Positive-definite Functions, Exponential Sums and the Greedy Algorithm: a Curious Phenomenon

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Yale University

August 12, 2020

The Big Picture

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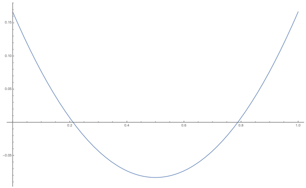

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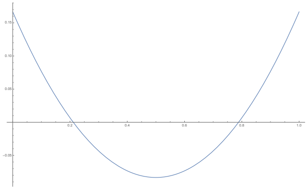

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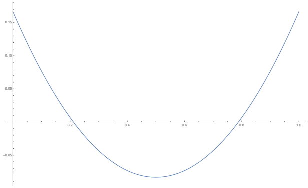

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We define a sequence of points by starting with an arbitrary initial set $\{x_1, \ldots, x_m\} \subset [0,1]$ and then greedily setting

$$x_n = \arg\min_{x \in \mathbb{T}} \sum_{k=1}^{n-1} f(x - x_k).$$

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Figure: $f(x)$

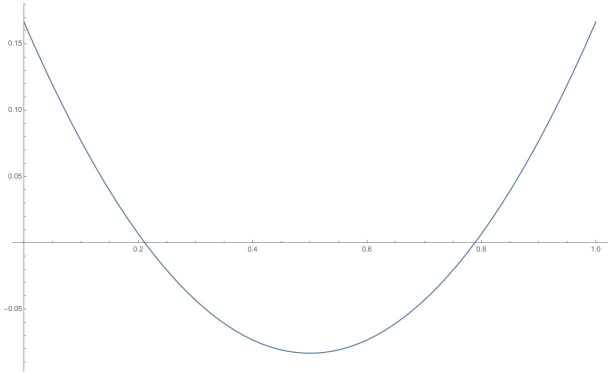

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Figure: $f(x) + f(x - .5)$

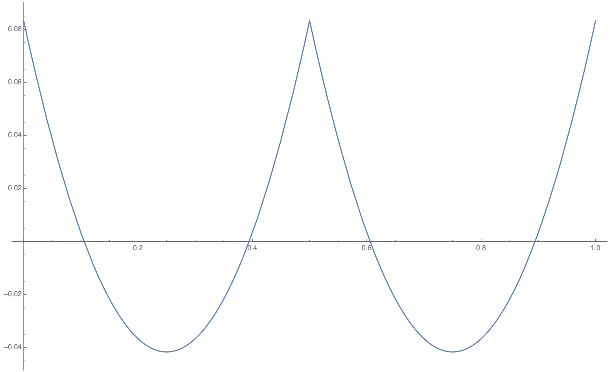

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Figure: $f(x) + f(x - .5) + f(x - .25)$

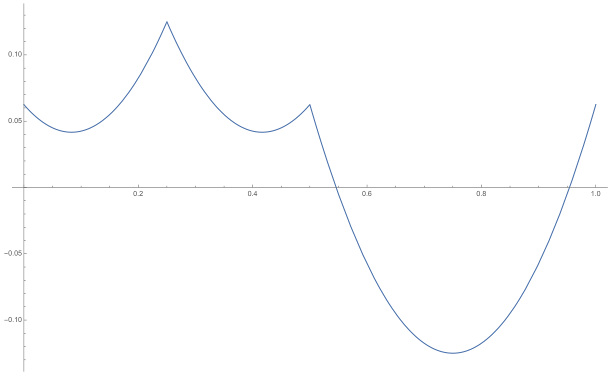

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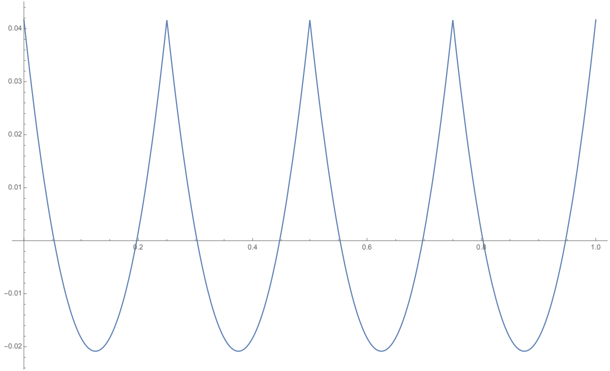
Figure: $f(x) + f(x - .5) + f(x - .25) + f(x - .75)$



$$0, .5, .25, .75, \ldots$$

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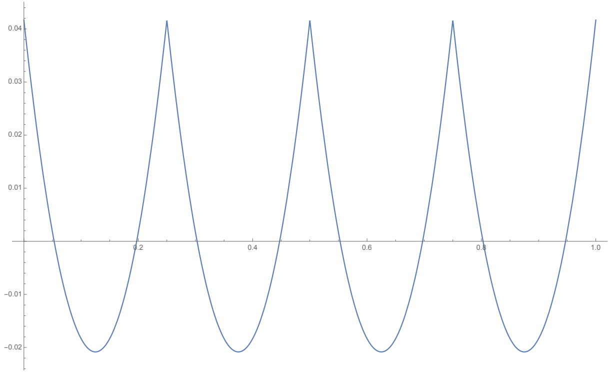

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We see that this produces an **extremely** regular sequence.

Talk Structure

1. Two Friendly Sequences

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These two sequences were both cooked up to be optimally regular, but they are very differently built–let's take a closer look.

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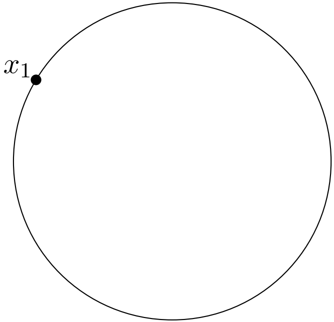

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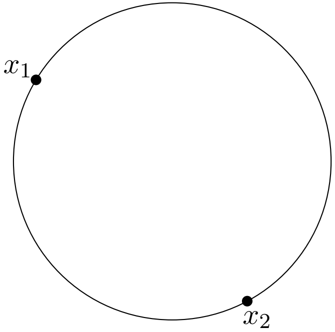

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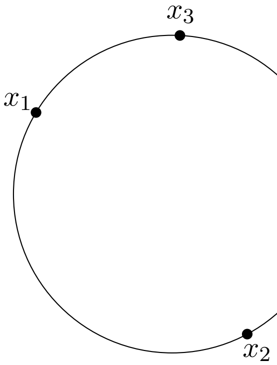

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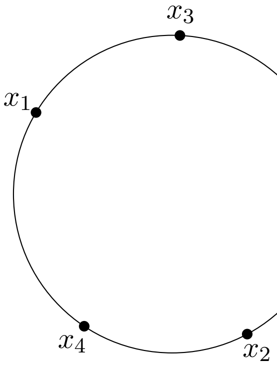

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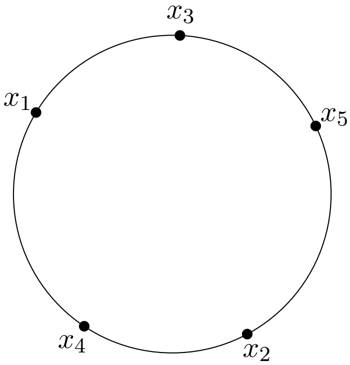

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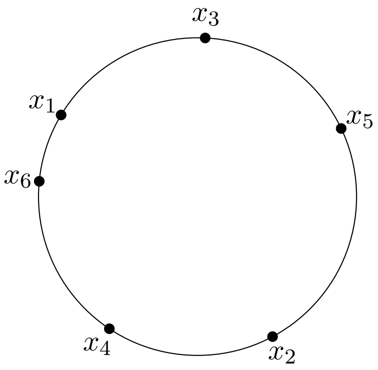

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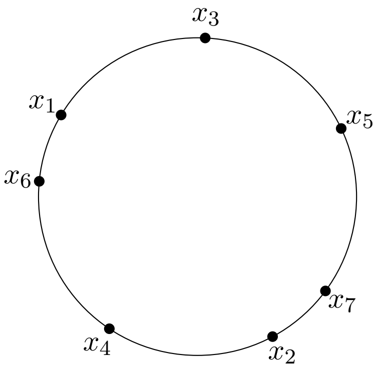

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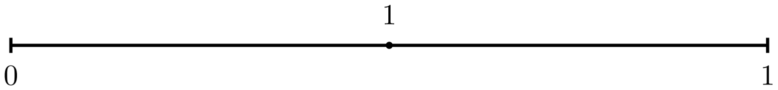

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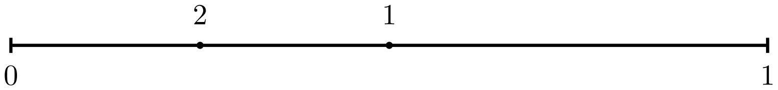

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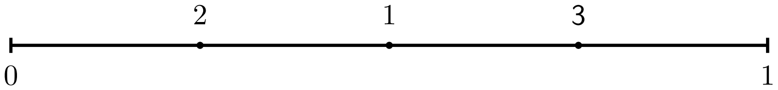

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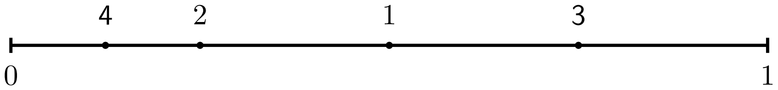

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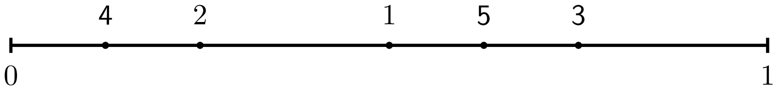

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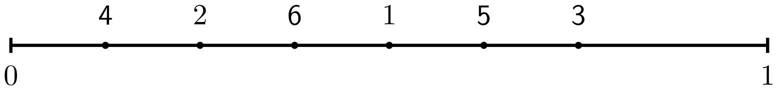

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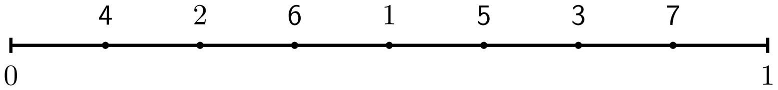

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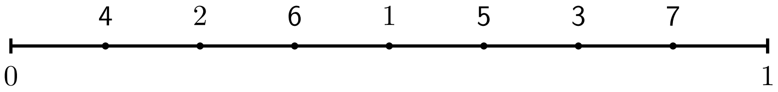

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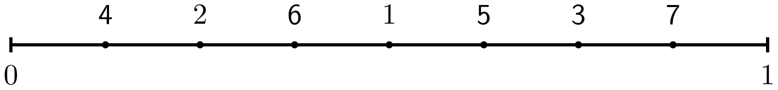

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The van der Corput sequence uses the regularity of binary expansions of numbers to produce uniformity. Note that it greedily "fills in the gaps"–at each step, it places a point at the midpoint of the longest empty interval. We'll come back to this...

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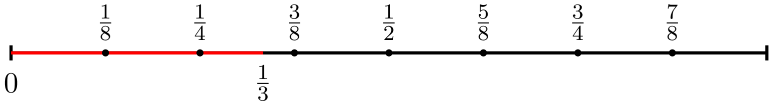

Figure: 7 terms of the van der Corput sequence; 2 lie in $(0, 1/3)$.

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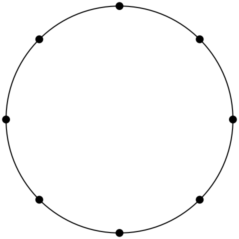

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It's very easy to compute the exponential sum

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integrating f over the unit interval exactly.

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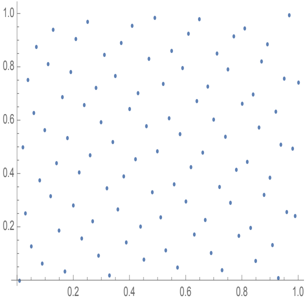

Figure: The first 100 terms of the van der Corput sequence

Discrepancy

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- The question naturally arises: can a discrepancy asymptotically on the order of $1/N$ be achieved?
- van der Corput sequence is always perfectly uniform after 2^n terms, attaining this bound. But! in between powers of 2, it accumulates a logarithmic error term.

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Up to constants, the Kronecker and van der Corput sequences achieve this lower bound.

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$$f(x) = \sum_{i=1}^{n} |x - x_i|^{-1}.$$

We can imagine a shifted $1/|x|$ function placed over each point:

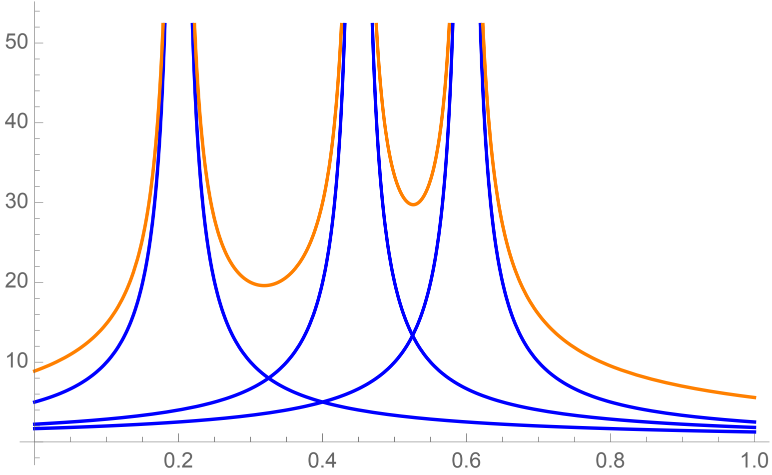

Figure: The potential of a point when charges are placed at .2,.6, and .45

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The resulting sequence has remarkable distribution properties!

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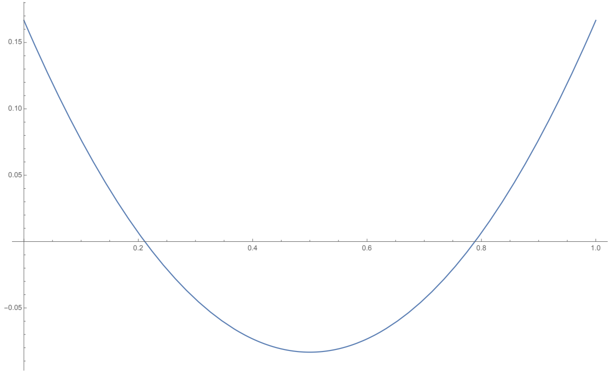
Figure: $f(x)$



0

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Figure: $f(x) + f(x - .5)$

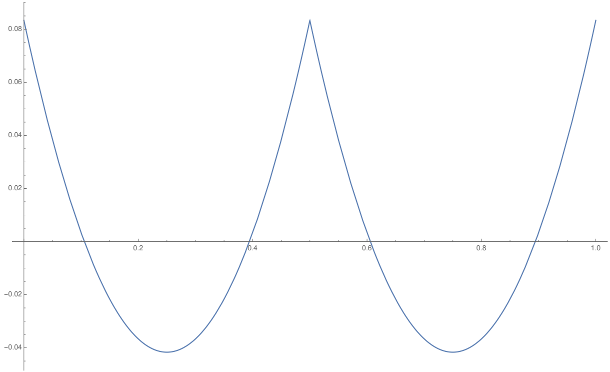

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Figure: $f(x) + f(x - .5) + f(x - .25)$

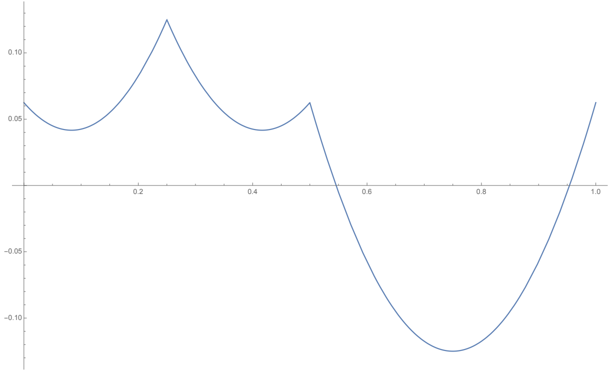

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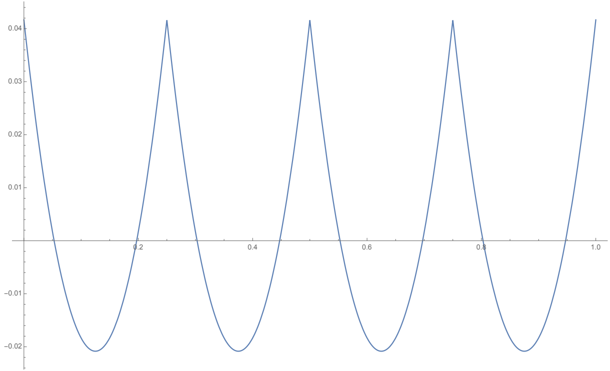
Figure: $f(x) + f(x - .5) + f(x - .25) + f(x - .75)$



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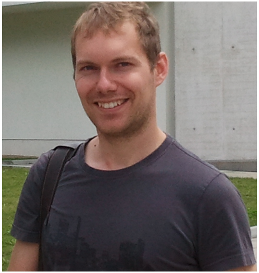

Figure: Florian Pausinger

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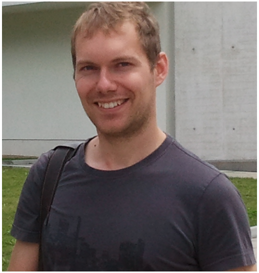

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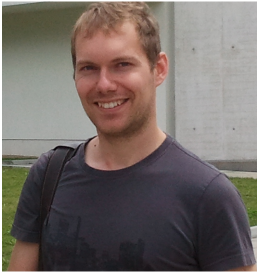

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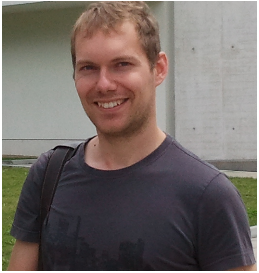

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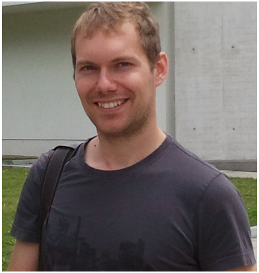

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Then the greedy algorithm running on f *and the initial set* $\{0\}$ *yields a van der Corput sequence.*

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where $\tilde{c} > 0$ depends on the initial set.

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Later in the talk, we will present the (very slick!) proof.

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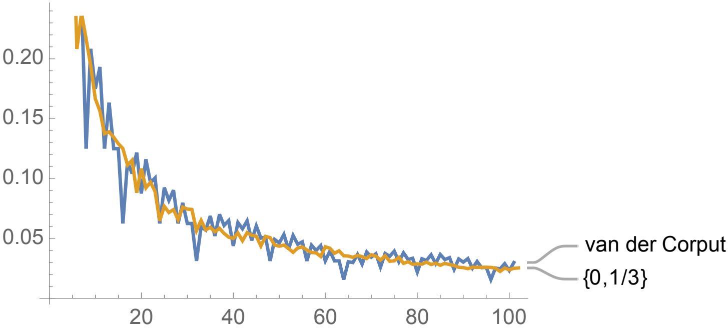

Figure: Discrepancy of van der Corput vs Algorithm running on $\{0, 1/3\}$

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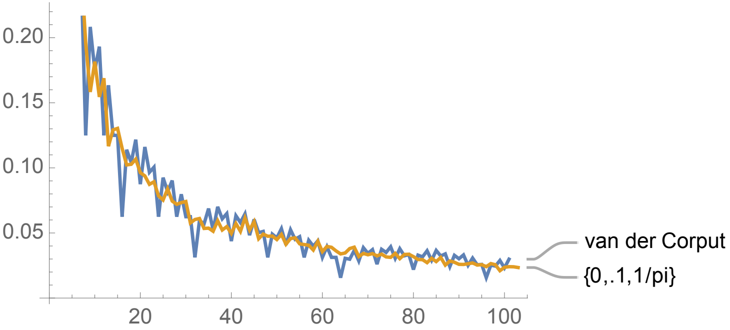

Figure: Discrepancy of van der Corput vs Algorithm running on $\{0, 1/10, 1/\pi\}$

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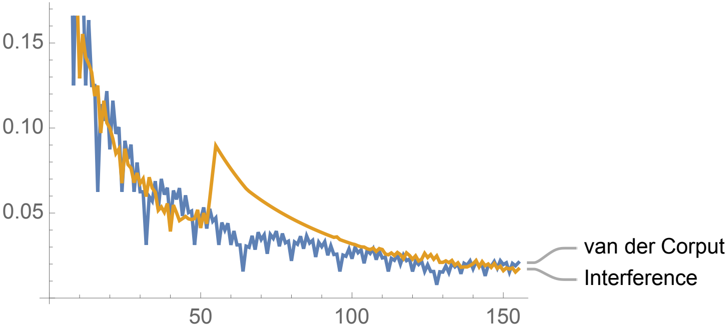

Figure: Discrepancy of van der Corput vs Algorithm running on $\{0, .6\}$ for 50 points, then add $\{.5, .51, .52\}$ to the sequence and run for another 100

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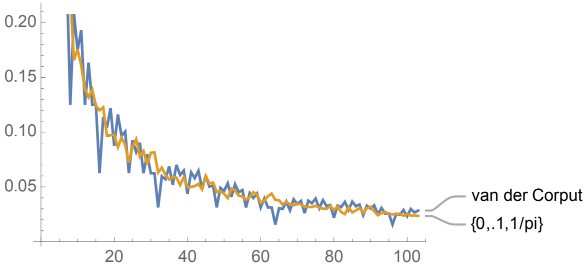

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Curious Phenomena

Conjecture 1 For all initial sets $\{x_1, \ldots, x_m\}$, and all even f such that $\hat{f}(k) > ck^{-2}$ for all $k \neq 0$, the greedy algorithm

$$x_n = \arg\min_{x \in \mathbb{T}} \sum_{k=1}^{n-1} f(x - x_k)$$

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(Proinov showed that this is optimal, no sequence can do better.)

Conjecture 2 For all initial sets $\{x_1, \ldots, x_m\}$, and all even f such that $\hat{f}(k) > ck^{-2}$ for all $k \neq 0$, the greedy algorithm

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We really suspect both these to be true based on the numerics, but the results we can prove are much looser bounds.

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$V(f)$ is a constant (only depends on f, not the set of points).

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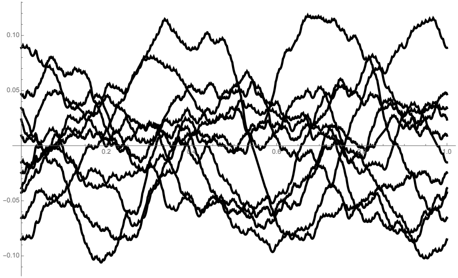

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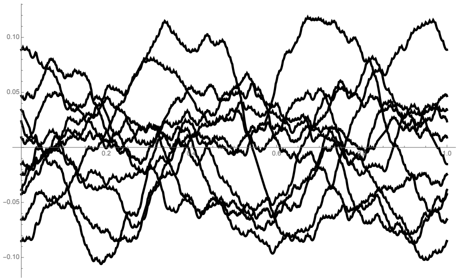

Figure: The functions $f_{100}, f_{110}, f_{120} \ldots, f_{200}$.

Somehow, all the shifted functions f balance out extremely nicely in such a way that the energy of the system stays low.

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In fact, the sequences defined via the algorithm appear, empirically, to be competitive with van der Corput and Kronecker sequences (which are known to be optimal) on all of the regularity measures discussed at the beginning: Combinatorially, Analytically, Numerically, and Geometrically. However, a proof is evasive, and it is an open question whether or not they truly are.

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people in number theory/combinatorics think of this as "diaphony", whereas the Sobolev norm is more analytical and shows up in PDEs.

Proof of Pausinger's Theorem

We now present a proof of Pausinger's Theorem:

Theorem (Pausinger '20)

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Thus

$$\sum_{m,\ell=1}^{n} f(x_m - x_\ell) \le nf(0). \qquad (\diamond)$$

Proof of Pausinger's Theorem

On the other hand, we have

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\sum_{m,\ell=1}^{n} f(x_m - x_\ell) &= \sum_{k\in\mathbb{Z}} \widehat{f}(k) \sum_{m,\ell=1}^{n} e^{2\pi i k(x_m - x_\ell)} \\
&= \sum_{k\in\mathbb{Z}} \widehat{f}(k) \left(\sum_{m=1}^{n} e^{2\pi i k x_m}\right) \left(\sum_{m=1}^{n} e^{2\pi i k(-x_m)}\right) \\
&= \sum_{k\in\mathbb{Z}} \widehat{f}(k) \left(\sum_{m=1}^{n} e^{2\pi i k x_m}\right) \overline{\left(\sum_{m=1}^{n} e^{2\pi i k x_m}\right)} \\
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\end{aligned}$$

Thus, combining with $\diamond$ from the previous slide,

$$\sum_{k\in\mathbb{Z}} \widehat{f}(k) \left|\sum_{m=1}^{n} e^{2\pi i k x_m}\right|^2 \leq n f(0).$$

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so $\|\mu_n\|_{\dot{H}^{-1}} \lesssim n^{-1/2}$. Finally, by LeVeque's Inequality, we can bound the discrepancy as

$$D_n \lesssim \|\mu_n\|_{\dot{H}^{-1}}^{2/3} \lesssim n^{-1/3}$$

and we have the desired result. □

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Higher Dimensions

The problem on the sphere with Riesz kernel $|x - y|^{-1}$ dates back to physicist J.J. Thomson in 1904, yet, to this day, only a handful of cases are known:

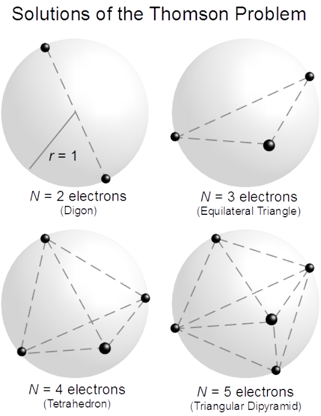

Figure: From Wikipedia

Higher Dimensions

If even the sphere poses a challenge, how can we hope to solve this on general manifolds?

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This has been researched, and greedy sequences constructed this way (with any kernel) are called *Leja Points*. López-García and Wagner have a wealth of results on the 1-dimensional circle alone.

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The scaling of the proof is fundamentally different in higher dimensions, and yields stronger bounds!

Wasserstein Distance

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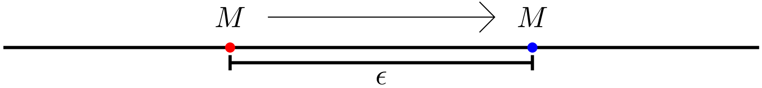

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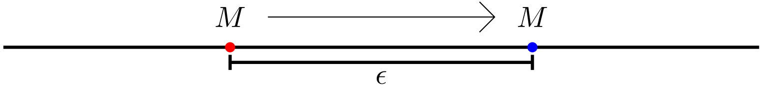
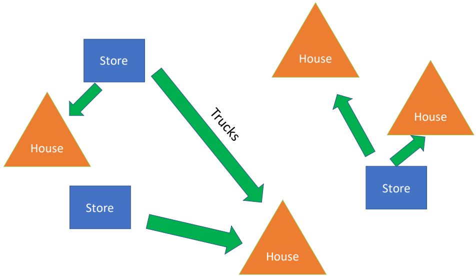


Figure: Transporting a point mass of weight M by distance ϵ incurs a cost of $M \cdot \epsilon$.

Figure: The Wasserstein distance between the blue and red point distributions which each have 2 point masses of weight $1/2$ is $\frac{1}{2}(.1) + \frac{1}{2}(.5) = .3$

Wasserstein Distance

Figure: Transporting between a point distribution on stores and houses



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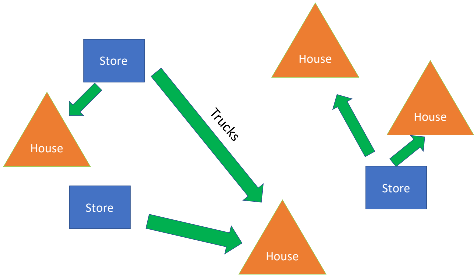

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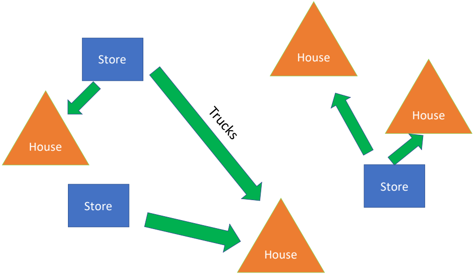
Wasserstein Distance

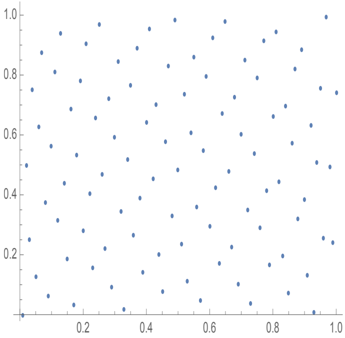
Figure: Transporting between a point distribution on stores and houses



In our setting, every point on the unit interval has a "house": We are interested in measuring the Wasserstein distance between the point measure μ_N from our sequence and the uniform distribution dx.

Wasserstein Distance

Here's the van der Corput sequence mapped to $[0,1]^2$ by $(\frac{i}{100}, x_i)$:



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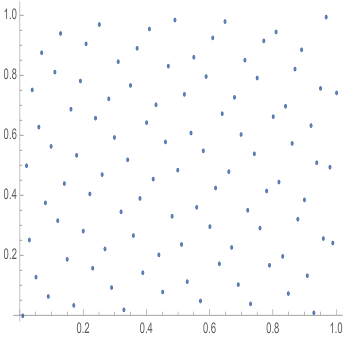

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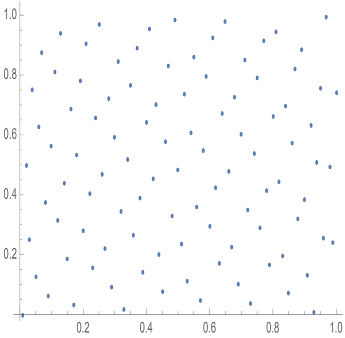

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We can imagine taking the Wasserstein distance between the (normalized) sum of Dirac measures on the points and the uniform distribution on the unit square: we would need to "smudge" each point to transport its mass continuously over nearby points, and W_1 measures how much smudging we need.

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Formally, the $p-$Wasserstein distance between two measures μ and ν is defined as

$$W_p(\mu,\nu) = \left(\inf_{\gamma \in \Gamma(\mu,\nu)} \int_{M \times M} |x-y|^p d\gamma(x,y) \right)^{1/p}$$

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where $|\cdot|$ is the metric and $\Gamma(\mu, \nu)$ denotes the collection of all measures on $M \times M$ with marginals μ and ν (also called the set of all couplings of μ and ν).
In 1-d, we have

$$W_2(\mu, dx) \lesssim \|\mu\|_{\dot{H}^{-1}},$$

so W_2 seems like a good generalization of diaphony to higher dimensions.

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For any d-dimensional manifold M, there is a constant $c > 0$ such that, for any set of N points $\{x_1, \ldots, x_N\}$ on M, we have

$$W_1\left(\frac{1}{N}\sum_{i=1}^{N}\delta_{x_i}, dx\right) \geq cN^{-1/d}.$$

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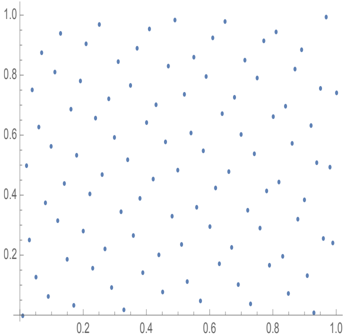

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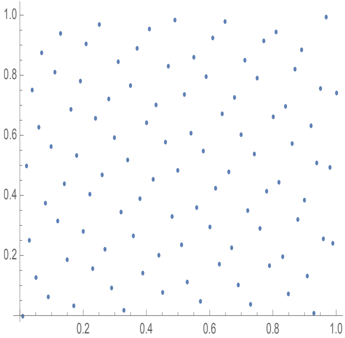

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We may imagine that each point on the plot is actually a very small disc, and we see that the vast majority of the area is outside these discs; thus, we would need to carry most of the point mass by (much) more than the radius of the discs.

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Theorem (B & Steinerberger '20)

Let x_n be a sequence obtained on a $d-$dimensional compact manifold, by starting with an arbitrary set $\{x_1, \dots, x_m\}$ and greedily setting

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Then

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

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This result is optimal in $d \geq 3$, but nobody knows what the best discrepancy is (or if this implies that these sequences obtain it)!

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- Other types of functions that work?

Thank you!