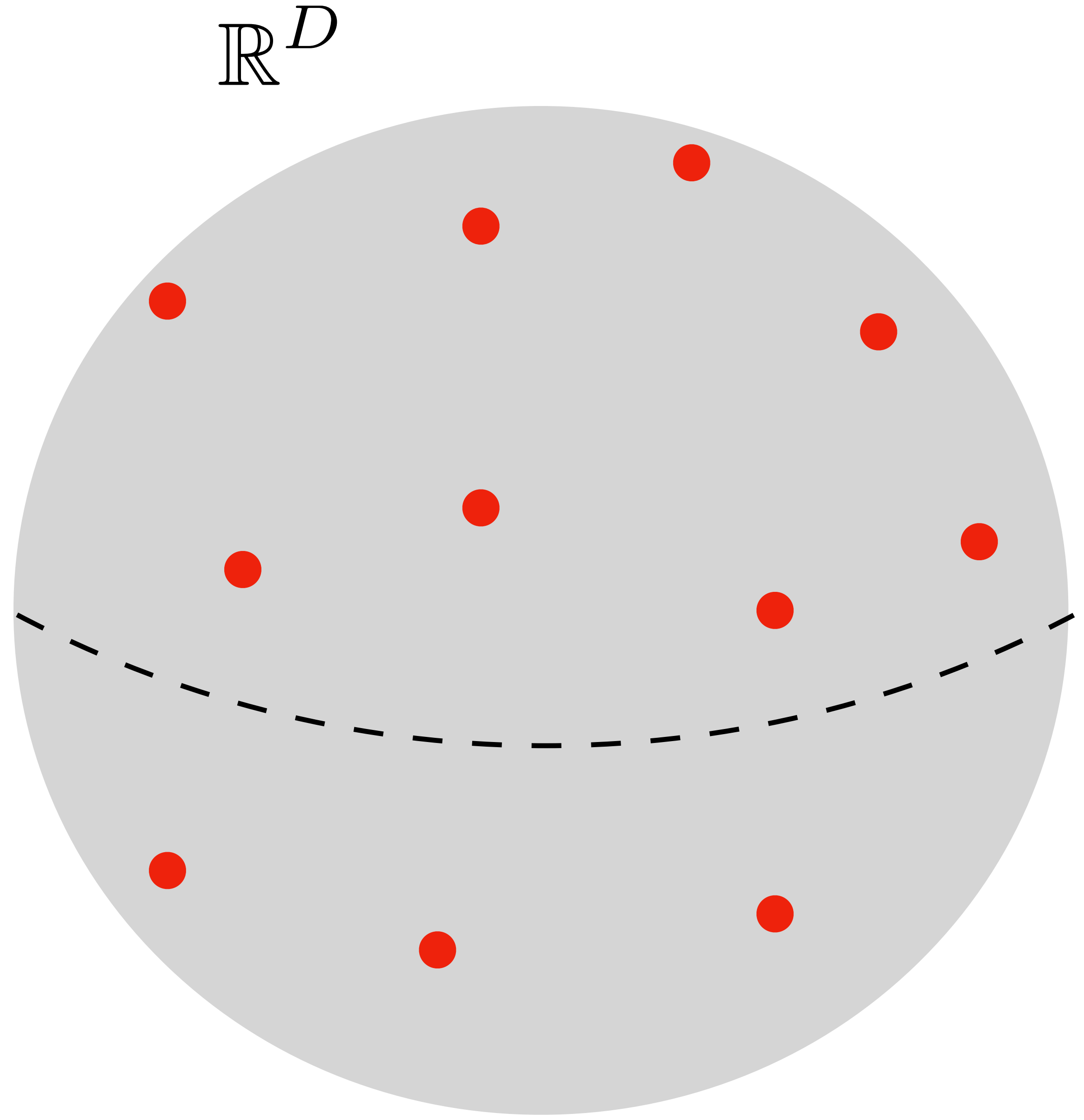

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Main Idea?

1. Apply LSH.
2. Run discrepancy after.

Basics of Discrepancy Minimization

"Simplest" PSD Kernel:

- Linear kernel: $K(x, y) = x^\intercal y$

- 1-dimensional :-): $K(x, y) = x \cdot y$

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- **You know** $p_1, \ldots, p_n \in \mathbb{R}$
- **You don't know** q

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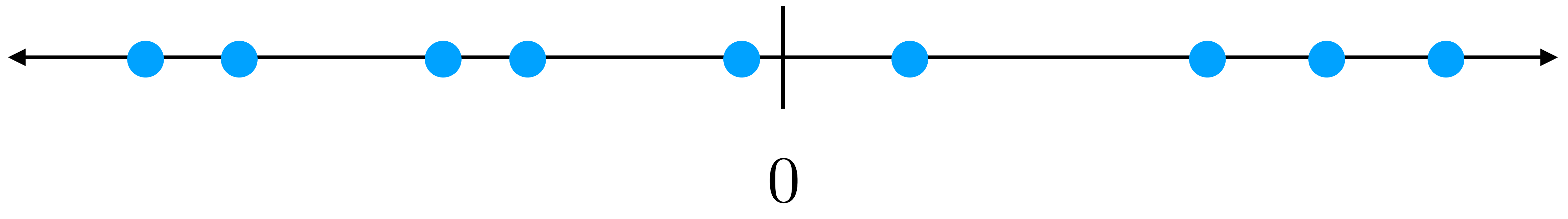

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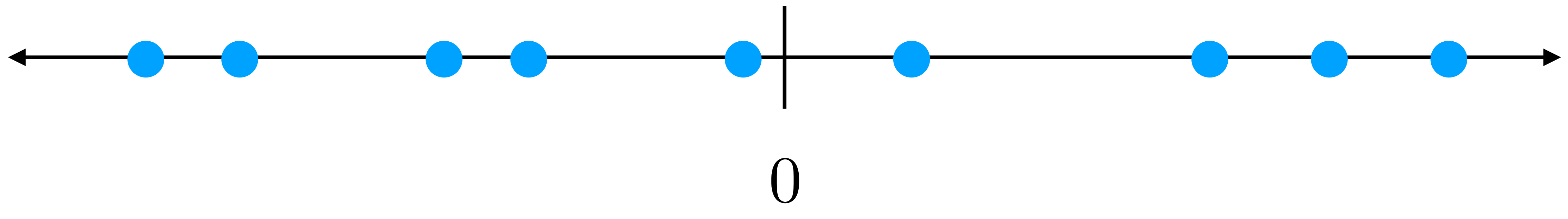

Random signs: $|q| \cdot \left(\sum_{i=1}^{n} p_i^2 \right)^{1/2}$

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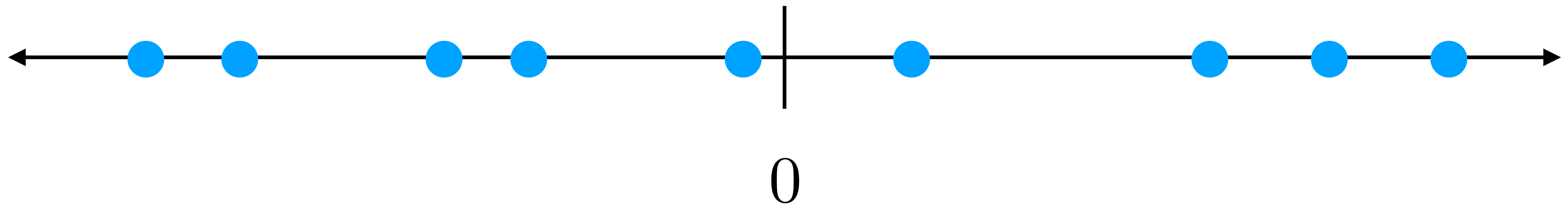


Random signs: $|q| \cdot \left(\sum_{i=1}^{n} p_i^2 \right)^{1/2}$

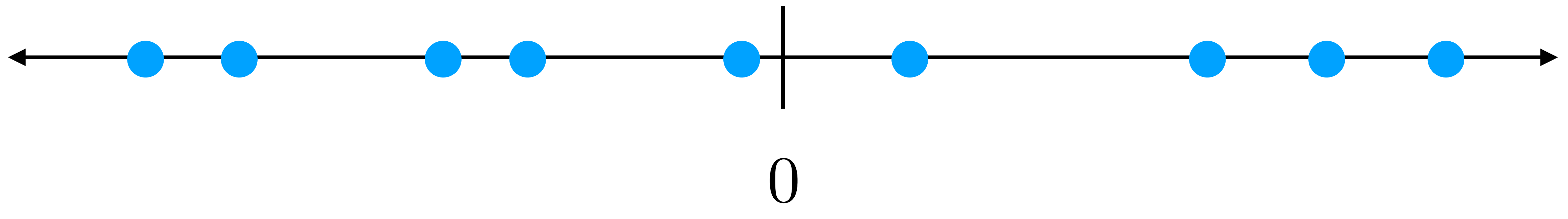
Greedy balance:

Basics of Discrepancy Minimization

"Simplest" PSD Kernel:

- Linear kernel: $K(x, y) = x^\intercal y$

- 1-dimensional :-): $K(x, y) = x \cdot y$



- "Discrepancy Minimization Task:"
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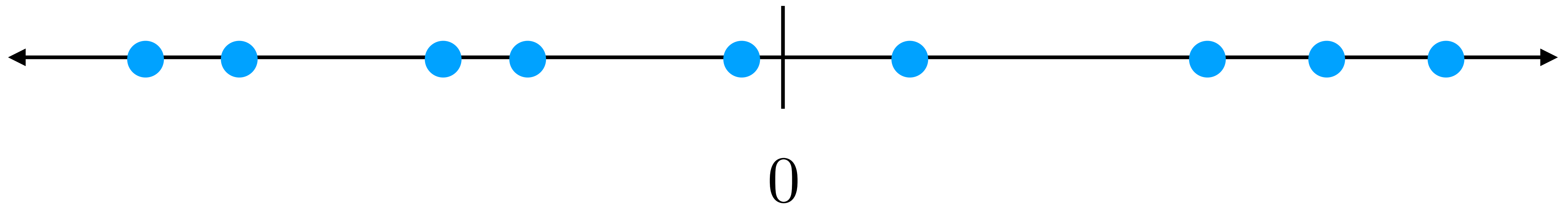

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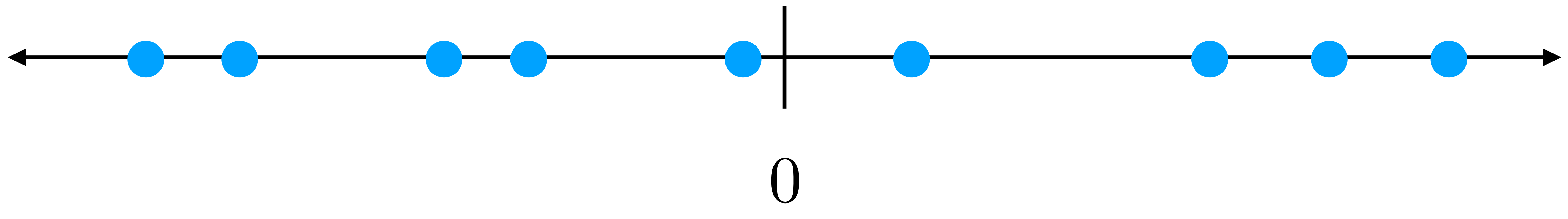

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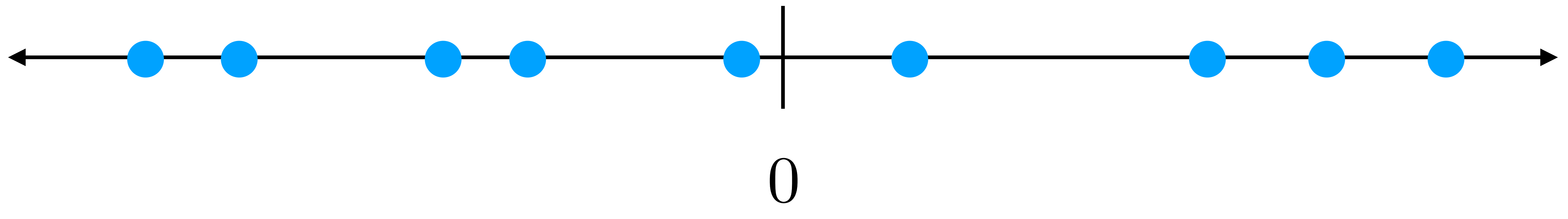

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"Gram-Schmidt Walk"

[Bansal, Dadush, Garg, Lovett '17]

"Self-balancing Walk"

[Alweiss, Liu, Sawhney '20]

$$\tilde{O}(1) \cdot \|\phi(q)\|_2 \cdot \max_i \|\phi(p_i)\|_2$$

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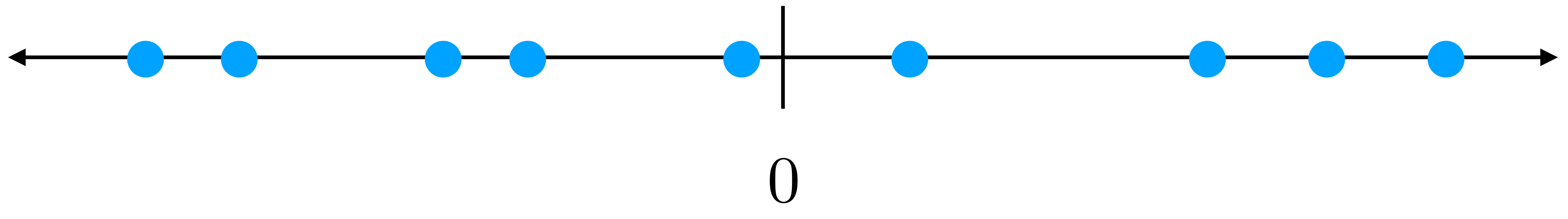

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$$\gamma_2(K) = \min_{\phi} \max_{q,p} \|\phi(q)\|_2 \|\phi(p)\|_2$$

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[Phillips-Tai '20]
PSD of Bounded Kernel Directly Applies

$K \colon \mathbb{R}^d \times \mathbb{R}^d \to [0,1]$

PSD and Radially Decaying

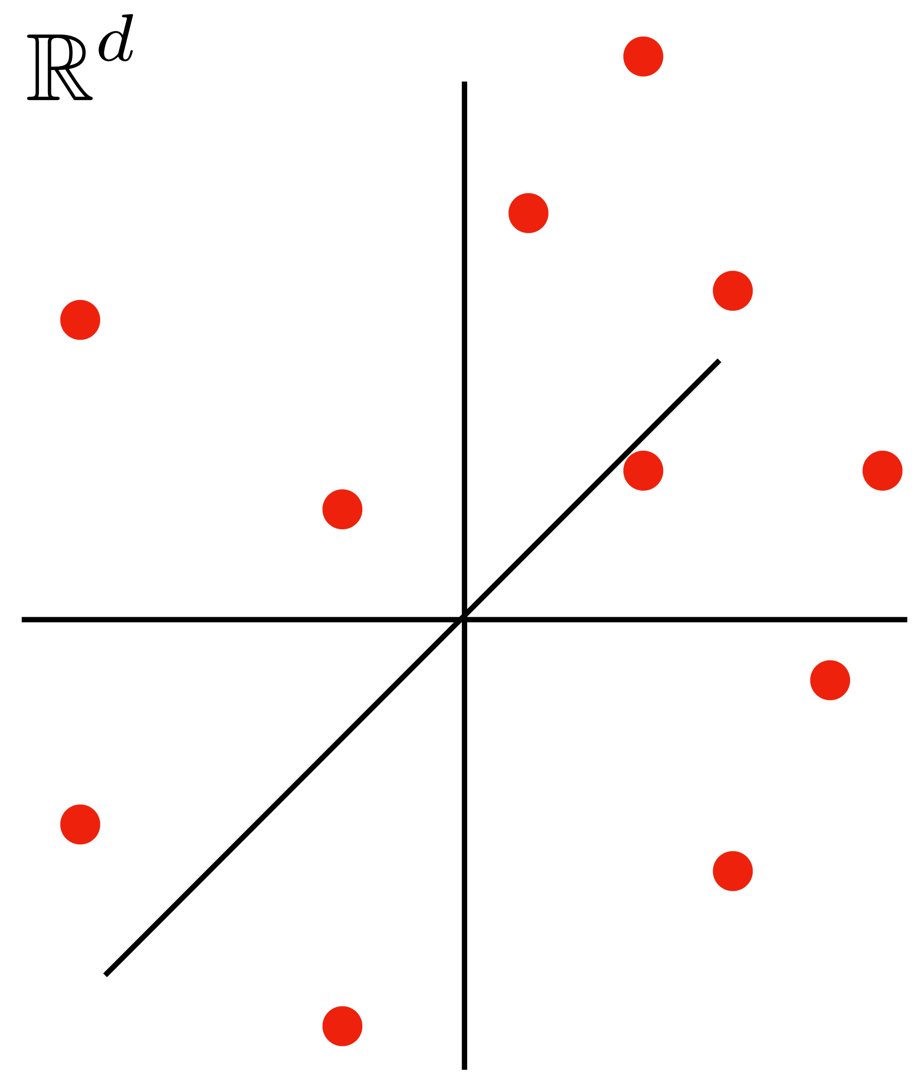
$$\tilde{O}(1) \cdot \underbrace{\max\{\|\phi(q)\|_2 \cdot \|\phi(p)\|_2\}}_{\gamma_2\text{-norm}}$$

$$\begin{aligned}\|\phi(p)\|_2^2 &= \langle \phi(p), \phi(p) \rangle \\ &= K(p,p) = 1\end{aligned}$$

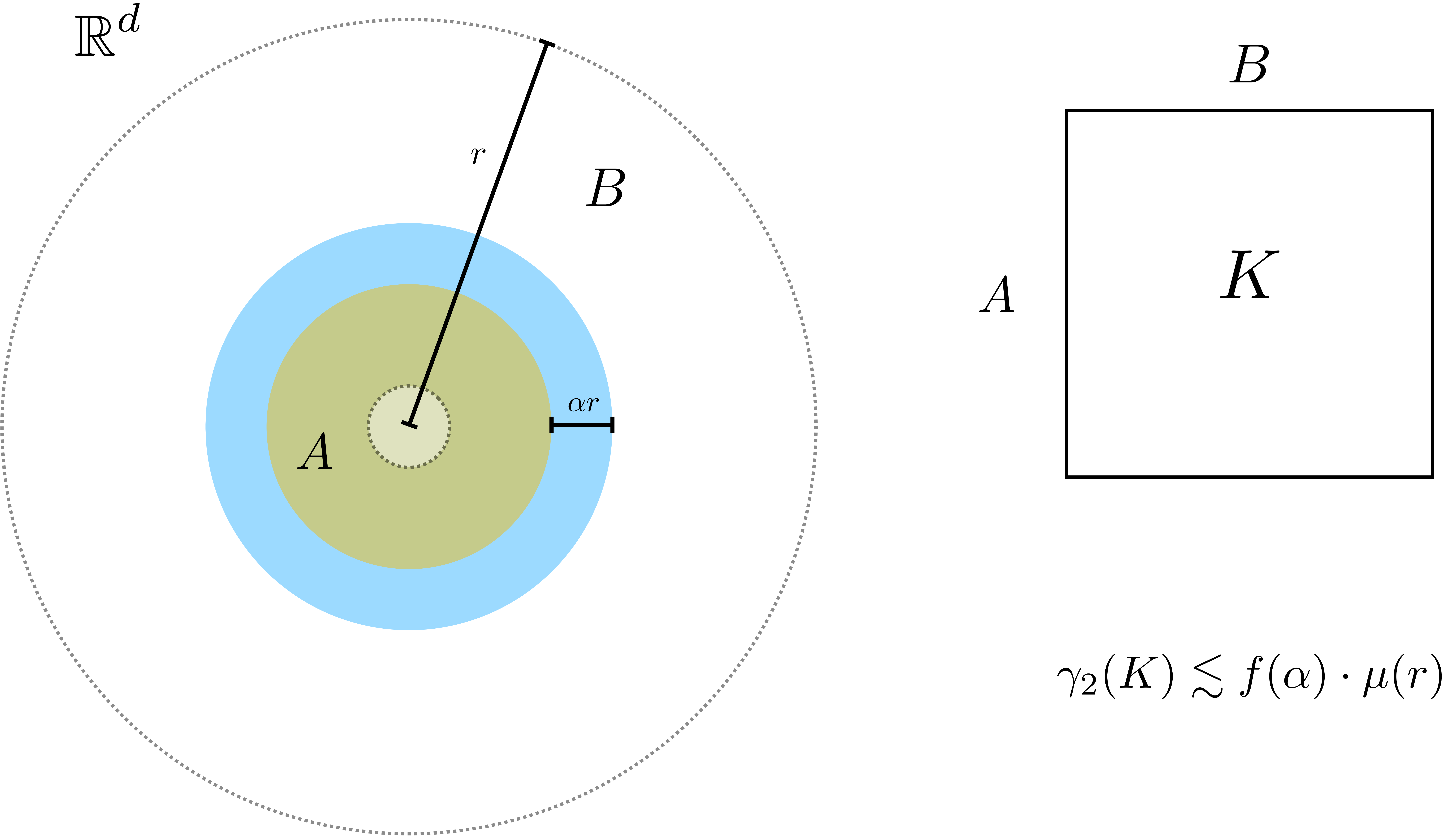
$$\implies \gamma_2\text{-norm} \leq 1$$

What if we could…

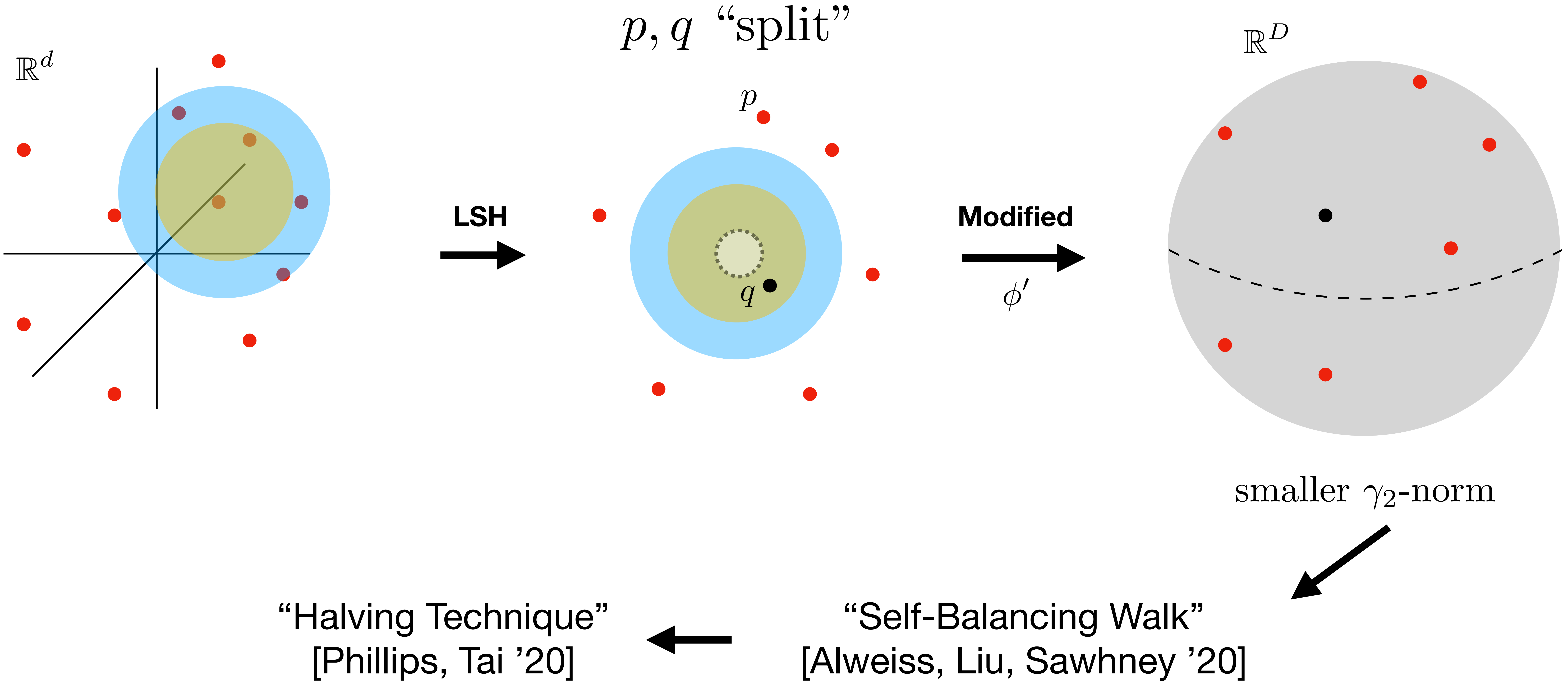
1. Decompose dataset efficiently (LSH)
2. For each part, find *better* embedding ϕ with smaller γ_2-norm.



$$K : \mathbb{R}^d \times \mathbb{R}^d \to [0, 1]$$


$\mathbb{R}^d$
r
B
αr
A
B
K
A
$\gamma_2(K) \lesssim f(\alpha) \cdot \mu(r)$

At “scale” R:


$\mathbb{R}^d$
LSH
p, q “split”
p
q
Modified
ϕ'
$\mathbb{R}^D$
smaller γ_2-norm
“Self-Balancing Walk”
[Alweiss, Liu, Sawhney ’20]
“Halving Technique”
[Phillips, Tai ’20]

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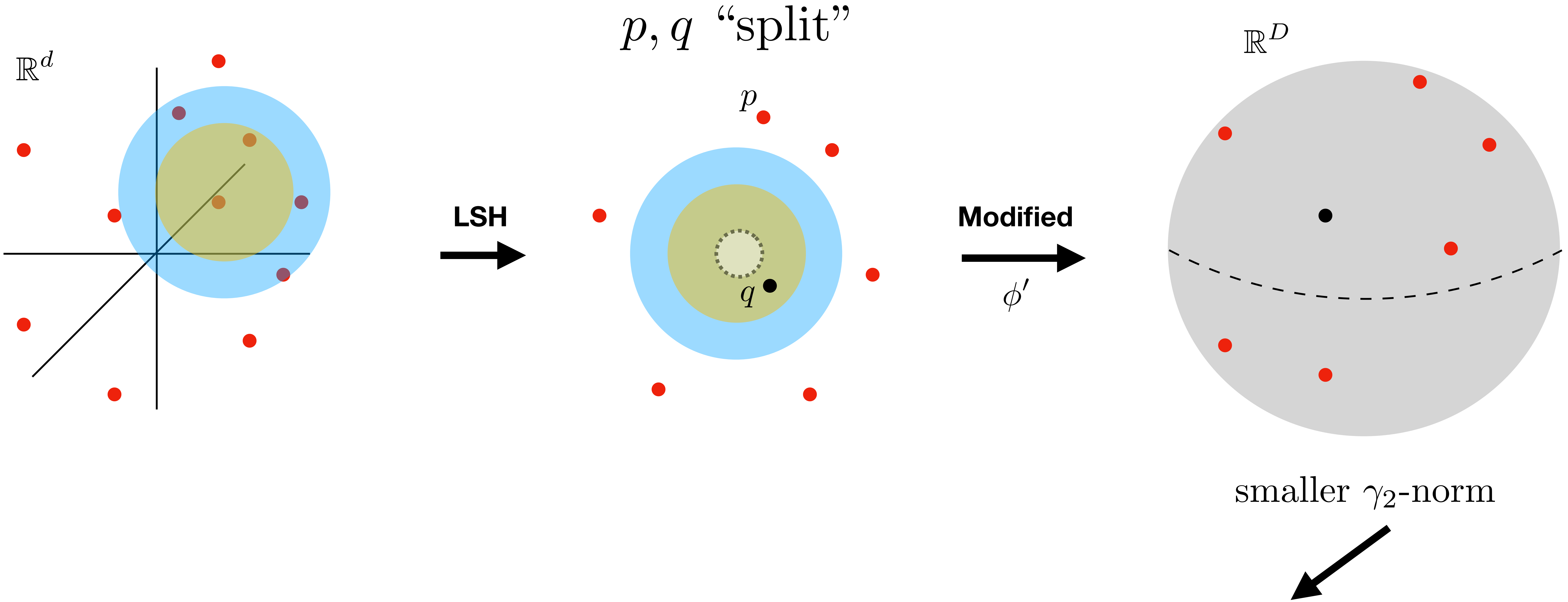

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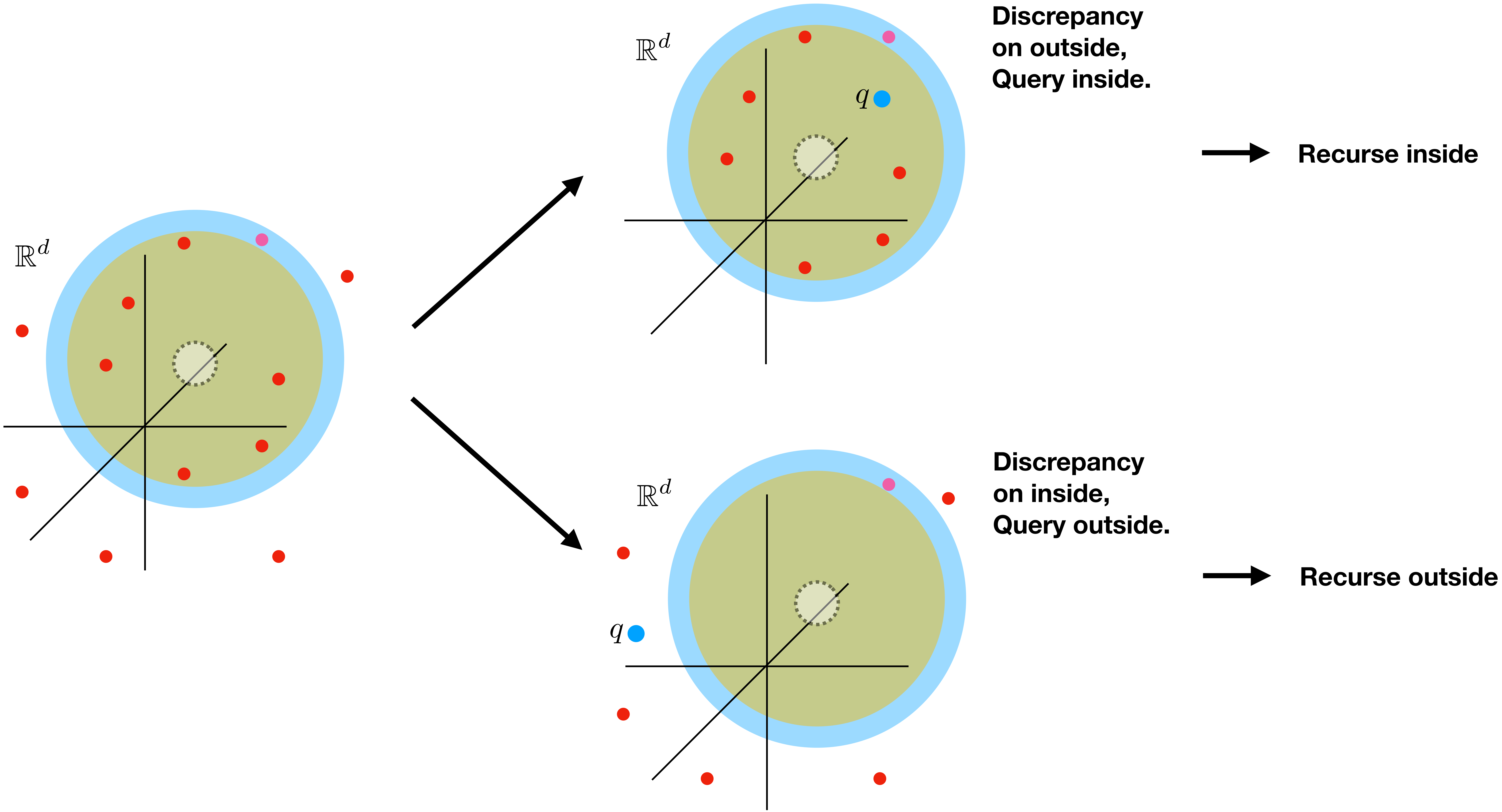
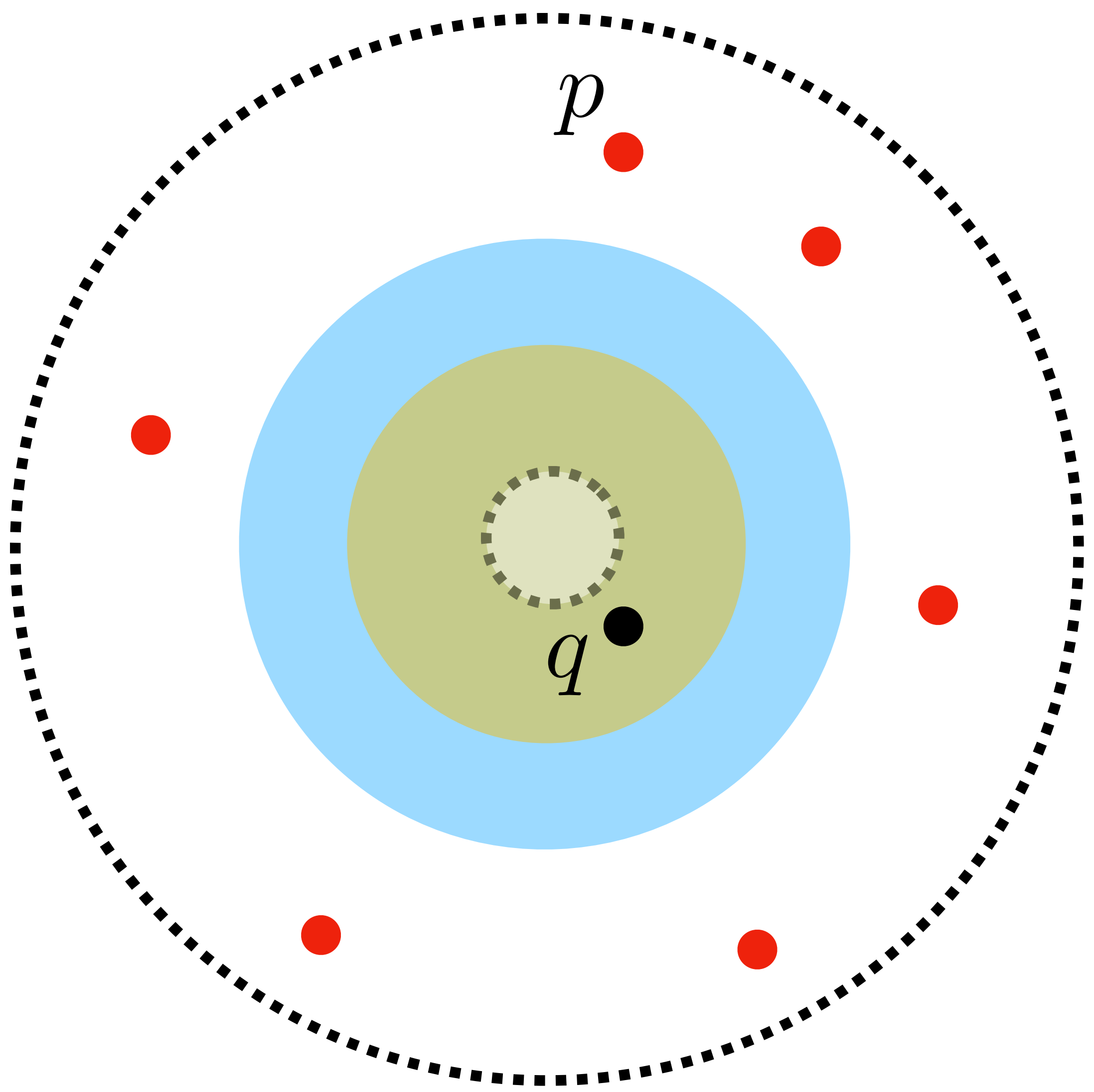
$$\underbrace{O(\log \Phi)}_{\text{scales}} \times \underbrace{O(\log n)}_{\text{“caught”}} \times \underbrace{O(\gamma_2/(\epsilon\mu(R)))}_{\text{coreset size}}$$

Data Structure



Why we need smoothness:



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$$K(p,q) \approx \mu(R)$$

Tension:

- How thick of a shell can I fit between a query and many dataset points at particular length?

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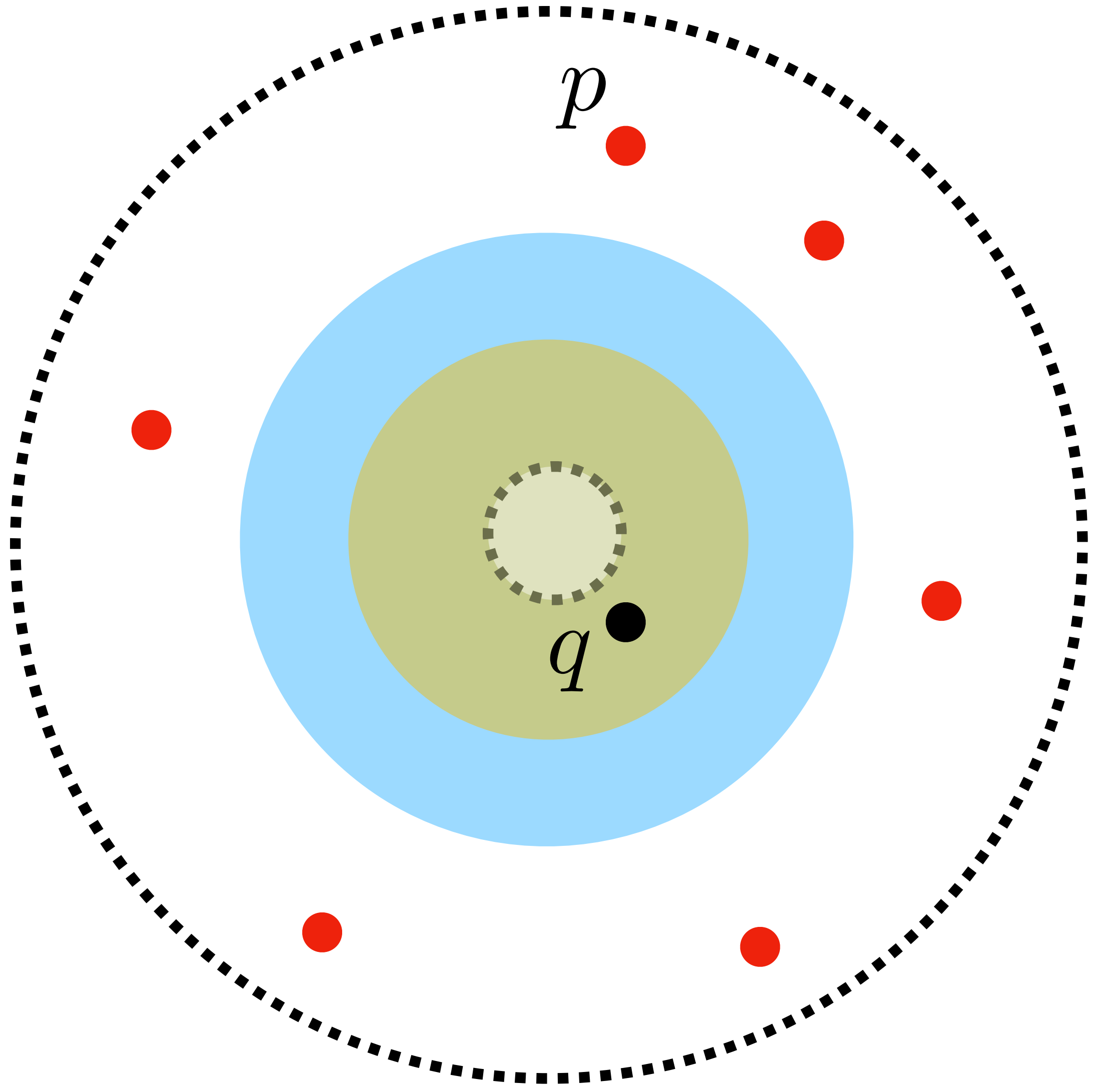

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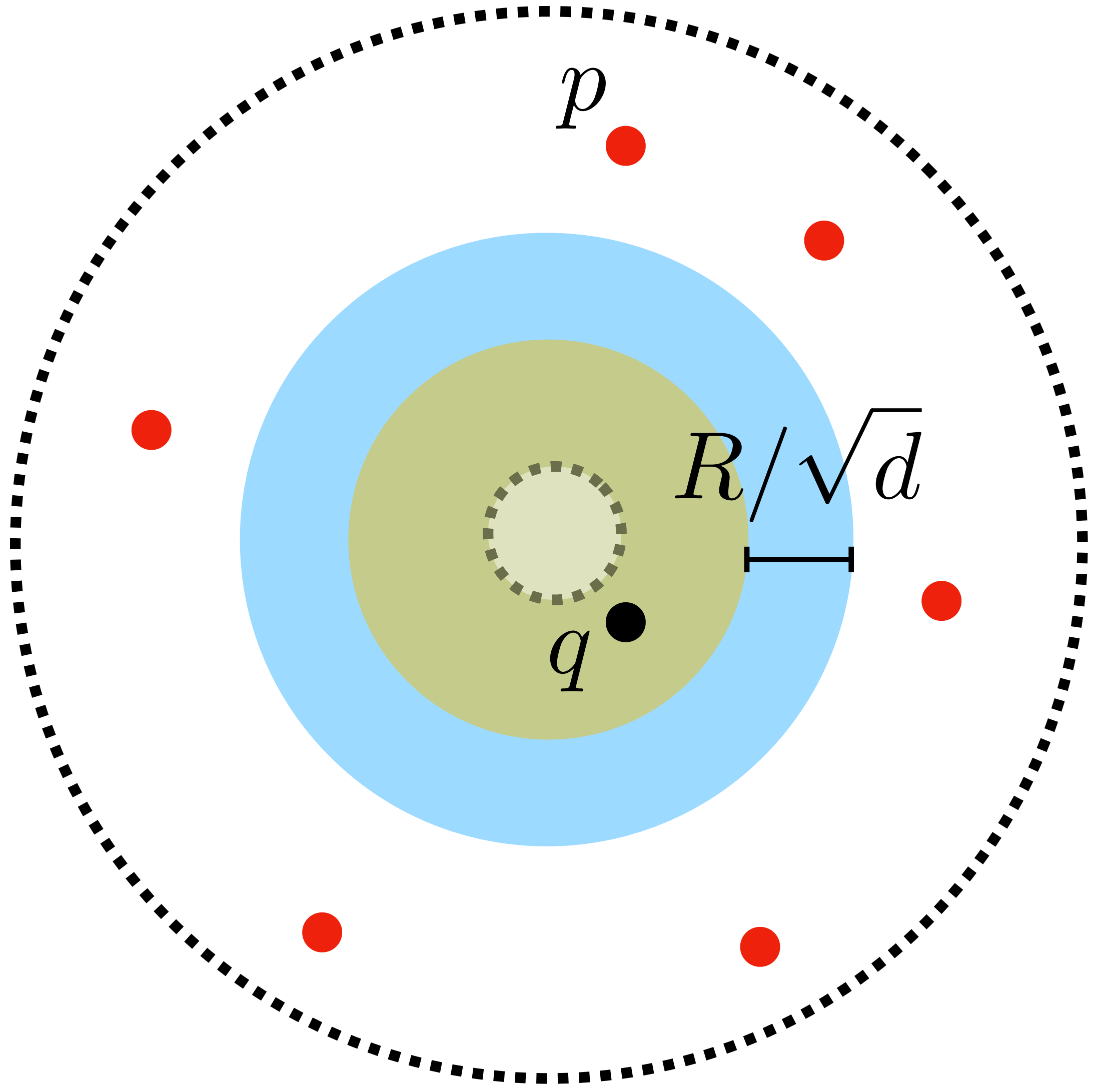

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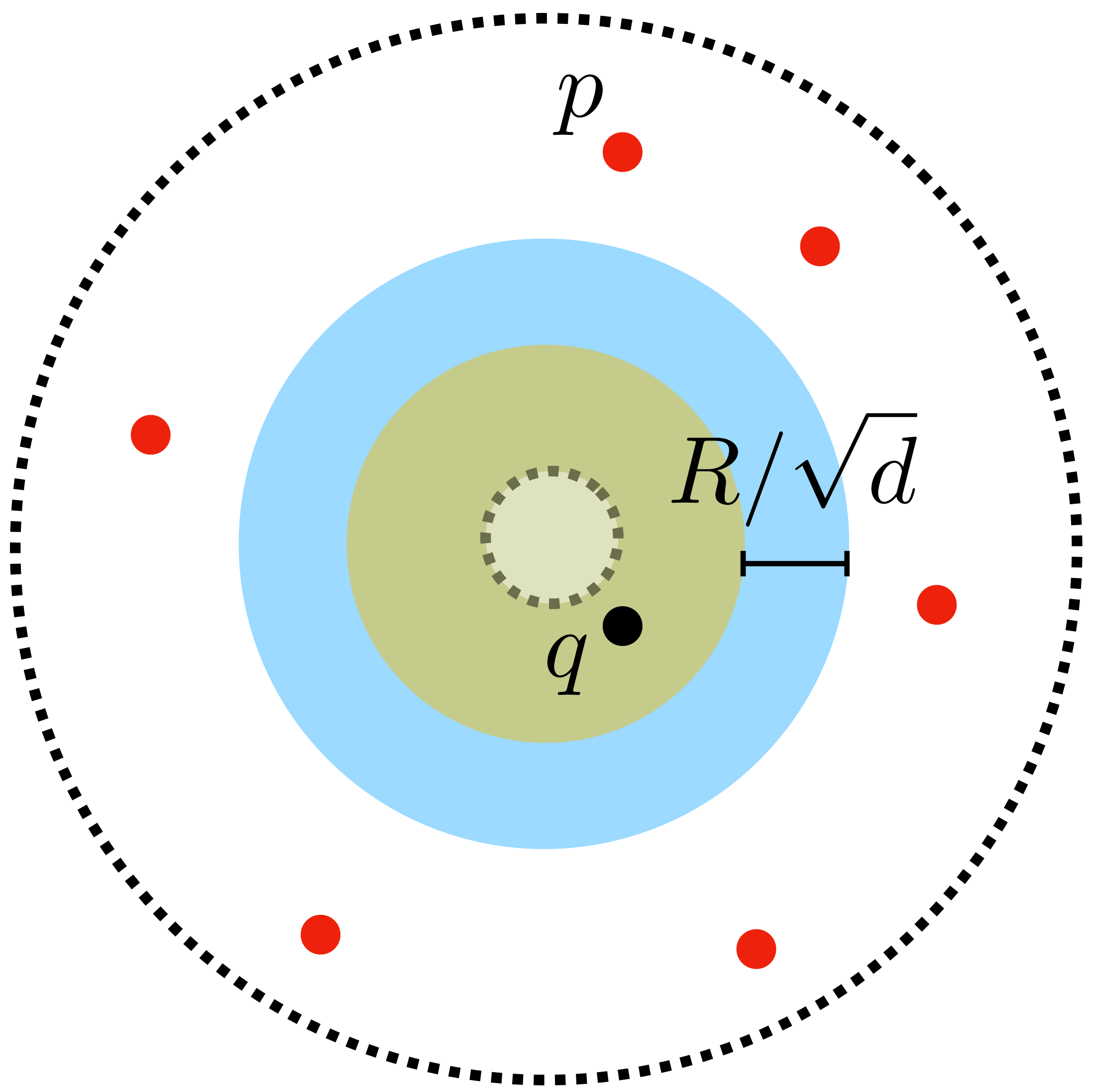

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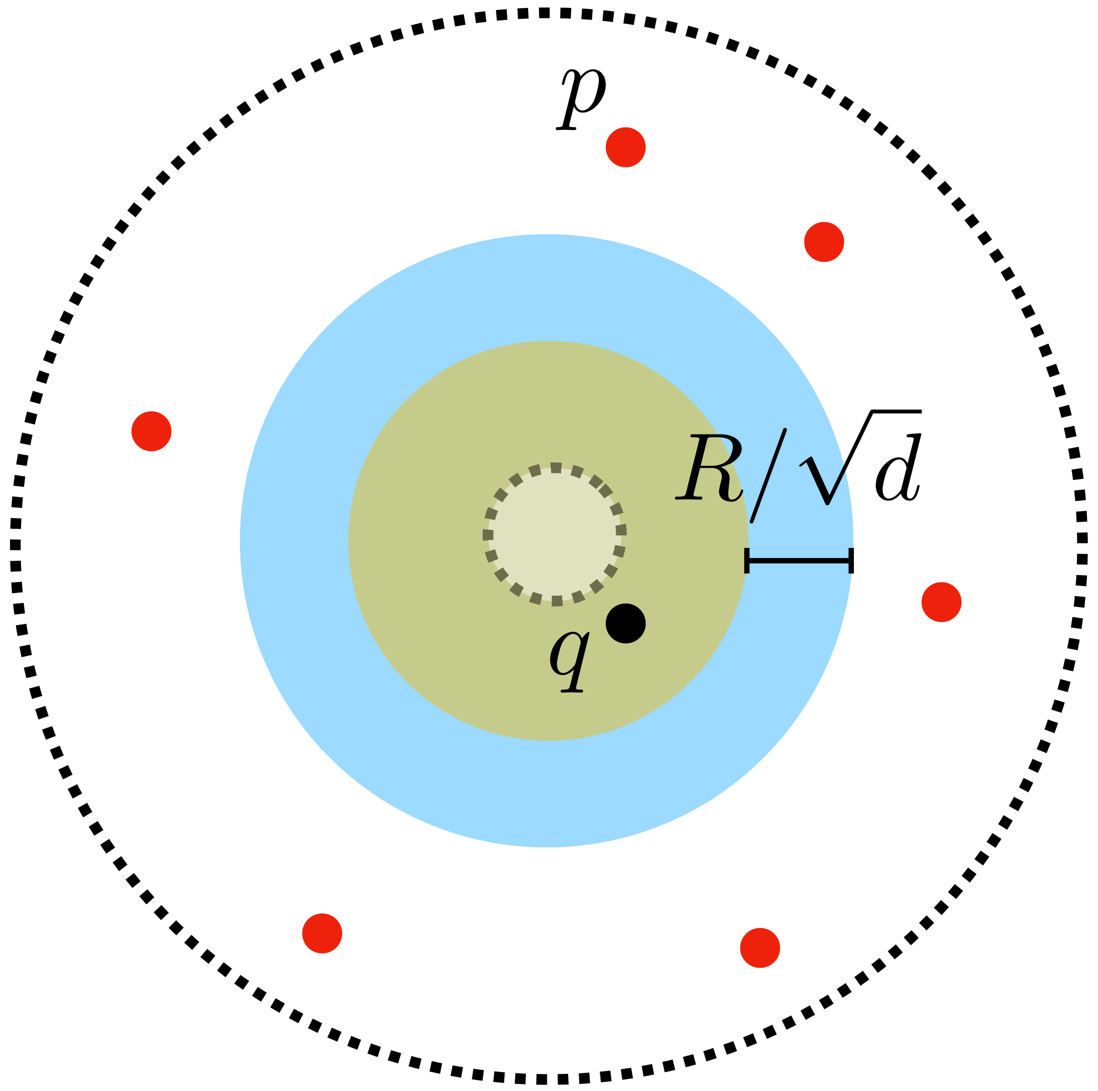

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$$\mu(R) \text{ vs. } \mu(R/\sqrt{d})?$$

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Open Problems

1. Non-smooth kernels?

2. Preprocessing is slower.