An Optimization Perspective on the Construction of Low Discrepancy Point Sets

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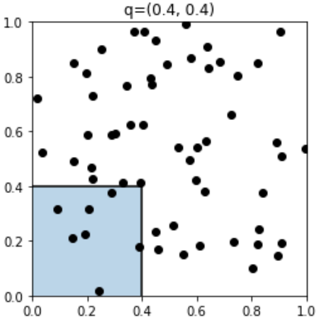
PhD Defense, 18/07/2024

The L_∞ star discrepancy

Approximate volume of boxes $[0,q) \subseteq [0,1)^d$ by the proportion of points inside.

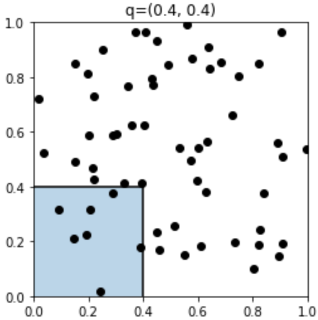


The L_∞ star discrepancy

L_∞ star discrepancy

For P a point set in $[0;1]^d$,

$$d^*_\infty(P) = \sup_{q \in [0;1)^d} \left| \frac{|P \cap [0,q)|}{|P|} - \lambda([0,q)) \right|.$$



Local discrepancy:

$D(q,P) = |7/60 - 0.16| = 0.044$

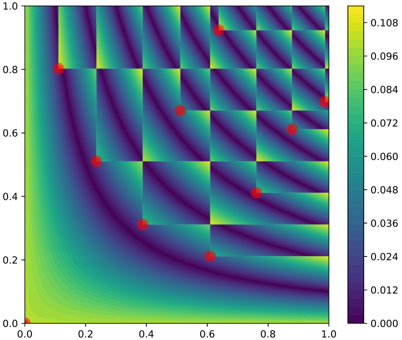


Figure: Discrepancy heatmap for 10 points in dimension 2

Why discrepancy?

- Covering a search space uniformly: design of experiments, non-adaptive black-box optimization, Quasi-Monte Carlo methods
- **Koksma-Hlawka inequality**: Discrepancy is a bound for the error of approximating an integral

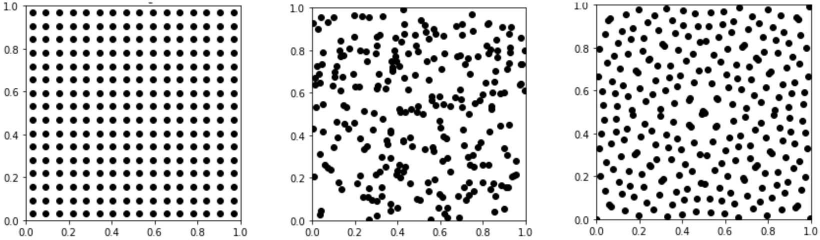
$$\left| \int_{[0,1]^d} f(x) d\lambda^d(x) - \frac{1}{|P|} \sum_{p \in P} f(p) \right| \leq Var(f) d_\infty^*(P)$$

How many samples do you need for a desired error bound?

Summary

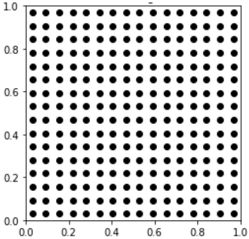
- Background
- Optimal constructions and beyond
- Set extraction and heuristic construction
- From sets to sequences

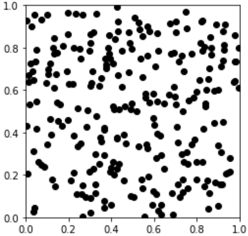
Some point sets

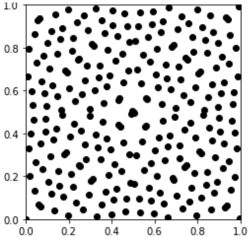


- Grid points: $O(n^{-1/d})$

Some point sets

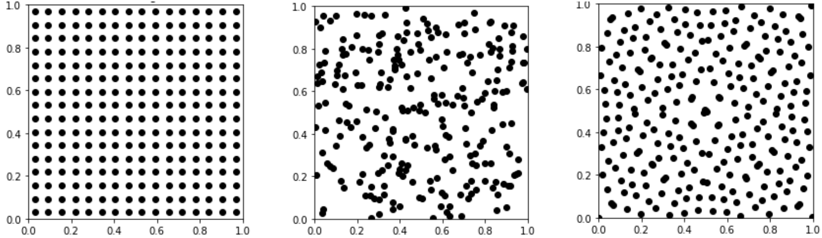






- Random points: $\Theta(\sqrt{d/n})$

Some point sets



- Sobol' (and low-discrepancy sequences in general): $O\left(\frac{\log^d(n)}{n}\right)$

Sets vs Sequences

- Sequence: Infinite sequence of points. Any prefix big enough has low discrepancy
- Set: Finite set of points, good only for a specific n

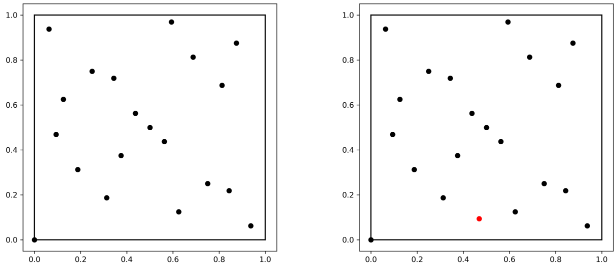


Figure: The Sobol' sequence for 20 and 21 points

A specific construction: the Fibonacci set

- Kronecker sequence: Given $\alpha \in \mathbb{R} \setminus \mathbb{Q}$, we define the sequence $(x_n)_{n\in\mathbb{N}} = \{\{i\alpha\} : i \in \mathbb{N}\}$. These sequences are uniformly distributed [Weyl, 1916]
- Among these, one of the best is for $\alpha = \phi := (1+\sqrt{5})/2$: the Fibonacci sequence
- We can then associate it to a two-dimensional lattice of fixed size n, $P = \{(i/n, \{\phi i\}) : i \in \{0, \ldots, n-1\}\}$

A specific construction: the Fibonacci set

$$P = \{(i/n, \{\phi i\}) : i \in \{0, \ldots, n-1\}\}$$

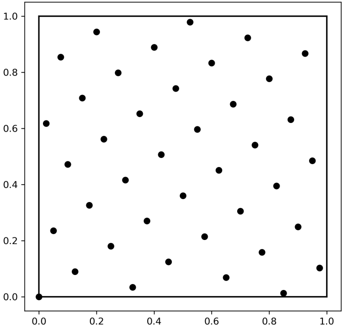


Figure: The Fibonacci set for 40 points

The minimal star discrepancy

- The optimal discrepancy order is unknown
- The asymptotic order is $O\left(\frac{\log^d(n)}{n}\right)$ for sequences, or $O\left(\frac{\log^{d-1}(n)}{n}\right)$ for sets. What happens for smaller n?
- The minimal star discrepancy, $d_\infty^*(n,d)$, is the best possible L_∞ star discrepancy value for a point set of size n in dimension d
- There is a bound by [Heinrich et al, 2001] showing that $d_\infty^*(n,d) \leq C\sqrt{d/n}$ for some constant C
- In general there is no constructive approach to obtain point sets matching these bounds

Very small instances: optimal values

- $d^*_\infty(n,d)$ is explicitly known in only a few specific cases
- [White, 1977] gave point sets for $n \leq 6$ in dimension 2
- 1-point sets for any d have been solved by [Pillard, Cools and Vandewoestyne, 2006], extended to 2 points by [Larcher and Pillichshammer, 2007]
- For the periodic L_2 discrepancy, [Hinrichs and Oettershagen, 2016] solved the problem for $n \leq 16$

Can we provide point sets matching $d^*_\infty(n,d)$?

Computing the star discrepancy

Calculating the discrepancy is a discrete problem, maximal values can only be reached on a grid defined by the points [Niederreiter, 1972].

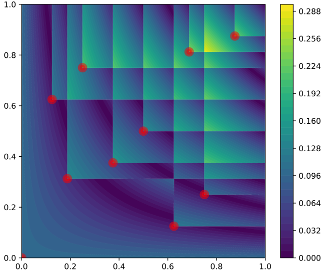


Figure: Critical boxes defined by a given point set in two dimensions.

Computing the star discrepancy

- From the discrete "positions-grid": $O\left(n^d\right)$, $O\left(n^d/d!\right)$ if we only count **critical boxes**
- Best known algorithm: $O\left(n^{1+d/2}\right)$ by [Dobkin, Eppstein and Mitchell, 1996]
- New parallel implementation by Alexandre D. Jesus as part of a GECCO paper[1]. It is based on the original work of Magnus Wahlström
- Best heuristic in higher dimensions: **Threshold Accepting** algorithm by [Gnewuch, Wahlström and Winzen, 2012]

Too expensive to evaluate!

[1] F. C., D. Vermetten, J. de Nobel, A. D. Jesus, C. Doerr, L. Paquete. Computing Star Discrepancies with Numerical Black-Box Optimization Algorithms. Proceedings of GECCO 2023

Summary

- Background
- **Optimal constructions and beyond**
- Set extraction and heuristic construction
- From sets to sequences

Optimal constructions[2]

Optimal L_∞^* star discrepancy set

Given an integer $n \geq 1$ and a dimension $d \geq 2$, find a set P of size n in dimension d of discrepancy $d_\infty^*(n,d)$.

- Our two non-linear programming formulations rely on the grid structure of the discrepancy calculation

[2] Constructing Optimal L_∞ Star Discrepancy Sets, F.C, C. Doerr, K. Klamroth and L. Paquete, submitted, 2023

First formulation

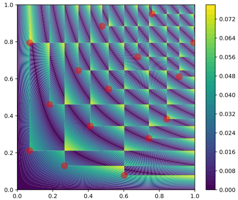
- Objective z is the discrepancy value
- Variables correspond to the points' coordinates (x_{2i-1}, x_{2i}), plus some ordering variables y_{ij}
- Add constraints for each box that could define the discrepancy, always lower-bounding z

First formulation

$\min \; z$

$$\text{s.t. } \frac{1}{n}\sum_{u=1}^{i} y_{uj} - x_{2i-1}x_{2j} \leq z + (1 - y_{ij})$$

$$\frac{-1}{n}\left(\sum_{u=1}^{i-1} y_{uj} - 1\right) + x_{2i-1}x_{2j} \leq z + (1 - y_{ij})$$



For each box, we need:

- the number of points inside: $\sum_{u=1}^{i} y_{uj}$
- its volume: $x_{2i-1}x_{2j}$
- to verify it is critical: $1 - y_{ij}$

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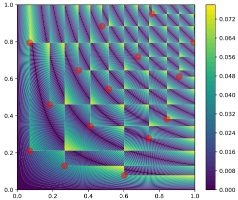

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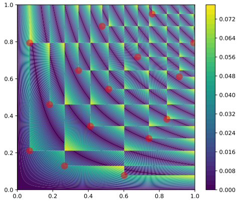

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Bonus constraints: Breaking symmetries

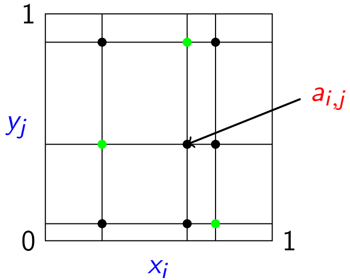
Proposition [CDKP, 2023]

- There is an optimal configuration *in two dimensions* with the points in general position
- Lower bound on the discrepancy of $1/n$ if $n \geq 4$ for $d \geq 2$

- There is an optimal configuration in general position where no coordinate is smaller than $1/n$ if $n \geq 4$
- Transitivity of the ordering variables

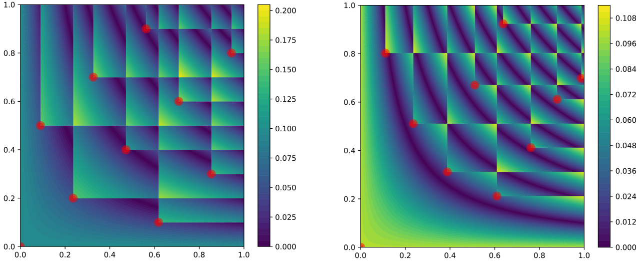
A second formulation

We split the problem in two parts: finding the coordinates and finding an assignment.



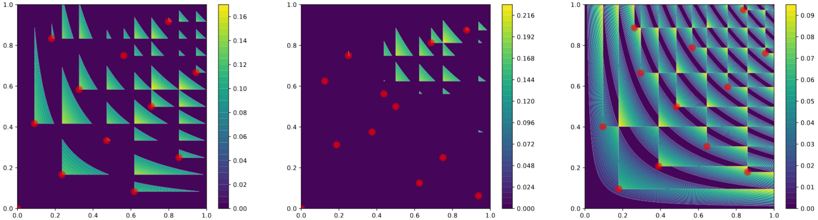
Results: a visible difference

- First model better in 2D, second better in 3D: solutions up to $n = 21$ points in 2D and $n = 8$ in 3D.



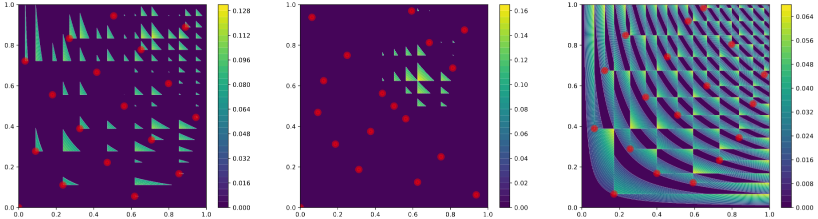
Left: 10 point Fibonacci set; **Right**: 10 optimally placed points.

Fibonacci vs Sobol' vs Optimal



Left: Fibonacci 12; **Middle**: Sobol' 12; **Right**: Optimal 12

Fibonacci vs Sobol' vs Optimal



Left: Fibonacci 18; **Middle**: Sobol' 18; **Right**: Optimal 18

Better point sets... and a new search direction for constructions?

The multiple-corner discrepancy

- Our models are not limited to the L_∞ star discrepancy.
- Star discrepancy breaks symmetries: one corner of $[0,1)^d$ is more important.
- Possible counter-measure: take each corner as an anchor, then take the worst star discrepancy.
- This multiple-corner discrepancy is an intermediate step between star and extreme discrepancies.
- In 2D, we need to introduce 3 more sets of "box constraints".

Comparison to our star optimal set

Optimizing the multiple-corner discrepancy leads to very little loss for the star discrepancy.

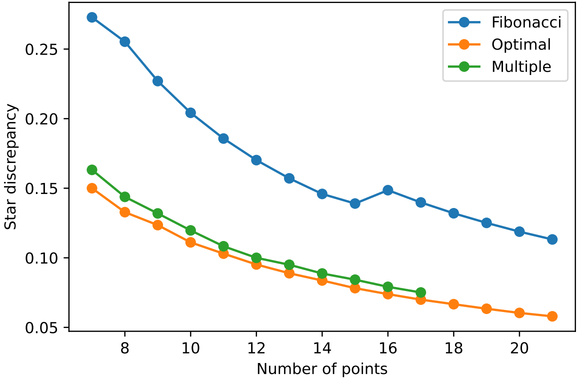


Figure: Comparison of our optimal sets with the Fibonacci set

Comparison to our star optimal set

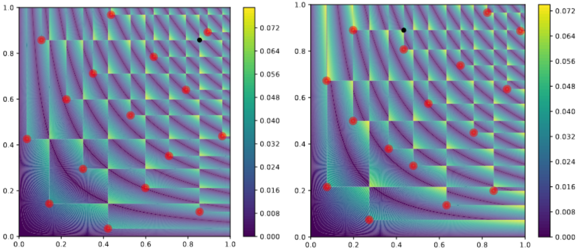


Figure: Optimal multiple-corner and star discrepancy sets for the star discrepancy.

Comparison to our star optimal set

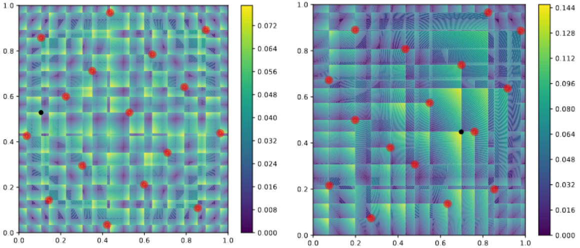
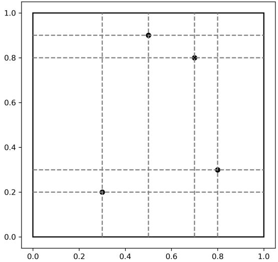


Figure: Optimal multiple-corner and star discrepancy sets for the multiple-corner discrepancy.

How to obtain good solutions for higher n?[3]

- Our models find excellent solutions quickly. Difficulty is proving optimality
- Two simple options: fixing the coordinates, or fixing the permutation, then solving the remaining problem



$$\pi(P) = (1,4,3,2)$$

[3] Transforming the Challenge of Constructing Low-Discrepancy Point Sets into a Permutation Selection Problem, F. C., C. Doerr, K. Klamroth and L. Paquete, arxiv 2024

The better choice: fixing the permutation

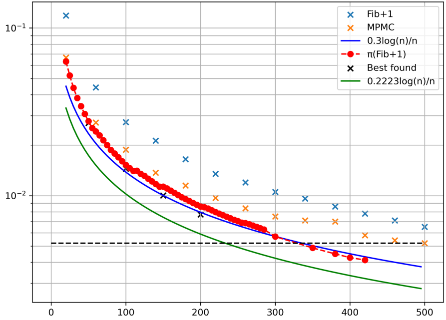


Figure: Best L_∞ star discrepancy values obtained by taking the permutation from the Fibonacci set *offset by 1*, compared with MPMC[4] and the Ostromoukhov upper bound[5]

[4] T. Konstantin Rusch, N. Kirk, M. M. Bronstein, C. Lemieux and D. Rus, Message-Passing Monte Carlo: Generating low-discrepancy point sets via Graph Neural Networks, 2024

[5] V. Ostromoukhov, Recent Progress in Improvement of Extreme Discrepancy and Star Discrepancy

(Nearly?) Optimal sets: Conclusion

- Best point sets known to this day in $2D$
- New structure observed for low-discrepancy point sets
- Changing the paradigm: from a point construction problem to a permutation selection one

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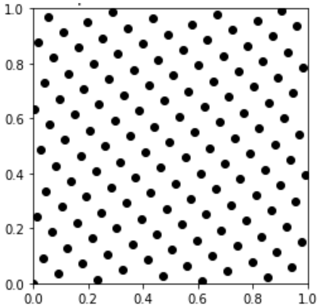
Subset Selection[6]

Star Discrepancy Subset Selection

Given two integers $n \geq 1$ and $k \leq n$, and a point set P, find a subset $P' \subseteq P$ of size k such that $P' := \arg\min_{P_k \subseteq P, |P_k|=k} d^*_\infty(P_k)$.



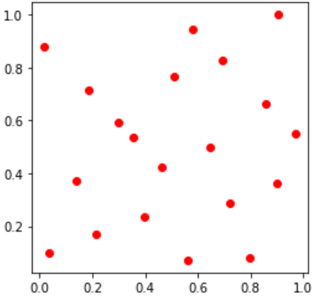


Figure: Selecting 20 points out of 140 from the Fibonacci set.

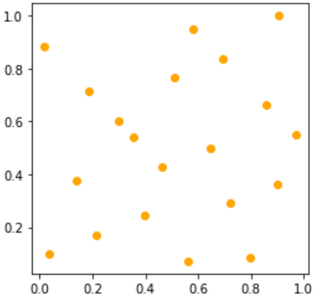
[6] F. C., C. Doerr, and L. Paquete. Star discrepancy subset selection: Problem formulation and efficient approaches for low dimensions. Journal of Complexity, 2022

A difficult problem

Proposition [CDP 2022]

The Star Discrepancy Subset Selection Problem is NP-hard.

- Given n, the best subset of size k is not necessarily contained in the best subset of size $h > k$



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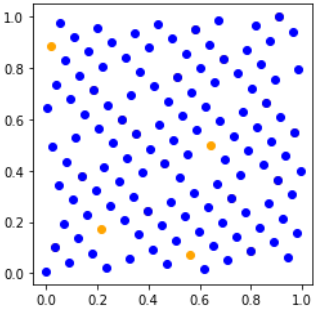
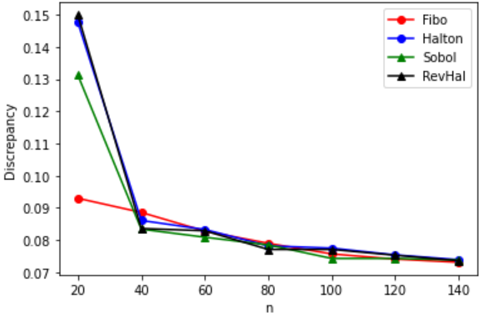


- Mixed Integer Linear Programming formulation is very similar to the one for optimal sets!
- Simply add a binary variable term to each point variable
- Branch-and-Bound: how good could our future point set theoretically be, given choices made so far?

MILP and Branch-and-Bound

- Both algorithms give substantially better low-discrepancy points sets than the well-known ones in lower dimensions (dimension 2 here)
- Similar plots for other values of n



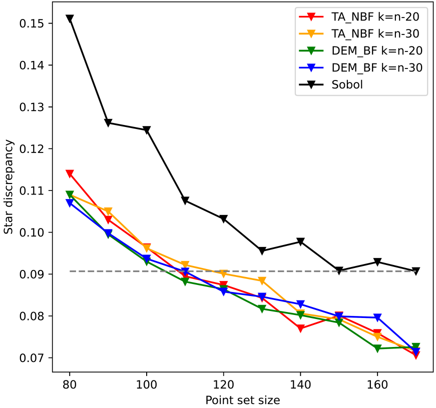
Best subset discrepancies for $k = 20$

Tackling higher dimensions: Swap heuristic[7]

- Keep a current best subset
- At each step try to replace a selected point by a non-selected point
- Main Limitation: computing star discrepancies

[7] F. C., C. Doerr, and L. Paquete. Heuristic approaches to obtain low-discrepancy point sets via subset selection. Journal of Complexity, 2024

Results



Best discrepancy values obtained in dimension 6 for $k = 80$ to 170.

Extracting sets: Conclusion

- We provide a way of solving a common problem for practitioners, in a wide range of (n, d) settings
- At the same time, the resulting sets have the lowest discrepancy values known in the majority of tested settings

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The L_2 discrepancy

L_2 star discrepancy

For P a point set in $[0;1]^d$,

$$d_2^*(P) = \Big(\int_{[0,1)^d} D(q,P)^2 dq\Big)^{1/2},$$

where $D(q,P)$ is the local discrepancy.

- The main advantage of the L_2 discrepancy is that it is very easy to compute using the Warnock formula [Warnock, 1972].

$$(d_2^*)^2(P) = \frac{1}{3^d} - \frac{n}{2^{d-1}} \sum_{i=1}^{n} \prod_{k=1}^{d} (1-(x_k^{(i)})^2) + \sum_{i,j=1}^{n} \prod_{k=1}^{d} (1-\max(x_k^{(i)}, x_k^{(j)}))$$

The Warnock formula

$$(d_2^*)^2(P) = \frac{1}{3^d} - \frac{n}{2^{d-1}} \sum_{i=1}^{n} \prod_{k=1}^{d} (1 - (x_k^{(i)})^2) + \sum_{i,j=1}^{n} \prod_{k=1}^{d} (1 - \max(x_k^{(i)}, x_k^{(j)}))$$

Individual point weights

The Warnock formula

$$(d_2^*)^2(P) = \frac{1}{3^d} - \frac{n}{2^{d-1}} \sum_{i=1}^{n} \prod_{k=1}^{d} (1-(x_k^{(i)})^2) + \sum_{i,j=1}^{n} \prod_{k=1}^{d} (1-\max(x_k^{(i)}, x_k^{(j)}))$$

Interaction between pairs of points

The Kritzinger sequence

Kritzinger, 2022

Given a starting point p_1, we define the sequence $P = (p_i)_{i \in \mathbb{N}}$, such that

$$p_k := \arg \min_{p \in [0,1)^d} d_2^*(P_{k-1} \cup \{p\}),$$

where $P_{k=1}$ is the set containing the first $k-1$ elements of P.

In 1d, this comes down to finding

$$\arg \min_{p \in [0,1)} (n+1)(1-p^2) + (1-p) + 2\sum_{i=1}^{n}(1-\max(x_i,p))$$

Computing the Kritzinger sequence

- [Kritzinger, 2022] Points have a very specific structure. Computations up to around 1500 points

Proposition [F.C. 2024]

There exists an algorithm to compute the next point in the Kritzinger sequence in linear time.

- I also introduced exact and heuristic methods for higher dimensions

A million points

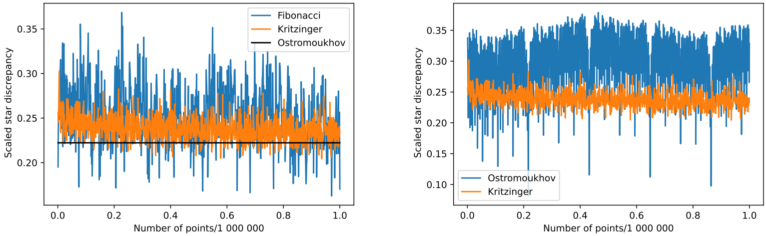

Figure: One million points with the Kritzinger sequence, compared to the Fibonacci sequence and the Ostromoukhov sequence.

Going forward: L_2 subset selection

- Same problem as before: optimizing for L_2 instead of L_∞
- Only linear dependency on d
- Flexibility: Any measure where a point's contribution can be identified
- Very good initial results for low dimensions

A measure for the future?

- L_2 allows for the construction of low-discrepancy L_∞ sequences
- It can easily be adapted: weighted, multiple-corner, periodic...
- Now even making good L_∞ sets! MPMC, L_2 subset selection

Is the L_2 discrepancy a good surrogate
for the L_∞ discrepancy?

Conclusion

- We have introduced methods to construct sets, extend sequences or extract from a given set
- For any n and d combination, at least one of the methods presented can be applied
- Resulting sets are far better, discrepancy-wise, than previous constructions

Further work

- Can we generalize these constructions to obtain new construction methods?
- Can we prove a better relationship between L_2 and L_∞ for sets used in practice? Or obtain a separate surrogate for L_∞?
- Is the star discrepancy really what we should optimize? Is multiple-corner a good compromise?
- How to know which measure and point sets should be used for which applications?

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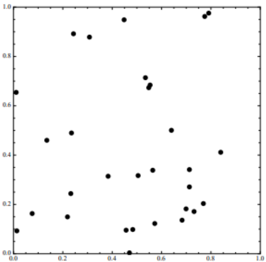
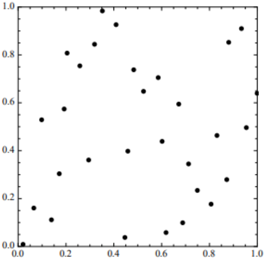
Thank you for your attention!

Steinerberger's energy functional

By gradient descent, minimize:

$$E[X] = \sum_{\substack{1 \le m,n \le N \\ m \ne n}} \prod_{k=1}^{d} \left(1 - \log(2\sin(|x_{m,k} - x_{n,k}|\pi))\right)$$





Kritzinger in 2D and 3D

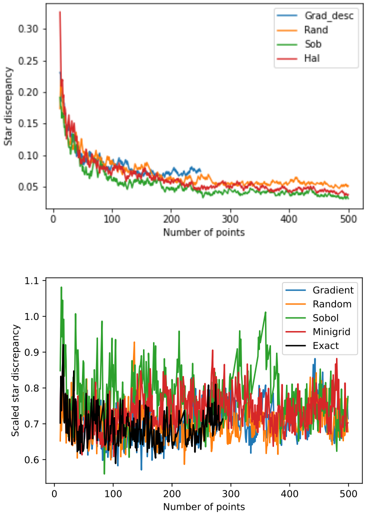


Figure: Kritzinger sequence in 2D and 3D

Kritzinger in 2D and 3D

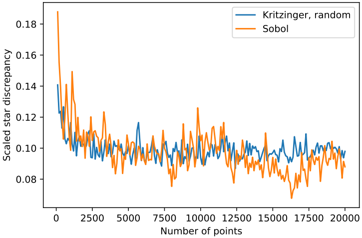


Figure: 20K points in 2D for the Kritzinger sequence

Exact approaches: Branch-and-Bound

- **Upper-bound**: Best set found so far.
- **Lower-bound 1**:

$$LB_1(P_A, P_R, P_N) := \max_{q \in \Gamma(P_A)} \left\{ \lambda(q) - \frac{1}{k} \min \{k, D(q, P_A) + D(q, P_N)\}, 0 \right\}$$

Exact approaches: Branch-and-Bound

- **Lower-bound 2**:

$$LB_2(P_A, P_R, P_N) := \max_{q \in \Gamma(P_A)} \left\{ \frac{1}{k} \overline{D}(q, P_A) - \lambda(q), 0 \right\}.$$

- When we reach a candidate subset, this will give us the local discrepancy for all closed boxes without recomputing.
- Only the first lower bound needs to be updated when rejecting a point.

Bracketing covers

- Most recent paper by Gnewuch, Pasing and Weiss, based on a generalization of the Faulhaber inequality.
- $N_{[],\delta} \leq \max(1.1^{d-101}, 1)\frac{d^d}{d!}(\delta^-1+1)^d$.
- Improved bounds from Thiémard's algorithm by Gnewuch:

$$N_{[],\delta} \leq \frac{d^d}{d!}\epsilon^{-d}$$

(t, m, d)-nets

(t, m, d)-net

For a given dimension d, integer base b, a positive integer m and an integer $0 \leq t \leq m$, a point set P of size b^m in $[0,1)^d$ is called a (t, m, d)-net in base b if each b-adic elementary interval of order $m-t$ contains b^t points of P.

- Elementary interval of order k: $J = \prod_{i=1}^{d} \left[\frac{a_i}{b^{d_i}}, \frac{a_i+1}{b^{d_i}} \right($, where $\sum_{i=1}^{d} d_i = k$ and $0 \leq a_i < b^{d_i}$

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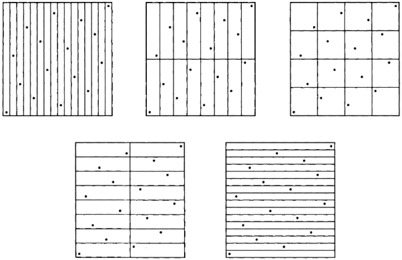

Figure: Order 4 dyadic intervals for a binary net in $d=2$

Digital (t, m, d)-nets

- One of the methods to build (t, m, d) nets in base b.
- Introduce d matrices over $\mathbb{F}_b$: $C_1, \ldots, C_d$.
- Given an integer n, write its b-adic expansion: $n = \sum_{i=0}^{m-1} a_{n,j} b^j$ and a_n the vector with the $a_{n,j}$.
- $x_{n,i} = \sum_{j=0}^{m-1} (C_i a_n)_j b^{-j}$ is the $i-th$ coordinate of the n-th point of our set.
- Some well-known digital nets in base 2: Hammersley sequence and Sobol' sequence.

Negative dependent variable

- Attempt to combine the good asymptotic behaviour of low-discrepancy sequences with that of random points when there are fewer points.
- For the moment: improved constants in the bounds for the star discrepancy of random sets (Monte-Carlo or LHS)

An NLP formulation: quick sketch

$$\min \; z$$

$$\text{s.t.} \quad \frac{1}{m}\sum_{u=1}^{i} y_{uj} - x_{2i-1}x_{2j} \le z + (1 - y_{ij}) \qquad \forall i,j = 1,\dots,m, j \le i \tag{2a}$$

$$\frac{-1}{m}\left(\sum_{u=1}^{i-1} y_{uj} - 1\right) + x_{2i-1}x_{2j} \le z + (1 - y_{ij}) \quad \forall i = 2,\dots,m, j = 1,\dots,i-1 \tag{2b}$$

$$\frac{-1}{m}\left(\sum_{u=1}^{m} y_{uj} - 1\right) + x_{2j}\cdot 1 \le z \qquad \forall j = 1,\dots,m \tag{2c}$$

$$\frac{-(i-1)}{m} + x_{2i-1}\cdot 1 \le z \qquad \forall i = 1,\dots,m \tag{2d}$$

An assignment-like formulation

$$
\begin{aligned}
\min\ & z \\
\text{s.t. } & \frac{1}{m}\sum_{u=1}^{i}\sum_{v=1}^{j} a_{uv} - x_i y_j \leq z & \forall i,j = 1,\dots,m \quad & \text{(3a)} \\
& \frac{-1}{m}\sum_{u=1}^{i-1}\sum_{v=1}^{j-1} a_{uv} + x_i y_j \leq z & \forall i,j = 1,\dots,m+1 \quad & \text{(3b)} \\
& x_{m+1} = 1,\ y_{m+1} = 1 & & \text{(3c)} \\
& x_{i+1} - x_i \geq \varepsilon & \forall i = 1,\dots,m-1 \quad & \text{(3d)} \\
& y_{i+1} - y_i \geq \varepsilon & \forall i = 1,\dots,m-1 \quad & \text{(3e)} \\
& \sum_{i=1}^{m} a_{ij} = 1 & \forall j = 1,\dots,m \quad & \text{(3f)} \\
& \sum_{j=1}^{m} a_{ij} = 1 & \forall i = 1,\dots,m \quad & \text{(3g)} \\
& \forall i = 1,\dots,m, x_i, y_i \in [0,1],\ \forall i,j = 1,\dots,m; a_{ij} \in \{0,1\}\ z \geq 0. & &
\end{aligned}
$$

MILP formulation

$$\begin{aligned}
\min \quad & z \\
\text{s.t.} \quad & z \geq h_{i,j} - \frac{1}{k} \sum_{\ell \in \Delta(P,i,j)} x_\ell & \text{for all } i,j \in [1..n+1] \\
& z \geq -h_{i,j} + \frac{1}{k} \sum_{\ell \in \overline{\Delta}(P,i,j)} x_\ell & \text{for all } i,j \in [1..n] \\
& \sum_{i=1}^{n} x_i = k \\
& x_i \in \{0,1\} & \text{for all } i \in [1..n] \\
& z \in \mathbb{R}_{\geq 0}
\end{aligned}$$

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