Optimal Transport and Point Distributions on the Torus

Stefan Steinerberger

Point Distribution Webinar, September 2020

UNIVERSITY of WASHINGTON

The Story in 2 Slides

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where D_N is the discrepancy and Var denotes Hardy-Krause variation. Hardy-Krause is tricky: it tends to grow exponentially in the dimension.

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The point of this talk is to discuss a new type of notion. I propose we look at something called the Wasserstein distance

$$W_1 = W_1\left(\frac{1}{N}\sum_{k=1}^{N}\delta_{x_k}, dx\right) \qquad \text{as a measure of regularity.}$$

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

Moreover, this inequality is sharp. $\|\nabla f\|_{L^\infty}$ is, I would argue, a lot more natural than Hardy-Krause.

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is not really useful until $N \gg d^d$. In contrast,

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

has no such hidden costs. The price: $W_1 \gtrsim N^{-1/d}$.

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- Computing the Wasserstein Distance for some classical sequences (which is a very nice thing: it's not some abstract quantity, it can actually be computed)
- What does this mean for Numerical Integration?

Gaspard Monge (1746 – 1818)

1781: 'Sur la théorie des déblais et des remblais'

Roughly: 'On the Theory of Rubble and Embankments'

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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

Optimal Transport

Suppose we are given two measure μ and ν having same total mass and want to transport one to the other. (In all our applications, μ will be the measure induced by the points and $\nu = dx$.)

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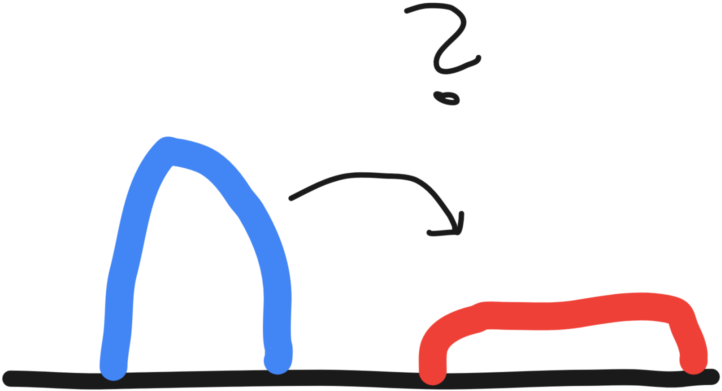

Optimal Transport

Think of both measures as being a collection of little boxes. Suppose it costs $\delta \cdot \varepsilon$ to move a box of weight ε distance δ. What is the cheapest way to move the boxes to the desired goal?

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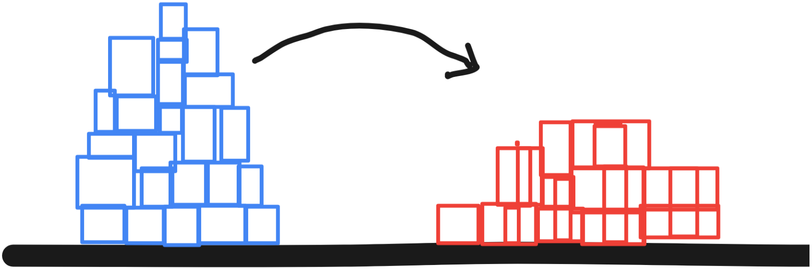
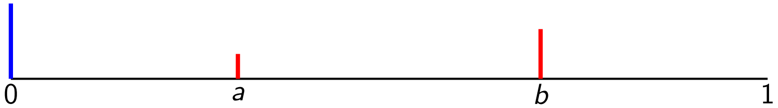
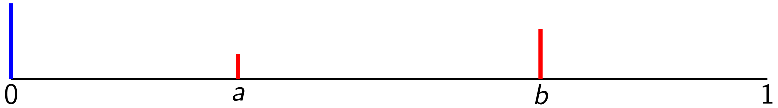


Wasserstein Distance



One unit of mass in 0 (blue), 1/3 unit of mass in a, 2/3 mass in b.

Wasserstein Distance



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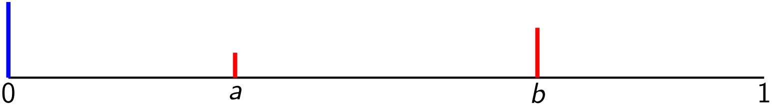
$$W_1(\mu, \nu) = \frac{a}{3} + \frac{2b}{3}$$

This is the *Earth Mover Distance*, the physical cost.

Wasserstein Distance



One unit of mass in 0 (blue), $1/3$ unit of mass in a, $2/3$ mass in b.

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This is the *Earth Mover Distance*, the physical cost. There also exists an L^p-version of this, where $p > 1$, which leads to the $p-$Wasserstein distance

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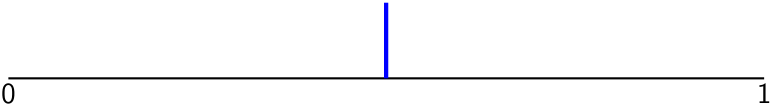
$$W_p(\mu, \nu) = \left(\frac{1}{3} a^p + \frac{2}{3} b^p \right)^{1/p}$$

Wasserstein Distance



One unit of mass in $1/2$ (blue). How much do I pay for the transport to dx?

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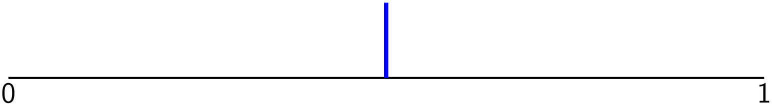

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$$W_1(\mu, dx) = \int_0^1 \left| x - \frac{1}{2} \right| dx = \frac{1}{4}.$$

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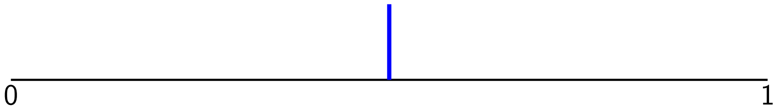

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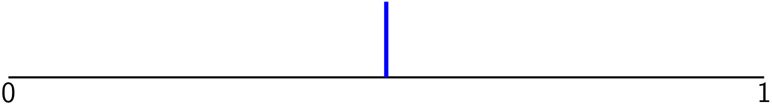

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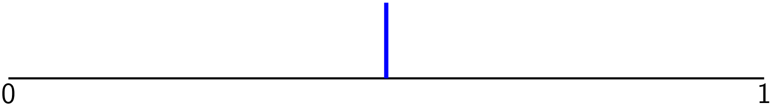

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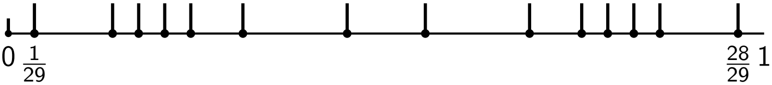
Hölder's inequality implies that $W_p \geq W_1$. For this talk: feel free to replace everything by W_1 (in fact, I assume that for most of the talk the W_1 and the W_2 behave similarly).

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



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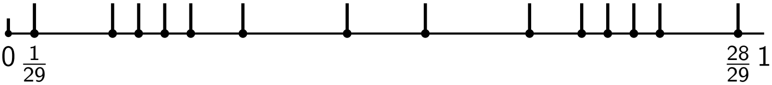

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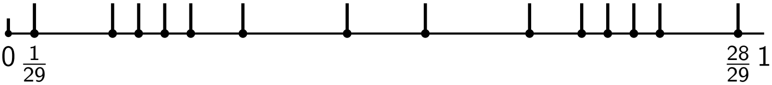

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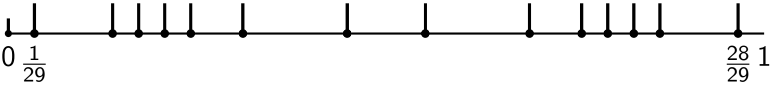

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Theorem (S. 2018)

For primes p

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

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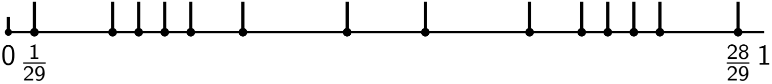

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This tells us that we have to move most particles roughly distance $\sim p^{-1/2}$. This is in line with the heuristic that these are ‘random’.

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It is natural to compare this to the **discrepancy**

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

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Theorem

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

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

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Theorem (Cole Graham 2020)

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

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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.

Irrational Rotations: Kronecker sequences

Theorem (S 2018)

$$W_2 \left(\frac{1}{N} \sum_{n=1}^{N} \delta_{\sqrt{2} \cdot n \mod 1}, \ dx \right) \lesssim \frac{\sqrt{\log N}}{N}$$

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Theorem (Cole Graham 2020)

For every $(x_n)_{n=1}^{\infty}$ in $[0,1]$, there are infinitely many N such that

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

Something Very Nice

Theorem (R. Peyre, 2018)

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$$W_2(\mu, dx) \lesssim \left(\sum_{\ell \neq 0} \frac{1}{\ell^2} \left| \frac{1}{N} \sum_{k=1}^{N} e^{2\pi i \ell x_l} \right|^2 \right)^{1/2}.$$

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This is reminiscent of the Erdős-Turan inequality.

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Cole Graham (arXiv:1910.14181) has similar results on the torus, Bence Borda (arXiv:2005.04925) on compact Lie groups.

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The upper bound is also known as **Zinterhof's diaphony**.

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The upper bound is also known as **Zinterhof's diaphony**. This allows us to easily deal with the van der Corput sequence

$$\frac{1}{2}, \frac{1}{4}, \frac{3}{4}, \dots$$

Theorem (Proinov)

For the van der Corput sequence

$$W_2\left(\frac{1}{N}\sum_{n=1}^{N} \delta_{x_n}, dx\right) \lesssim \frac{\sqrt{\log N}}{N}$$

The Coffee Shop Problem: Irregularities of Distributions

How to place your coffee shops?

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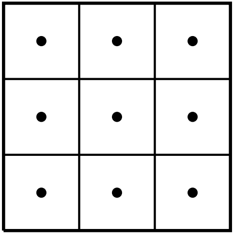

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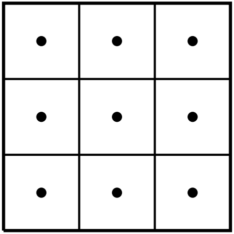

Question. Is there a sequence $(x_n)_{n=1}^{\infty}$ on $[0,1]^2$ such that

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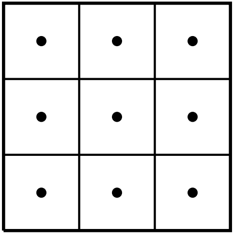

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(Recall, Cole Graham: on $[0,1]$, no sequence has $\lesssim N^{-1}$.)

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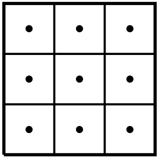

Theorem (Louis Brown and S, 2019)

Let $d \geq 2$ and let $\alpha \in \mathbb{R}^d$ be badly approximable. Then the Kronecker sequence $x_k = k\alpha \mod 1$ satisfies

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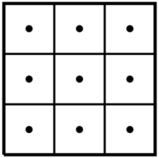

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In $d \geq 3$, this seems to be fairly easy to do. **Open Problem.** But $d = 2$ appears subtle, are there other constructions?

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This has an interesting analogue in Analytic Number Theory: **Zinterhof's Diaphony**. For $\{x_1, \dots, x_N\} \subset [0,1]$, Zinterhof's diaphony F_N is given by

$$F_N = \left(\sum_{\ell \neq 0}\frac{1}{\ell^2}\left|\frac{1}{N}\sum_{k=1}^{N} e^{2\pi i \ell x_l}\right|^2\right)^{1/2}.$$

It has never been generalized to higher dimensions.

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Theorem (Louis Brown and S, 2019)

For each $t > 0$,

$$\boxed{W_2(\mu, dx)^2 \lesssim_d \inf_{t>0}\left[t + \sum_{\substack{k\in\mathbb{Z}^d \\ k\neq 0}} \frac{e^{-\|k\|^2 t}}{\|k\|^2}\left|\frac{1}{N}\sum_{n=1}^{N} e^{2\pi i\langle k, x_n\rangle}\right|^2\right]}$$

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Some of them can probably be attacked via Exponential Sums?
Others (nets?) via explicit constructions?

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We recall that

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

What if the function is twice-differentiable? Or in other smoothness classes?

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Likewise, we have

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When N is large, some kind of lattice structure (sphere packing?) is presumably optimal (see also Hinrichs, Novak, Ullrich, Wozniakowski, 2016).But $N = 1000$ in $d = 30$? ($2^{30} \gg 1000$)

A Final Application

The following is **very classical**. Let $f : [0,1]^d \to \mathbb{R}$. Then there are points $\{x_1, \dots, x_N\} \subset [0,1]^d$ such that

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

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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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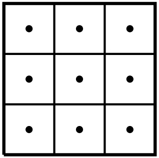

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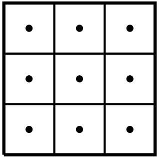

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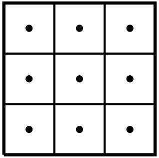

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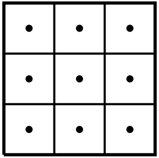

Sukharev (1979) showed that this leads to the smallest constant.
But what if we want to take a sequence? On-line sampling? We do not know how many points we get?

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 universal $c_\alpha > 0$ and all differentiable $f : \mathbb{T}^d \to \mathbb{R}$

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... this is **strange**. The grid should actually be the best....

Slight Improvement over a Classical Result

Theorem (Louis Brown and S, 2019)

We have, for some explicit constant c_d depending only on the dimension, for all differentiable $f : [0,1]^d \to \mathbb{R}$ sampled on the regular grid $(x_k)_{k=1}^N$

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This is sharp again (probably?): take $0 < \varepsilon \ll 1$ and

$$f(x) = \min\left\{\varepsilon, \min_{1 \leq i \leq N} \|x - x_i\|\right\}.$$

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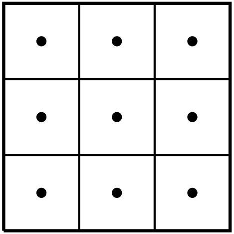
In contrast, the Wasserstein distance does not care very much about the underlying background. This makes it a **stable** notion. But there are lots of problems on, say, $\mathbb{S}^2$ as well, and we'll discuss some of them on Friday.



Thank you!