Optimal Coffee Shops, Numerical Integration and Kantorovich-Rubinstein Duality

Stefan Steinerberger

PIHOT, Kick-off Event, Jan 2021

UNIVERSITY of WASHINGTON

Leonid Kantorovich (1912 – 1986)

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USSR **Leonid Vital'yevich KANTOROVICH**

Head, Problems Laboratory of Economic-Mathematical Methods and Operations Research, Institute of Management of the National Economy

(1975)

An internationally recognized creative genius in the fields of mathematics and the application of electronic computers to economic affairs, Academician Leonid Kantorovich (pronounced kahntuhROHvich) has worked at the Institute of Management of the National Economy since 1971. He has been involved in advanced mathematical research since the age of 15; in 1939 he invented linear programming, one of the most significant contributions to economic management in the twentieth century. Kantorovich has spent most of his adult life battling to win acceptance for his revolutionary concept from Soviet

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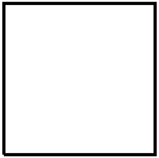
You want to open a coffee shop in the unit square (assume the coffee drinking population is evenly distributed in this square).



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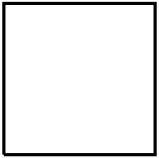

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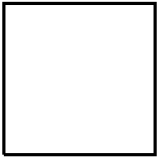

Where's the best place to put it? Clearly in the center but why? One could argue that you want to put it in the place x_0 such that 'the averaging walking distance'

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

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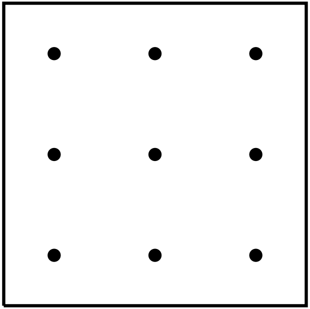

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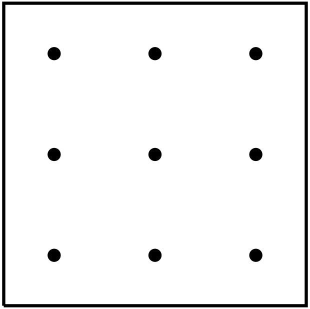
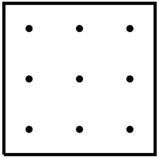


This is probably the best solution but it's less clear to me how one would prove that quickly.

Optimal Coffee Shops

Suppose now you open n coffee shops. How small can you make the Wasserstein distance of

$$W_1\left(\frac{1}{n}\sum_{k=1}^{n}\delta_{x_k}, dx\right)?$$



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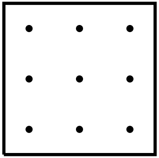

This type of example shows that

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

is possible.

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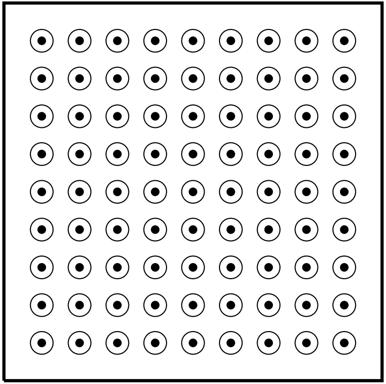

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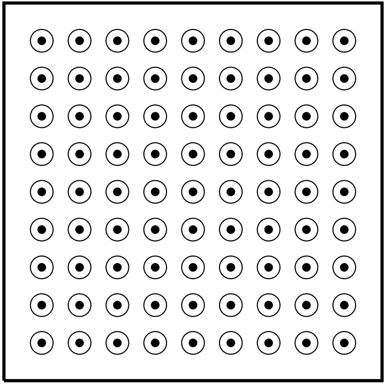

The total area they cover is $\varepsilon^2\pi$ which, for $\varepsilon \sim 0.01$ is much less than 1. So most of the unit square is distance at least $0.01/\sqrt{n}$ away from one of the points.

The Coffee Shop Problem

So we always have

$$W_1\left(\frac{1}{n}\sum_{k=1}^{n}\delta_{x_k}, dx\right) \geq \frac{c_2}{\sqrt{n}}$$

and this is best possible.

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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 $n \in \mathbb{N}$

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

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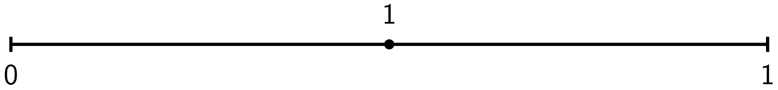

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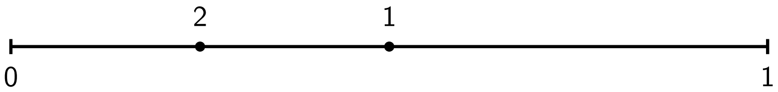

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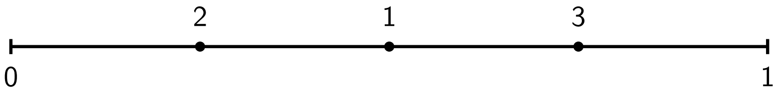

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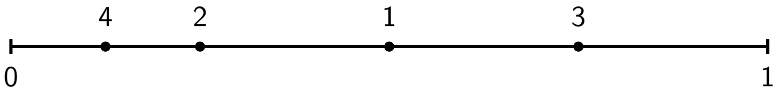

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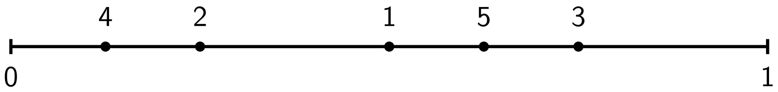

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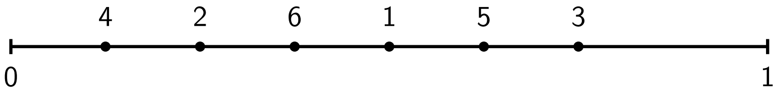

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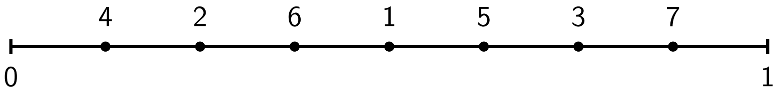

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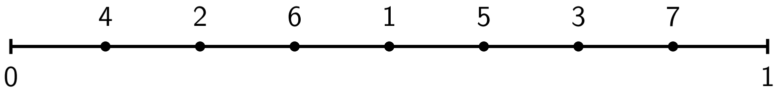

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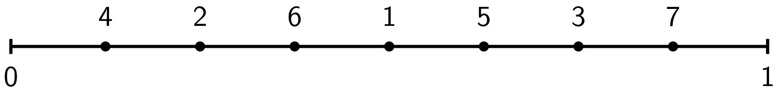

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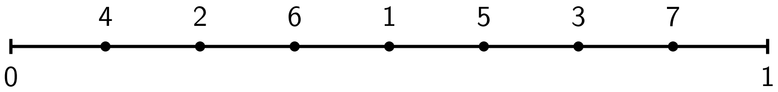

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Theorem (Louis Brown and S. 2019)

For the van der Corput sequence

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

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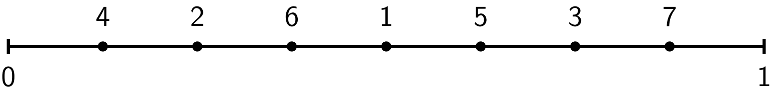

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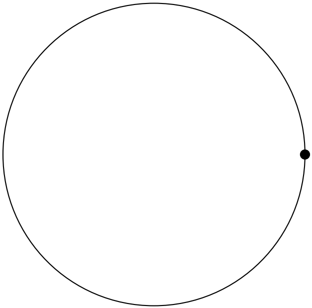
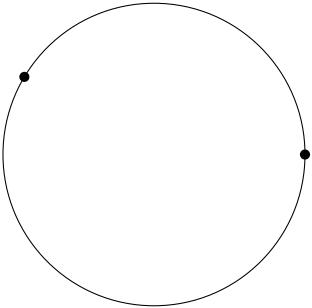
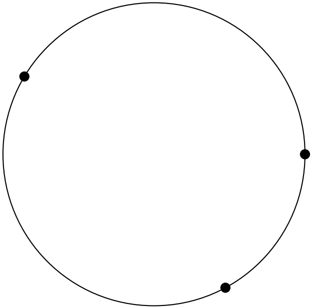
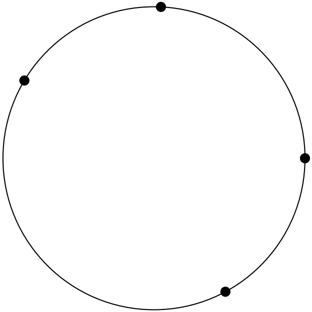
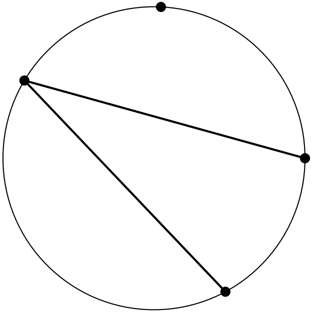
Almost solves the coffee shop problem.

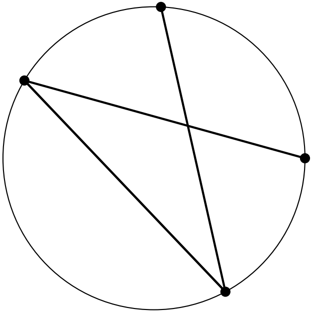


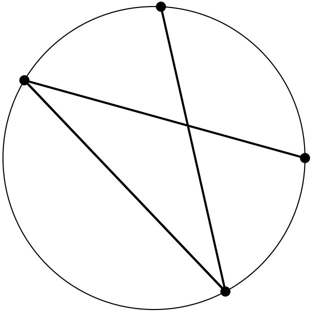






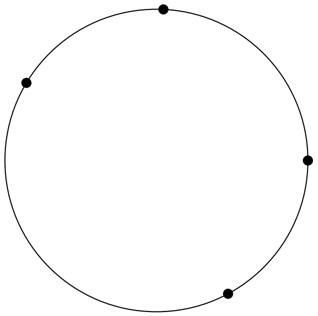


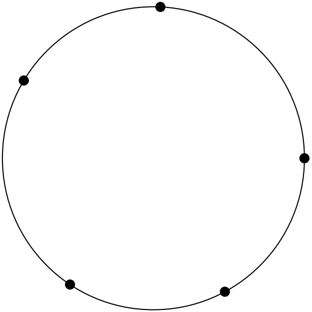


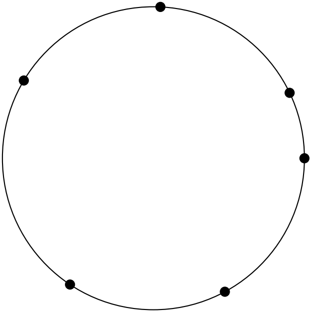


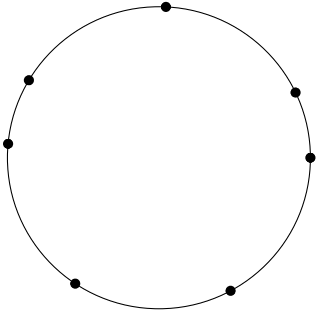
There is also a simple definition: for $\alpha \in \mathbb{R}$

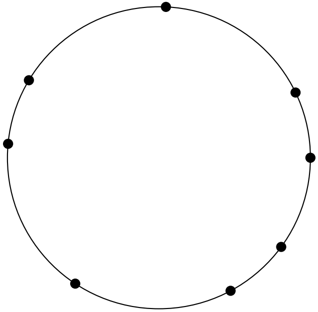
$$x_n = \{n\alpha\} = n\alpha - \lfloor n\alpha \rfloor$$

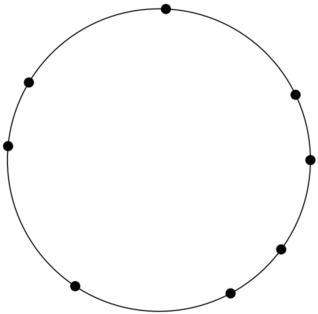


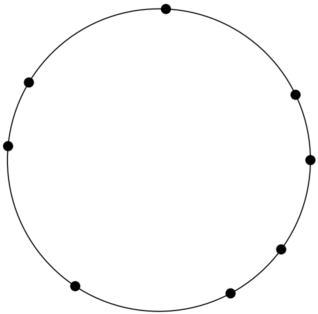












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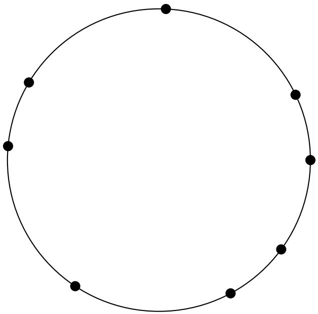

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Summary

For the van der Corput sequence and the Kronecker sequence

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I thought that it would be quite hard to beat this.

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Theorem (Cole Graham, 2020)

For **every** sequence 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 $n \in \mathbb{N}$.

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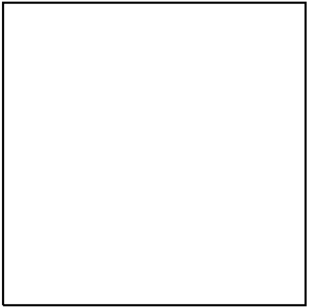
The Coffee Shop Problem is really harder in $d = 1$.

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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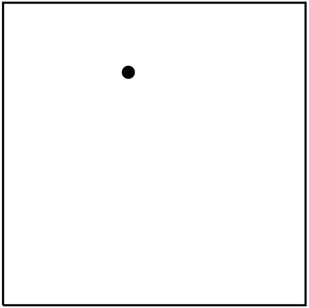

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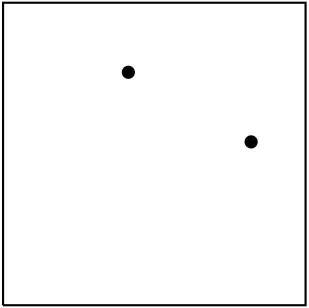

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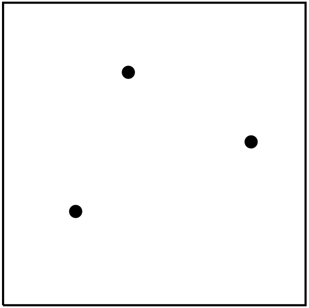

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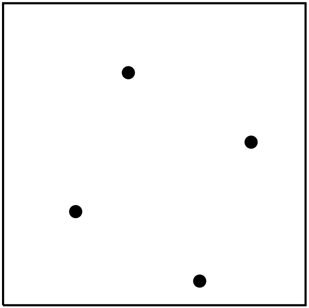

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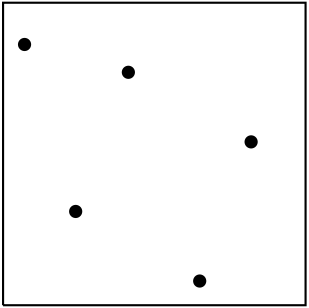

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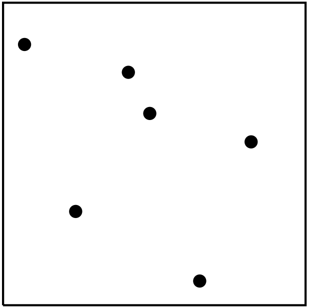

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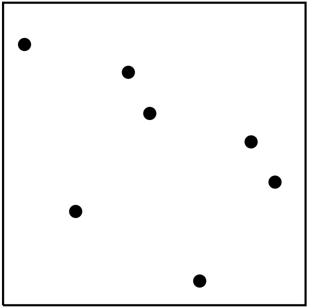

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'Badly approximable' is pretty subtle number theory – are there easier constructions?

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(Ajtai, Komlos & Tusnady 1984, Ambrosio, Stra & Trevisan 2016). So we are talking about a couple of logarithmic factors.

The Coffee Shop Problem for $d \geq 3$

As it turns out, the Coffee Shop Problem becomes somewhat easier in W_2 once $d \geq 3$ since N **random points** satisfy

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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 $N \in \mathbb{N}$

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

The larger p, the harder it becomes. Phase transition for each d?

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Theorem (R. Peyre, 2018)

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These types of **exponential sums** are well studied in Number Theory! Analytic Number Theory $\rightarrow$ Optimal Transport.

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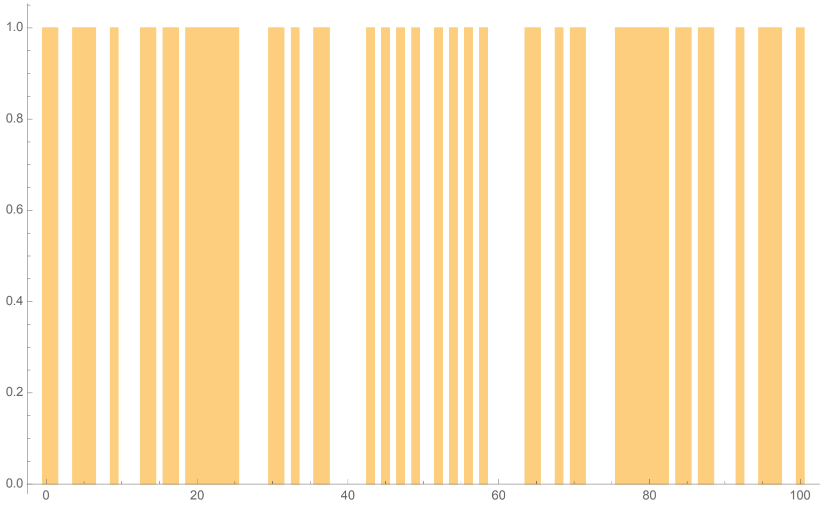
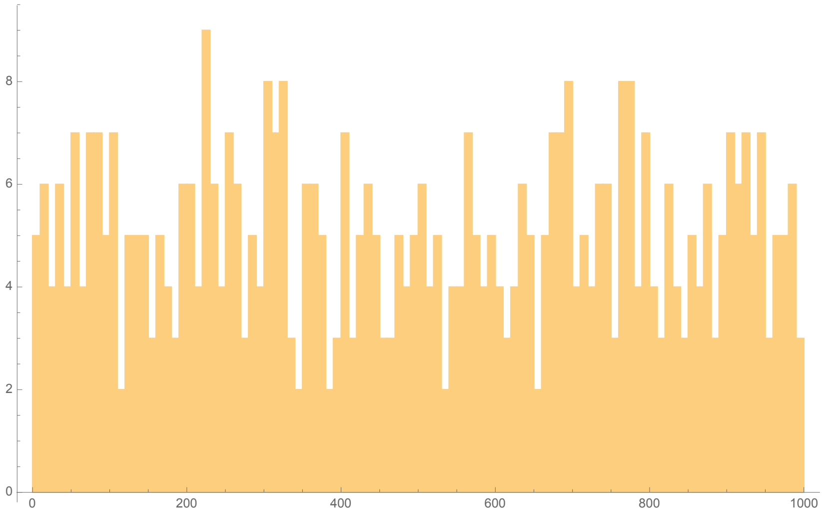
$$0, 1, 4, 5, 6, 7, 9, 13, 16, 20, 22, 23, 24, 25, 28$$

Quadratic residues mod 101



Quadratic residues mod 997



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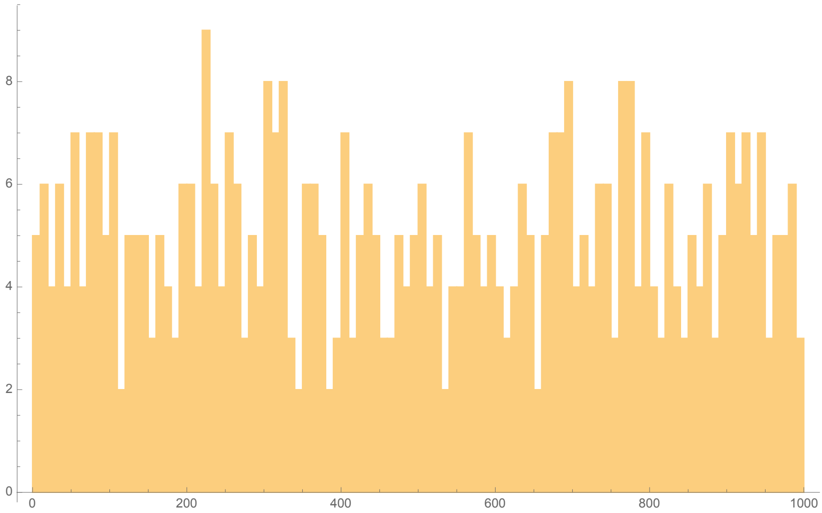
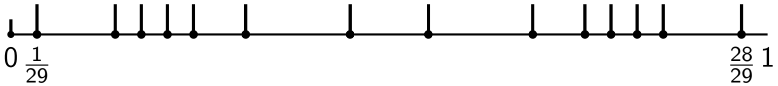


They seem 'random'.

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



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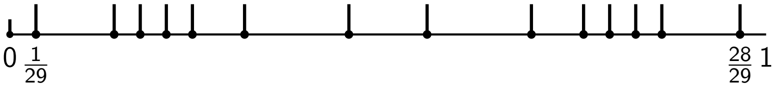

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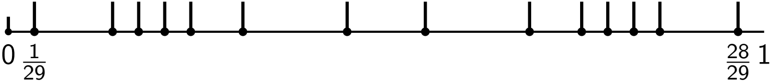

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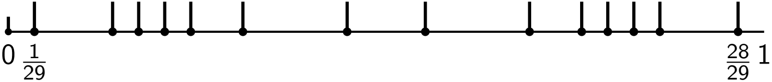

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Theorem (S. 2018)

For prime p

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

Compare to Existing Results

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Theorem

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

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

'There are exceptional sets but few.'

Theorem (Cole Graham 2020)

For primes p and $2 < q < \infty$

$$W_q\left(\frac{1}{p}\sum_{k=0}^{p-1}\delta_{\frac{k^2 \mod p}{p}}\right) \lesssim \frac{1}{\sqrt{p}}$$

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He also pointed out that

$$W_2\left(\frac{1}{p}\sum_{k=0}^{p-1}\delta_{\frac{k^2 \mod p}{p}}\right) \geq \frac{1}{\sqrt{12p}}$$

which shows that this result is sharp.

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This actually tells us something nice about $\sqrt{2}$: consider

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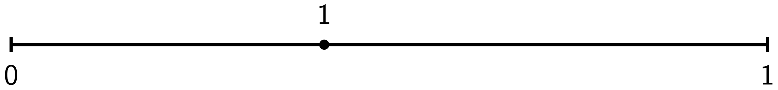

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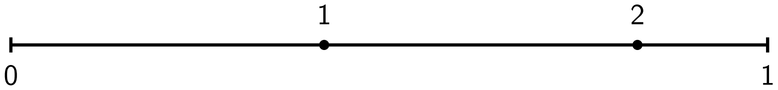

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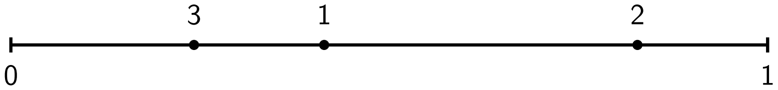

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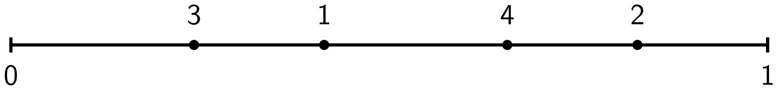

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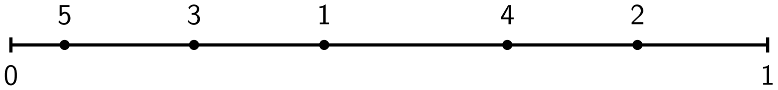

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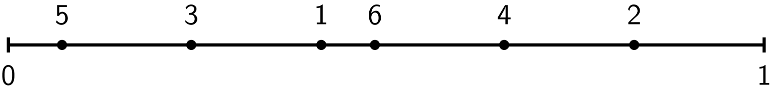

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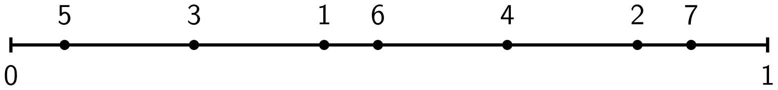

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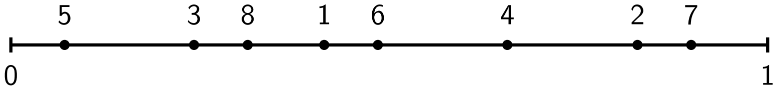

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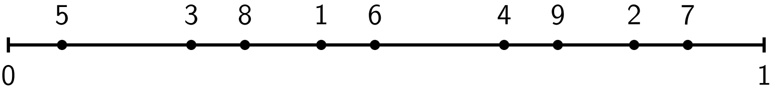

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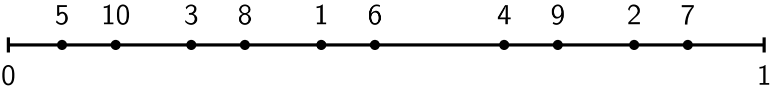

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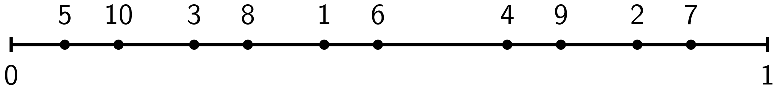

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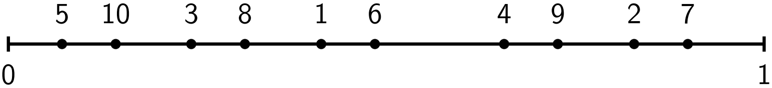

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For each interval $J \subset [0,1]$, the number of elements of $\{x_1, \ldots, x_N\}$ are in J is $= |J|N \pm \mathcal{O}(\log N)$.

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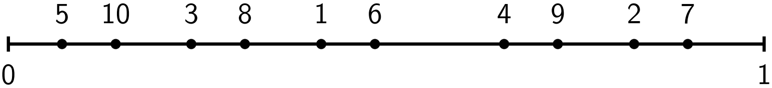

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Wasserstein Distance

The amount of mass that will be exported out of or imported into $J \subset [0,1]$ is, typically, $\mathcal{O}(\sqrt{\log N})$.

Moving towards Sampling

Suppose you have $f : [0,1]^d \to \mathbb{R}$ and you want to approximate

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This requires *some* assumptions on the function f. Here, we will capture this by using the size of the gradient $\|\nabla f\|_{L^p}$.

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The average distance from a point in $[0,1]^d$ to a point is $\sim N^{-1/d}$.

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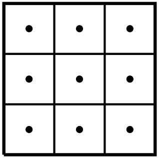

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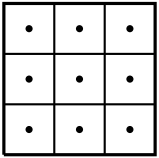

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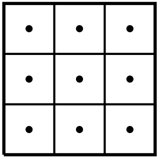

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Solutions of the Coffee Shop problem lead to good sequences of points!

Theorem (Louis Brown and S, 2019)

Let $d \geq 2$ and let $\alpha \in \mathbb{R}^d$ be a badly approximable vector. Then, for some $c_\alpha > 0$ and all differentiable $f : \mathbb{T}^d \to \mathbb{R}$ and all $N \in \mathbb{N}$

$$\left| \int_{\mathbb{T}^d} f(x)dx - \frac{1}{N} \sum_{k=1}^{N} f(k\alpha) \right| \leq c_\alpha \|\nabla f\|_{L^\infty(\mathbb{T}^d)}^{(d-1)/d} \|\nabla f\|_{L^2(\mathbb{T}^d)}^{1/d} N^{-1/d}.$$

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- Uniformly for a sequence and
- better L^p-spaces.
- In fact, this even generalizes to the standard classical grid for which we also obtain an improvement.

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Kantorovich-Rubinstein duality (special case)

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

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

where W_1 denotes the $1-$Wasserstein (or Earth Mover's) Distance.

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This got me interested in Kantorovich-Rubinstein duality. In the simplest possible setting, it says the following.

Kantorovich-Rubinstein duality (special case)

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

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

where W_1 denotes the $1-$Wasserstein (or Earth Mover's) Distance.

We know from all the previous arguments that

$$\inf_{x_1,\dots,x_N} W_1\left(\frac{1}{N}\sum_{k=1}^{N} \delta_{x_k}, dx \right) \sim \frac{1}{N^{1/d}}$$

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Can we trade one against the other? **Generally not**. Consider

$$W_1(\delta_{x_0}, \delta_{x_1}) = \sup_f |f(x_0) - f(x_1)|.$$

Kantorovich-Rubinstein Inequalities?

What I would like to know

If $f : [0,1]^d \to \mathbb{R}$ is Lipschitz and $\{x_1, \dots, x_N\} \subset [0,1]^d$, are there inequalities of the form

$$\left| \int_{[0,1]^d} f(x)dx - \frac{1}{N}\sum_{k=1}^{N} f(x_k) \right| \leq \|\nabla f\|_{X_p} \cdot W_p\left(\frac{1}{N}\sum_{k=1}^{N}\delta_{x_k}, dx\right)?$$

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- Certainly such inequalities exist: pick the Banach space $X_p = L^{\infty}$. That works (follows from Kantorovich-Rubinstein).
- The question is: can you pick a larger Banach space (corresponding to a smaller norm)?
- And what is the best space for a given p?

Kantorovich-Rubinstein Inequalities?

What I would like to know (special case, $p = \infty$)

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

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- I can *almost* prove it.

Kantorovich-Rubinstein Inequalities?

Theorem (S, 2020)

For any $f : [0,1]^d \to \mathbb{R}$ and any $\{x_1, \ldots, x_N\} \subset [0,1]^d$,

$$E = \left| \int_{[0,1]^d} f(x)dx - \frac{1}{N} \sum_{k=1}^{N} f(x_k) \right|$$

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- Improves Bakhalov in the case of the grid.

An Interesting Lemma

Lemma (S, 2020)

Let μ be a measure on $\mathbb{R}^d$ such that

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$$\left| \int_{\mathbb{R}^d} f(x) d\mu \right| \leq c_d \cdot R \cdot \mu(\mathbb{R}^d)^{\frac{d-1}{d}} \cdot \|\nabla f\|_{L^{d,1}(\|x\| \leq R)}$$

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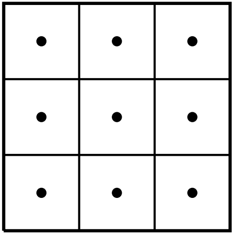
I thought that this was quite interesting because its ‘doubly isoperimetric’, both with respect to the measure and the function. I am pretty sure the scaling is best possible.



THANK YOU!