Five Short Stories about Optimal Transport

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PIMS Summer School, July 2022

UNIVERSITY *of* WASHINGTON

Outline

- Fekete Points
- Analytic Number Theory
- Irregularities of Distributions: the Coffee Shop Problem
- Coffee Shop Sampling
- Sparsity of Kantorovich Solutions

Fekete Points

Fekete (1923)

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Über die Verteilung der Wurzeln bei gewissen algebraischen Gleichungen mit ganzzahligen Koeffizienten.

Von

M. Fekete in Budapest.

(‘On the distribution of roots of certain algebraic polynomials with integer coefficients’)

Problem (Fekete Points on $\mathbb{S}^2$)

What is

$$\max_{x_1,\dots,x_n\in\mathbb{S}^2} \prod_{\substack{k,\ell=1\\k\neq\ell}}^{n} \|x_k - x_\ell\|_{\ell^2(\mathbb{R}^3)}$$

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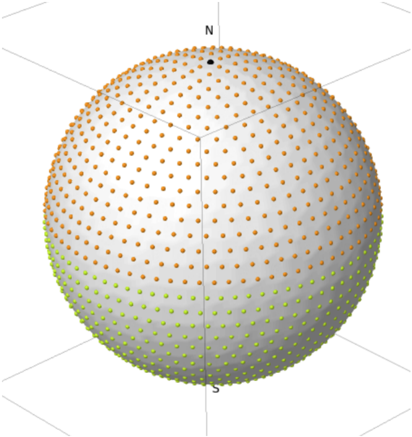
Taking a log, this is equivalent to

$$\min_{x_1,\ldots,x_n \in \mathbb{S}^2} \sum_{\substack{k,\ell=1 \\ k\neq\ell}}^{n} \log\left(\frac{1}{\|x_k - x_\ell\|_{\ell^2(\mathbb{R}^3)}}\right)$$

Diamond Ensemble (Beltran & Etayo)



(Picture by Beltran & Etayo)

The Smale Problems (1998)

Mathematical Problems for the Next Century[1]

Steve Smale

DEPARTMENT OF MATHEMATICS
CITY UNIVERSITY OF HONG KONG

Introduction. V. I. Arnold, on behalf of the International Mathematical Union has written to a number of mathematicians with a suggestion that they describe some great problems for the next century. This report is my response.

The Smale Problems (1998)

Problem 7: Distribution of points on the 2-sphere.

Let $V_N(x) = \sum_{1 \le i < j \le N} \log \frac{1}{\|x_i - x_j\|}$ where $x = (x_1, \ldots, x_N)$, the x_i are distinct points on the 2-sphere $S^2 \subset \mathbb{R}^3$, and $\|x_i - x_j\|$ is the distance in $\mathbb{R}^3$. Denote $\min_x V_N(x)$ by V_N.

Can one find $(x_1, \ldots, x_N)$ *such that*

$$V_N(x) - V_N \le c \log N \,, \qquad c \text{ a universal constant.} \tag{3}$$

[...]

This problem emerged from complexity theory, jointly with Mike Shub (see Shub-Smale, 1993). It is motivated by finding a good starting polynomial for a homotopy algorithm for realizing the Fundamental Theorem of Algebra.

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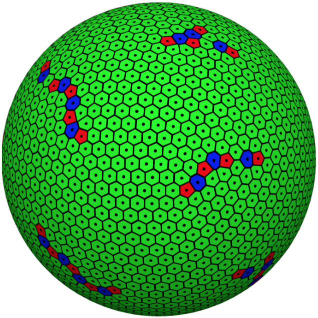
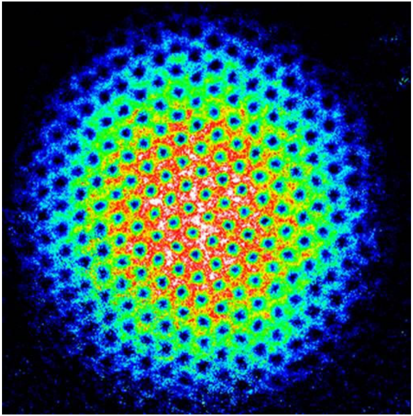


Figure 5.18: Examples of disconnected scars on a configuration resulting from optimizing $N = 1600$ points for $s = 4$.

(Picture by Calef, Ph.D. Thesis, Vanderbilt 2009)

Abrikosov Lattice (Nobel Prize in Physics 2003)

"When a Bose-Einstein condensate (BEC) is set into rapid rotation, vortices enter the condensate and arrange themselves into a regular lattice (Abrikosov lattice)."



(Picture by Peter Engels, JILA)

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You should think of, when $d \geq 3$,

$$G(x, y) \sim \frac{1}{\|x - y\|^{d-2}}$$

and $G(x, y) \sim -\log \|x - y\|$ when $d = 2$. On $\mathbb{S}^2$, the Green function is the logarithm (up to constants).

Theorem (S, 2019)

On compact manifolds without boundary in $d \geq 2$ dimensions

$$W_2\left(\frac{1}{n}\sum_{k=1}^{n}\delta_{x_k}, dx\right) \lesssim_M \frac{1}{n}\left|\sum_{\substack{k,\ell=1\\k\neq\ell}}^{n} G(x_k, x_\ell)\right|^{1/2} + \begin{cases}\frac{\sqrt{\log n}}{\sqrt{n}} & \text{if } d = 2\\ n^{-1/d} & \text{if } d \geq 3\end{cases}.$$

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Corollary

Points maximizing $\prod_{\substack{k,\ell=1\\k\neq\ell}}^{n} \|x_k - x_\ell\| \rightarrow \max$ *satisfy*

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Problem. Is the $\sqrt{\log n}$ necessary?

Analytic Number Theory

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Exponential Sum Estimates imply Wasserstein bounds.
Basically completely unexplored!

Quadratic residue in $\mathbb{F}_p$

If p is a prime number, then

$$\mathbb{F}_p = \mathbb{Z}/(p\mathbb{Z}) = \{0, 1, 2, \ldots, p-1\}$$

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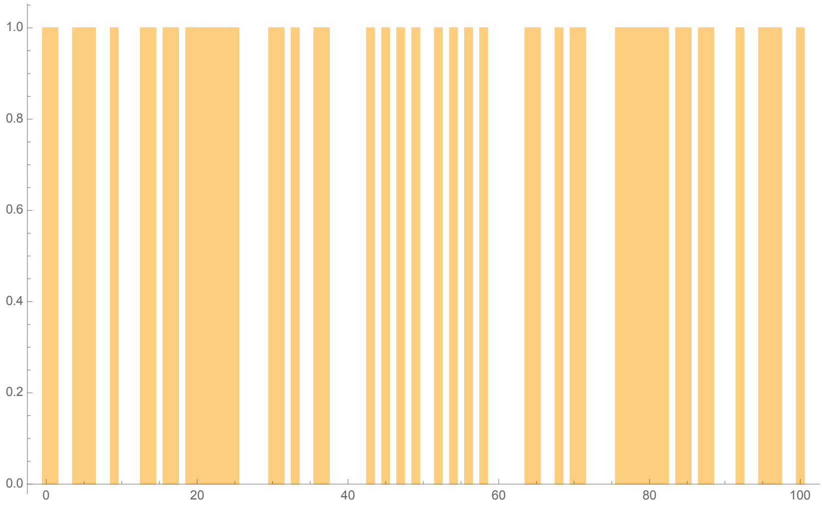
Question. How are quadratic residues distributed as $p \to \infty$?

Quadratic residues mod 101



Quadratic residues mod 499

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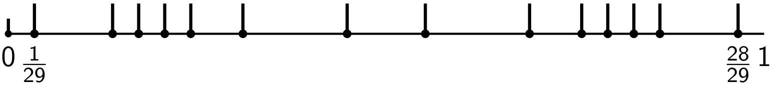
They seem ‘random’.

The Quadratic Residues in $\mathbb{F}_{29}$



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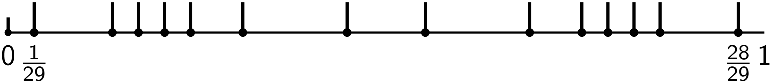

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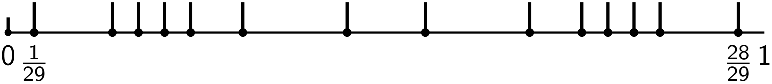

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Theorem (S. 2018)

For p prime

$$W_2\left(\frac{1}{p}\sum_{k=0}^{p-1}\delta_{\frac{k^2 \bmod p}{p}},\ dx\right) \lesssim \frac{1}{\sqrt{p}}$$

and this is optimal up to constants.

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It is natural to compare this to the Kolmogorov-Smirnov distance

$$\text{disc} = \sup_{0<z<1}\left|\frac{\#\left\{0 \le i \le p-1 : 0 \le \frac{i^2 \mod p}{p} \le z\right\}}{p} - z\right|$$

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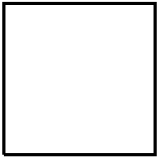
Theorem

$$\text{disc} \lesssim \frac{\log p}{\sqrt{p}} \qquad \text{(Polya-Vinogradov, 1918)}$$

$$\text{disc} \lesssim \frac{\log\log p}{\sqrt{p}} \qquad \text{(Vaughan-Montgomery (GRH), 1977)}$$

Irregularities of Distributions
The Coffee Shop Problem

You want to open a coffee shop in the unit square (assume the coffee drinking population is evenly distributed in this square).



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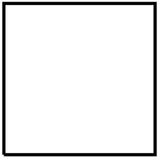

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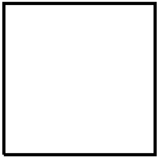

Where's the best place to put it? Clearly in the center but why? One could argue that you want to put it in the place x_0 such that 'the averaging walking distance'

$$W_1(\delta_x, dx) \qquad \text{is minimized.}$$

You want to open 9 coffee shops in the unit square.

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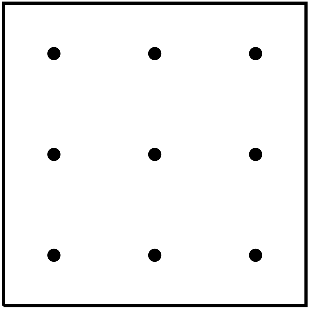

Suppose now you open n coffee shops on $[0,1]^2$. How small can you make the Wasserstein distance of

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It is not very hard to see that

$$\min_{x_1,\ldots,x_n} W_1\left(\frac{1}{n}\sum_{k=1}^{n}\delta_{x_k}, dx\right) \sim \frac{1}{\sqrt{n}}.$$

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The Coffee Shop Problem

Is there a sequence $(x_n)_{n=1}^{\infty}$ in $[0,1]^d$ such that for all $N \in \mathbb{N}$

$$W_p\left(\frac{1}{N}\sum_{k=1}^{N}\delta_{x_k}, dx\right) \leq c \cdot N^{-1/d} \qquad ?$$

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Let's start with $d = 1$.

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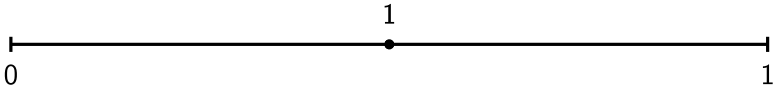

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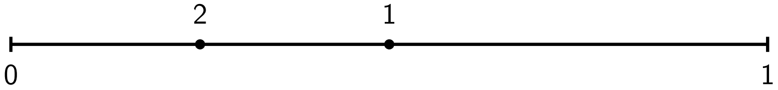

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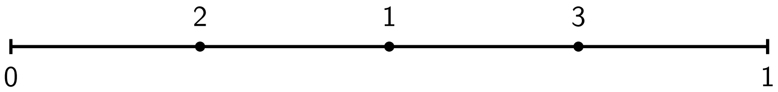

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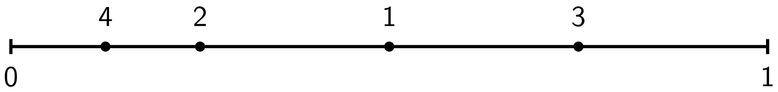

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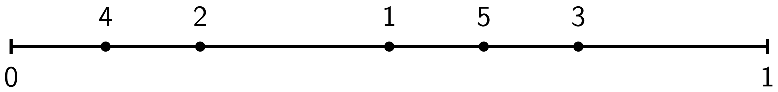

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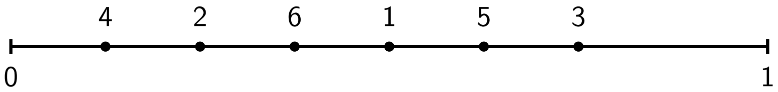

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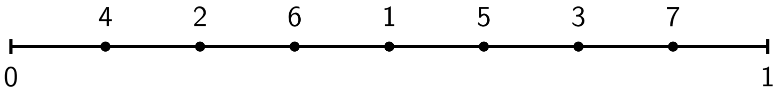

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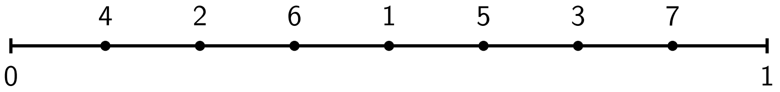

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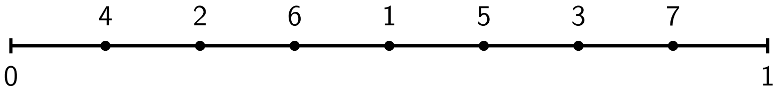

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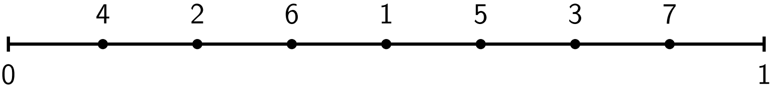

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Theorem (Louis Brown and S. 2019)

For the van der Corput sequence

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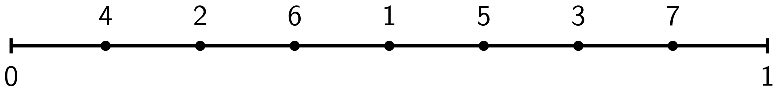

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Almost solves the coffee shop problem.

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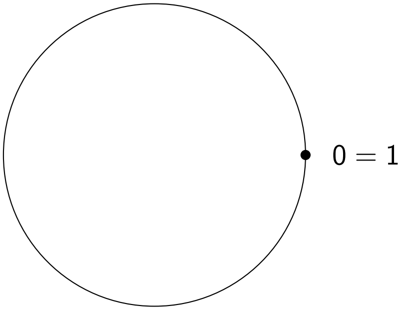

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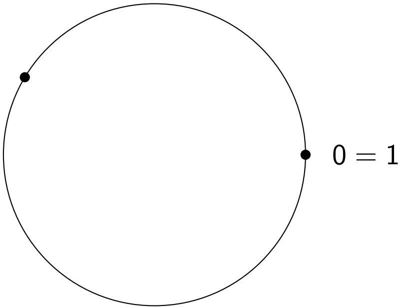

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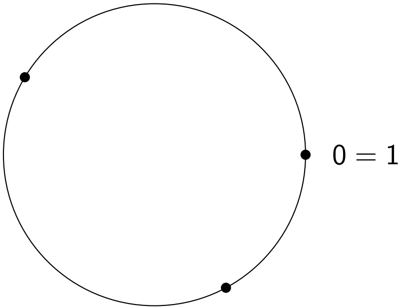

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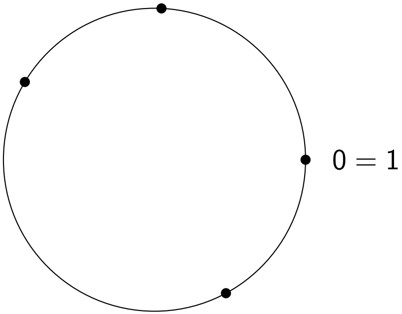

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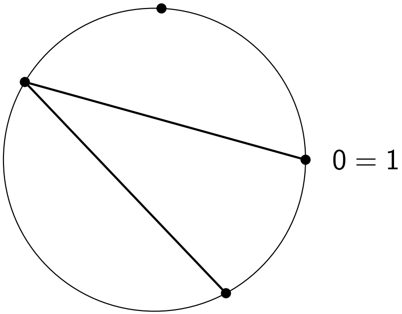

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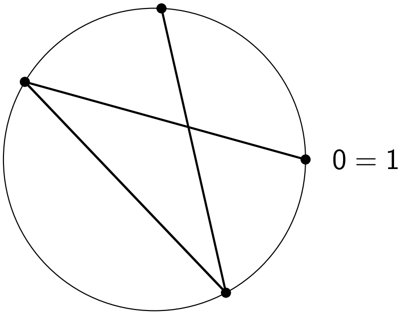

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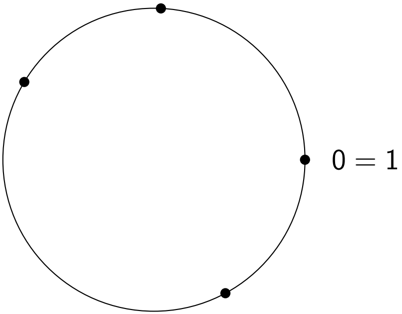

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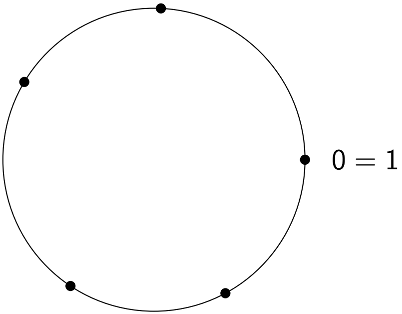

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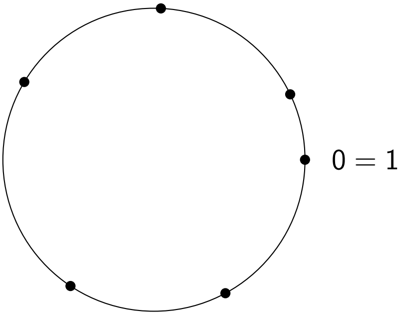

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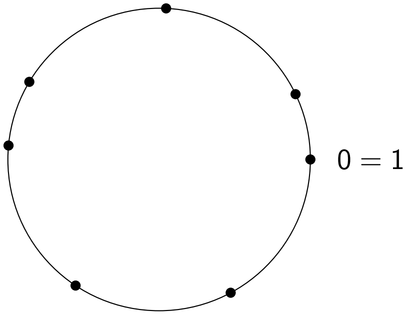

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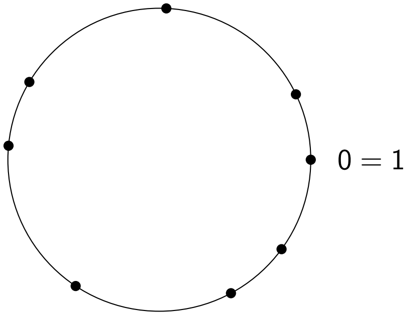
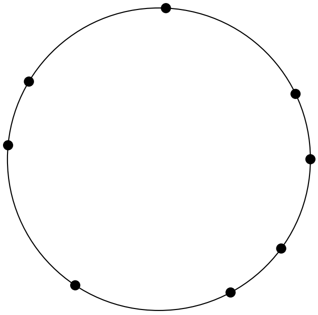
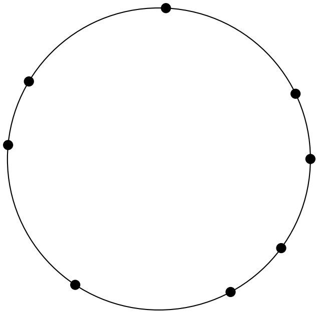


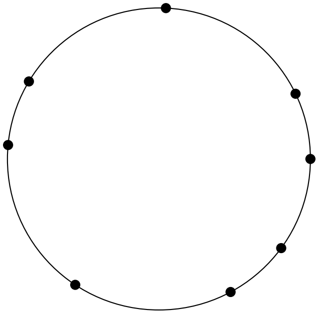




Theorem (S. 2018)

For suitable Kronecker sequences

$$W_2\left(\frac{1}{N}\sum_{k=1}^{N}\delta_{x_k}, dx\right) \leq c\frac{\sqrt{\log N}}{N}$$



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Almost solves the coffee shop problem.

Summary

For the van der Corput sequence and the Kronecker sequence

$$W_2\left(\frac{1}{N}\sum_{k=1}^{N}\delta_{x_k}, dx\right) \leq c\frac{\sqrt{\log N}}{N}$$

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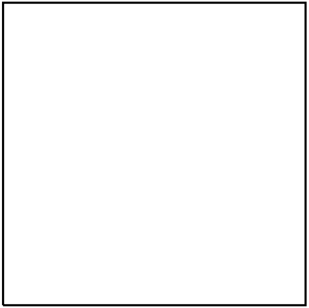
Theorem (Cole Graham, 2020)

For **every** sequence $(x_k)_{k=1}^{\infty}$ in $[0,1]$, the inequality

$$W_1\left(\frac{1}{N}\sum_{k=1}^{N}\delta_{x_k}, dx\right) \geq c\frac{\sqrt{\log N}}{n}$$

has to hold for **infinitely** many $N \in \mathbb{N}$.

The Coffee Shop Problem for $d = 2$



Similar construction as before: pick a vector $\alpha \in \mathbb{R}^2$ and define

$$x_n = n\alpha \pmod 1,$$

where the mod acts on each component independently.

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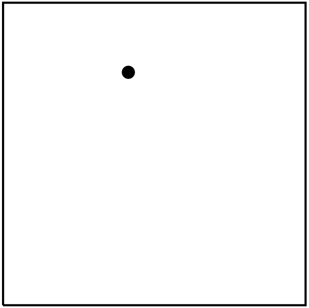

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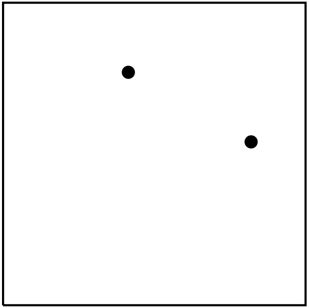

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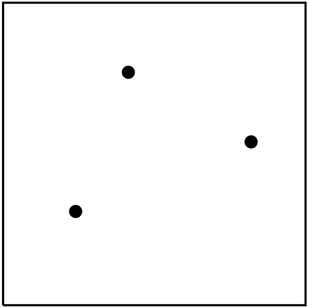

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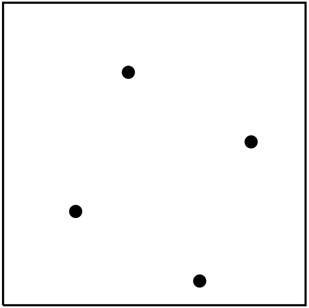

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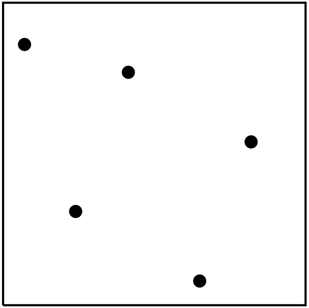

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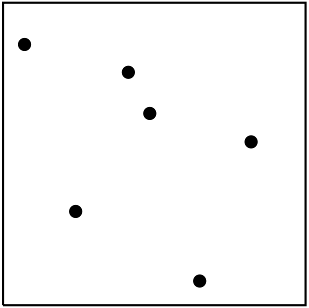

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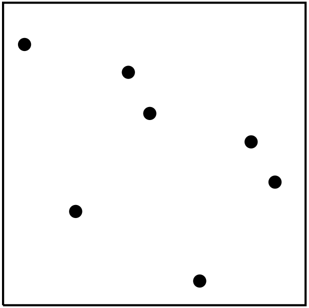

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'Badly approximable' is pretty subtle number theory – are there easier, nicer, more robust constructions?

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Problem

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What about W_p?

Coffee Shop Sampling

Theorem (Bakhalov, 1959)

Let $f : [0,1]^d \to \mathbb{R}$ be $L-$Lipschitz. Then there are points $\{x_1, \dots, x_N\} \subset [0,1]^d$ such that

$$\left| \int_{\mathbb{T}^d} f(x)dx - \frac{1}{N} \sum_{k=1}^{N} f(x_k) \right| \lesssim_d L \cdot \frac{1}{N^{1/d}}.$$

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Kantorovich-Rubinstein duality (special case)

If $f : [0,1]^d \to \mathbb{R}$ is $L-$Lipschitz and $\{x_1, \dots, x_N\} \subset [0,1]^d$, then

$$\left| \int_{[0,1]^d} f(x)dx - \frac{1}{N}\sum_{k=1}^{N} f(x_k) \right| \leq L \cdot W_1 \left(\frac{1}{N}\sum_{k=1}^{N} \delta_{x_k}, dx \right).$$

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Coffee Shop Problem!

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As we just saw, in dimension $d \geq 2$, we can even get

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W_2 is larger than W_1 so we can get further improvements!

- S, On a Kantorovich-Rubinstein Inequality (2021).
- F. Santambrogio, Sharp Wasserstein estimates for integral sampling and Lorentz summability of transport densities (2022)

Sparsity of Kantorovich Solutions

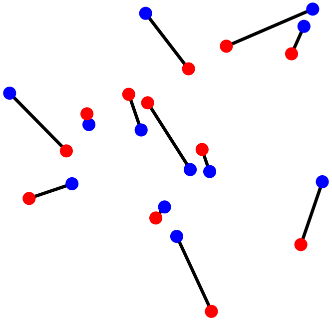
Theorem (Birkhoff, von Neumann)

If

$$\mu = \frac{1}{n}\sum_{i=1}^{n} \delta_{x_i} \qquad \text{and} \qquad \nu = \frac{1}{n}\sum_{i=1}^{n} \delta_{y_i},$$

then the solution of the Kantorovich optimal transport problem is Monge: the optimal transport map is a given by a bijection

$$\pi : \{x_1, \ldots, x_n\} \to \{y_1, \ldots, y_n\}.$$



What if

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and $m \neq n$? There are no Monge maps.

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and $m \neq n$? There are no Monge maps.

Intrinsic Kantorovich Sparsity (B. Hosseini & S, 2022)

There is a solution of the Kantorovich problem such that mass from each point in X is moved to at most $n/\gcd(m,n)$ different points in Y and that each point in Y receives mass from at most $m/\gcd(m,n)$ points in X.

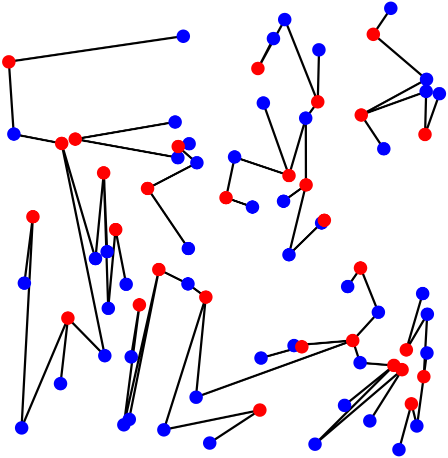


Figure: $m = 30$ red points are sent to $n = 50$ blue points. Each red point is transported to at most $30/\gcd(30, 50) = 3$ blue points, each blue points receives mass from at most $50/\gcd(30, 50) = 5$ red points.

Extension to weighted points

Intrinsic Kantorovich Sparsity (B. Hosseini & S, 2022)

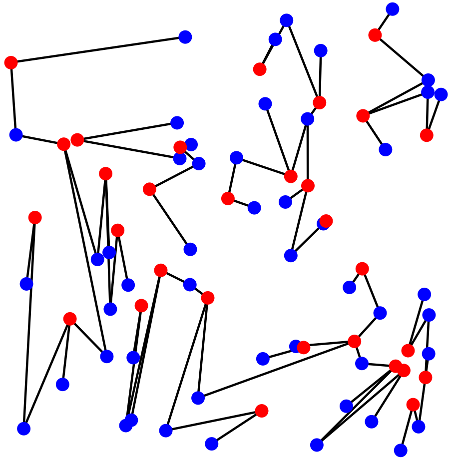
Let

$$\mu = \sum_{i=1}^{m} \frac{a_i}{b_i}\delta_{x_i} \qquad \text{and} \qquad \nu = \sum_{i=1}^{n} \frac{c_i}{d_i}\delta_{y_i}$$

be two probability measures with positive rational weights and let

$$B = \mathrm{lcm}(b_1, \ldots, b_m) \qquad \text{and} \qquad D = \mathrm{lcm}(d_1, \ldots, d_n).$$

There exists a solution of the Kantorovich problem such that mass from each point in X is moved to at most $D/\gcd(B, D)$ different points in Y and each point in Y receives mass from at most $B/\gcd(B, D)$ different points in X.



Thank you!