The L_2-Discrepancy of Latin Hypercubes

Nicolas Nagel

MCQMC
Waterloo University
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UNIVERSITY OF TECHNOLOGY
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The results from this talk originate from a project together with Ian Ruohoniemi and Dmitriy Bilyk (University of Minnesota)

- Two perspectives on discrepancy:
  - How *uniformly* can you distribute N points $\{\mathbf{x}^1, ..., \mathbf{x}^N\}$ on a set Ω?
  - How well does *quasi-Monte Carlo integration*

$$\int_\Omega f(\mathbf{x})\,\mathrm{d}\mathbf{x} \approx \frac{1}{N}\sum_{i=1}^{N} f(\mathbf{x}^i)$$

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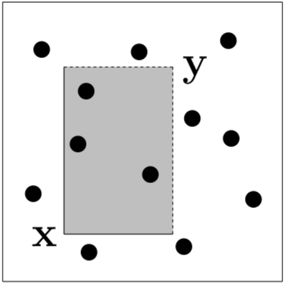
    perform at best?
- First point: compare to *test sets* (geometric)
- Second point: compare to a *function space* (analytic)
- In both cases: need notion of *uniformity*

- Example 1: $[0,1)^d$
- Test sets: axis parallel boxes $[\mathbf{x},\mathbf{y})$
- Discrepancy function (Note: unnormalization)

$$D_X(\mathbf{x},\mathbf{y}) := \#(X \cap [\mathbf{x},\mathbf{y})) - N|[\mathbf{x},\mathbf{y})|$$

- **Extremal L_p-discrepancy**

$$L_p^{\mathsf{extr}}(X)^p = \iint_{\mathbf{x}<\mathbf{y}} |D_X(\mathbf{x},\mathbf{y})|^p \,\mathrm{d}\mathbf{x}\,\mathrm{d}\mathbf{y}$$



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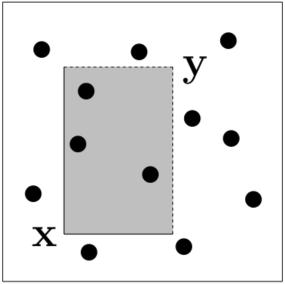

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- Warnock-type formula for $p = 2$

$$L_2^{\text{extr}}(X)^2 = \frac{N^2}{12^d} - \frac{N}{2^{d-1}} \sum_{\mathbf{x}\in X} \prod_{k=1}^{d} x_k(1-x_k) + \sum_{\mathbf{x},\mathbf{y}\in X} \prod_{k=1}^{d} (\min\{x_k, y_k\} - x_k y_k)$$

- Example 2: $[0,1)^d \simeq \mathbb{T}^d$
- Test sets: axis parallel, periodic boxes $[\mathbf{x}, \mathbf{y})$
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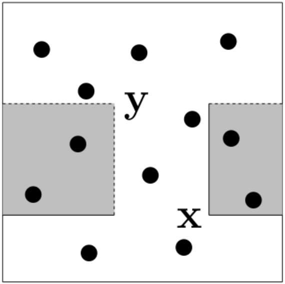

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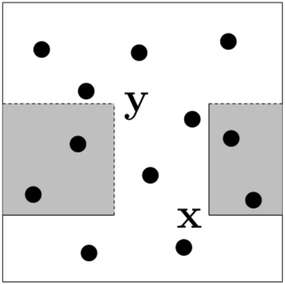

- $f \in \mathcal{H}^1_{\text{extr}}$ iff $f : [0,1) \to \mathbb{R}$ absolutely continuous, $f(0) = f(1) = 0$ and

$$\|f\|^2_{\mathcal{H}^1_{\text{extr}}} := \int_0^1 f'(x)^2 \, \mathrm{d}x < \infty$$

- $\mathcal{H}^d_{\text{extr}}$ via tensor product
- Kernel $K^{\text{extr}}(\mathbf{x}, \mathbf{y}) = \prod_{k=1}^d (\min\{x_k, y_k\} - x_k y_k)$ (*Brownian sheet*)
- Error functional

$$\mathcal{R}_X(f) := \int_{[0,1]^d} f(\mathbf{x}) \, \mathrm{d}\mathbf{x} - \frac{1}{N} \sum_{\mathbf{x} \in X} f(\mathbf{x}),$$

then

$$L_2^{\text{extr}}(X) = N \sup_{\|f\|_{\mathcal{H}^d_{\text{extr}}} \leq 1} |\mathcal{R}_X(f)|$$

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- Note the similarity to the Koksma-Hlawka inequality

- In this talk: extremal and periodic L_2-discrepancy on the torus
- Other aspects:
  - L_∞-discrepancy (no need for an underlying measure, optimal asymptotic generally unknown)
  - Star-discrepancy (only boxes $[\mathbf{0}, \mathbf{y})$ anchored in the origin)
  - Discrepancy on the sphere or projective plane (Stolarsky principle, 2-point homogeneous spaces, energies, ...)
  - Discrepancy for finite metric spaces ([Barg '21], [Barg, Skriganov '21]; connections to coding theory and combinatorics)

An observed relation

- Minimize QMC integration error $\Leftrightarrow$ minimize discrepancy
- Existence of asymptotically optimal point sets for QMC integration over Sobolev spaces of arbitrary (integer) smoothness and dimension known (digital net constructions by Goda, Suzuki, Yoshiki; based on work by Baldeaux, Dick, Hickernell, Kritzer, Kuo, Niederreiter, Nuyens, Pillichshammer, ...)

- Lower bounds [Roth '54; Hinrichs, Kritzinger, Pillichshammer '21]

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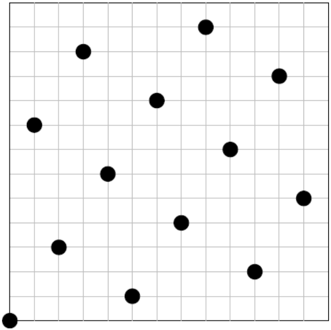
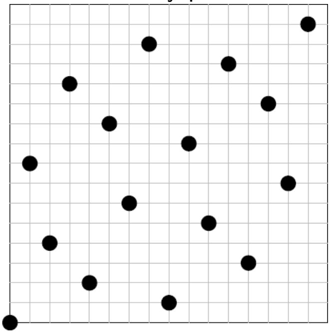
- Constructions matching (asymptotically) the lower bounds (for $d = 2$):

Fibonacci lattice



Hammersley point set



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$$L_2^{\text{extr}}(\text{Ham}_N)^2 = \frac{n}{64} + \frac{1}{72} - \frac{1}{144N^2}$$
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- Rational (=integration) lattice $\text{Lat}_{p/N} = \left\{ \left(\frac{k}{N}, \frac{kp \mod N}{N} \right) : k = 0, 1, \ldots, N-1 \right\}$ with $\gcd(p, N) = 1$

$$L_2^{\text{extr}}(\text{Lat}_{p/N})^2 = \frac{1}{16N^2} \sum_{r=1}^{N-1} \frac{1}{\sin\left(\frac{\pi r}{N}\right)^2 \sin\left(\frac{\pi p r}{N}\right)^2} + \frac{1}{72} - \frac{1}{144N^2}$$
$$L_2^{\text{per}}(\text{Lat}_{p/N})^2 = \frac{1}{4N^2} \sum_{r=1}^{N-1} \frac{1}{\sin\left(\frac{\pi r}{N}\right)^2 \sin\left(\frac{\pi p r}{N}\right)^2} + \frac{1}{9} + \frac{1}{36N^2}$$

- Similarities among the formulas noted when they were first computed
- For Hammersley point sets and rational lattices X with N points

$$L_2^{\mathrm{per}}(X)^2 = 4L_2^{\mathrm{extr}}(X)^2 + \frac{N^2+1}{18N^2}$$

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- Really a special relation (not true for general point sets)
- Can this be generalized? Is there a “deeper” reason for this relation?

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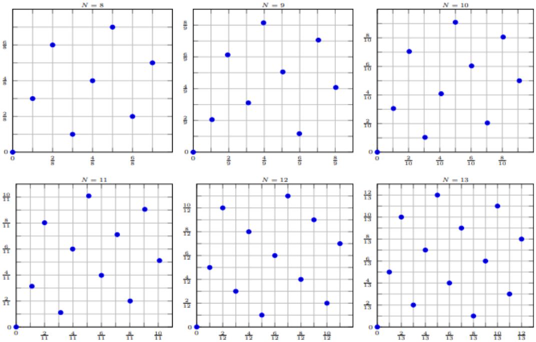

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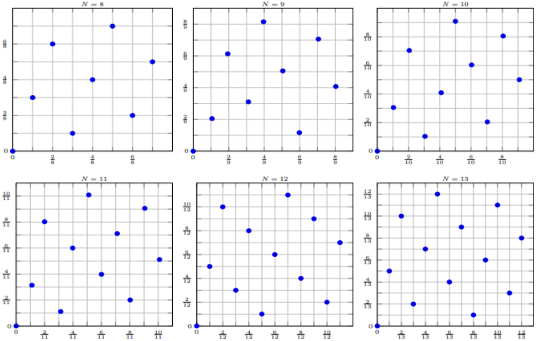

- All (approximate) permutations $\rightsquigarrow$ investigate **permutation sets**

$$X(\sigma) := \left\{ \frac{1}{N}(m, \sigma(m)) : m = 0, 1, ..., N-1 \right\}$$

- Are permutation sets good candidates for approximate global minimizers? (even optimality of Fibonacci lattices unknown)
- Are there combinatorial properties of a permutation σ that imply that $X(\sigma)$ is of low discrepancy? (permutation statistics)
- What makes permutation sets "special"?

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For the last question have the following:

Theorem: Relation for permutation sets [N]

For every permutation $\sigma : \{0, 1, ..., N-1\} \to \{0, 1, ..., N-1\}$ it holds

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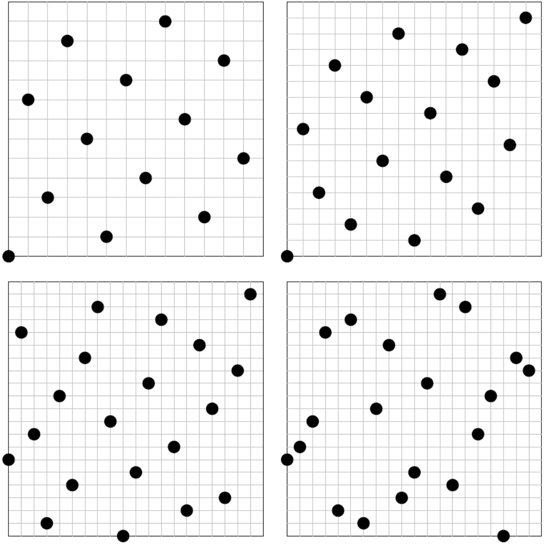
Note: Not a complete characterization of sets fulfilling this relation.

Permutation sets



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- Slight deviation from the usual terms: Latin squares ("sudokus") give Latin cubes (point sets of dimension 3)
- M-Latin hypercubes consist of $N = M^{d-1}$ elements
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Theorem: Relation for Latin hypercubes [N]

For every M-Latin hypercube of dimension d it holds

$$L_2^{\text{per}}(\mathcal{H})^2 - 2^d L_2^{\text{extr}}(\mathcal{H})^2 = \frac{(2M^2+1)^d + (M^2-1)^d - (1+2^d)M^{2d}}{6^d M^2}.$$

Even more general:

- Can define discrepancy for *weighted point sets* (X, w) where $w : X \to \mathbb{R}$
- Warnock-type formulas

$$L_2^{\text{extr}}(X,w)^2 = \sum_{\mathbf{x},\mathbf{y}\in X} w(\mathbf{x})w(\mathbf{y})\Bigg[\frac{1}{12^d} - \prod_{k=1}^{d}\frac{x_k(1-x_k)}{2} - \prod_{k=1}^{d}\frac{y_k(1-y_k)}{2} + \prod_{k=1}^{d}\left(\min\{x_k,y_k\} - x_k y_k\right)\Bigg]$$

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- Analogue for Latin hypercubes: weights $w : \frac{1}{M}\{0, 1, ..., M-1\}^d \to \mathbb{R}$ with constant row sums 1
- Same relation holds for this (linearly relaxed) case

- Immediate consequence:

$$L_2^{\text{per}}(\mathcal{H})^2 \geq \frac{(2M^2+1)^d + (M^2-1)^d - (1+2^d)M^{2d}}{6^d M^2} = \frac{d(2^{d-1}-1)}{6^d} \underbrace{M^{2d-4}}_{=N^{2\frac{d-2}{d-1}}} + \ldots$$

- Can be slightly improved in the constant:
- Let $\overline{G} := \{0, 1, \ldots, M-1\}^d$ and $G := \frac{1}{M}\overline{G}$ (*discretized torus*)

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Theorem: Expression of periodic discrepancy [N]

$$L_2^{\text{per}}(G, w)^2 = -\frac{1}{3^d}\left(\sum_{\mathbf{x}\in G} w(\mathbf{x})\right)^2 + \sum_{\mathbf{f}\in\overline{G}} \mu_{\mathbf{f}} \left|\sum_{\mathbf{x}\in G} w(\mathbf{x}) \exp(2\pi i \mathbf{f}\cdot\mathbf{x})\right|^2,$$

$$\mu_{\mathbf{f}} = \prod_{k=1}^{d} \begin{cases} \frac{1}{3} + \frac{1}{6M^2} & , f_k = 0 \\ \frac{1}{2M^2 \sin(\pi f_k/M)^2} & , f_k \neq 0 \end{cases}.$$

Theorem: Lower bound, Latin hypercube [N]

For every M-Latin hypercube $\mathcal{H}$ of dimension d with $N = M^{d-1}$

$$L_2^{\text{per}}(\mathcal{H}) \geq \left(\frac{d}{2 \cdot 3^d}\right)^{1/2} N^{\frac{d-2}{d-1}}$$

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For $d = 3$: lower bound of order $N^{1/2}$ (like random point sets)

- Upper bound via probabilistic considerations
- $\mathbb{E}L_2^{\text{per}}(\mathcal{H})^2$ for uniformly random $\mathcal{H}$

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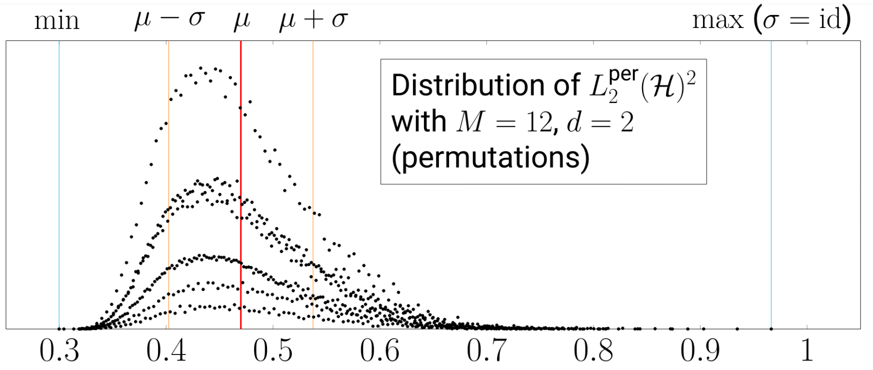

Theorem: Expected periodic discrepancy [N]

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Theorem: Upper bound, Latin hypercube [N]

For $d \geq 4$ there is an M-Latin hypercube of dimension d with

$$L_2^{\text{per}}(\mathcal{H}) \leq \left(\frac{d}{2 \cdot 3^d}\right)^{1/2} (1+o(1)) N^{\frac{d-2}{d-1}}.$$

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Thank you