Quasi-Monte Carlo on Product Spaces

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Overview

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Introduction

- Problem : Quasi-Monte Carlo integration over product spaces of the form $\mathcal{X}^s$ where $\mathcal{X} \subseteq \mathbb{R}^d$.

$$\mu = \frac{1}{\mathbf{vol}(\mathcal{X})^s} \int_{\mathcal{X}^s} f(\boldsymbol{x})\,\mathrm{d}\boldsymbol{x}.$$

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- This is fine for MC. For QMC we often find that $f \circ \tau \notin BVHK$

[Pillards and Cools (2005), Fang and Wang (1994)]

General Space $\mathcal{X}^s$

- Our estimates are equal weight rules

$$\hat{\mu} = \frac{1}{n}\sum_{i=1}^{n} f(\boldsymbol{x}_i), \quad \text{where} \quad \boldsymbol{x}_i = \phi(\boldsymbol{u}_i)$$

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  for random points $\boldsymbol{u}_i \in [0,1]^s$.
- Most interesting case : $d = 2$, such as, triangles, spherical triangles and discs.

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- For each finite n, $\mathrm{Var}(\hat{\mu})$ is bounded by a finite multiple of the Monte Carlo variance, uniformly over all $f \in L^2(\mathcal{X}^s)$.
- Under smoothness conditions on f and a sphericity constraint on the partitioning of $\mathcal{X}$ we show

$$\mathrm{Var}(\hat{\mu}) = O\left(\frac{(\log n)^{s-1}}{n^{1+2/d}}\right).$$

Overview

Special Case: $s = 1, d = 2, \mathcal{X}$ is Triangle.

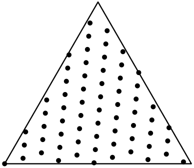

Figure: Kronecker Triangular Lattice using $3\pi/8$

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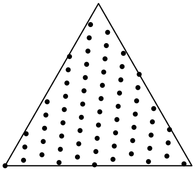

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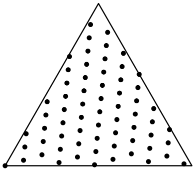

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- Kronecker Points. Uses badly approximable numbers.
- Convergence rate $O(\log n/n)$
- Fails for $d > 2$ and also for $d = 2, s > 1$ due to Littlewood conjecture.

[B. and Owen (2015a)]

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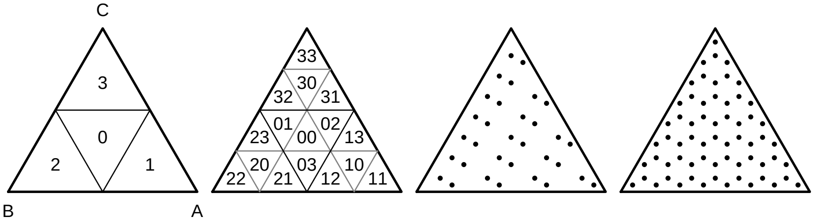

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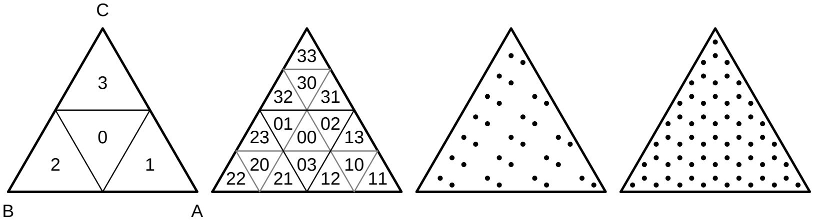

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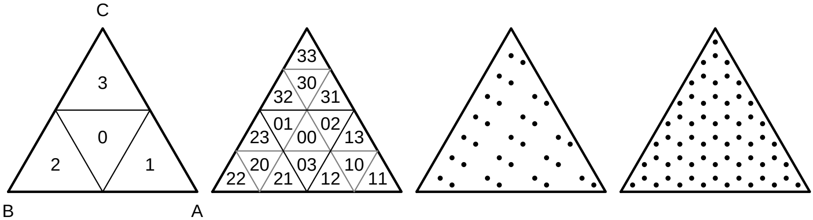

- Triangular van der Corput
- $n \geq 0$ in a base 4 representation $n = \sum_{k \geq 1} d_k 4^{k-1}$ where $d_k \in \{0, 1, 2, 3\}$
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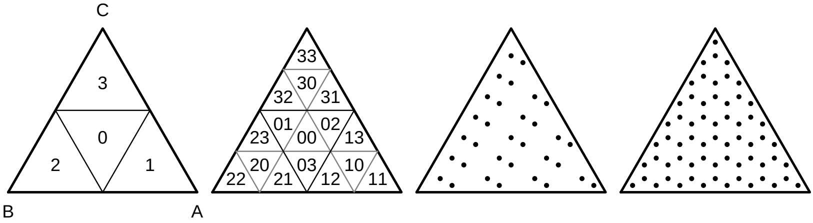

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- $n \geq 0$ in a base 4 representation $n = \sum_{k \geq 1} d_k 4^{k-1}$ where $d_k \in \{0, 1, 2, 3\}$
- $x_n = 0.d_1 d_2 \ldots$
- Discrepancy: $O(1/\sqrt{n})$. RMSE under randomization: $O(1/n)$.

[Brandolini et. al. (2013)]

Splits on the Triangle

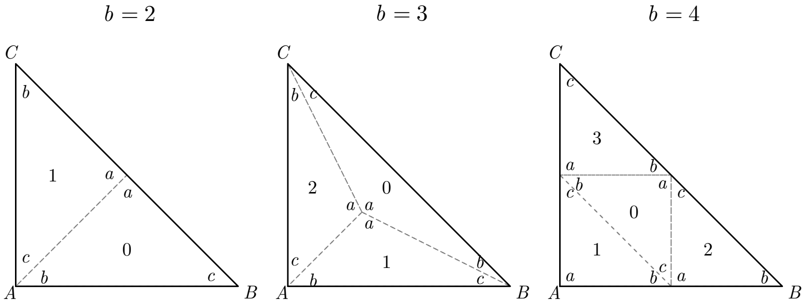

Figure: Splits of a triangle $\mathcal{X}$ for bases $b = 2$, 3 and 4. The subtriangles $\mathcal{X}_j$ are labeled by the digit $j \in \mathbb{Z}_b$.

Recursive Splits on the Triangle

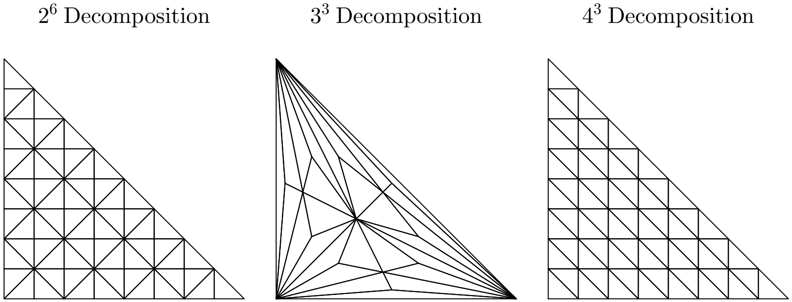

Figure: The base b splits from previous figure carried out to $k = 6$ or 3 or 4 levels.

Sphericity Constraint

Definition 1

Let $\mathbb{X}$ be a recursive split of $\mathcal{X} \in \mathbb{R}^d$ in base b. Then $\mathbb{X}$ satisfies the *sphericity condition* if there exists $C < \infty$ such that $\mathrm{diam}(\mathcal{X}_{a_1,\dots,a_k}) \le Cb^{-k/d}$ holds for all cells $\mathcal{X}_{a_1,\dots,a_k}$ in $\mathbb{X}$.

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Definition 2

A recursive split $\mathbb{X}$ in base b is convergent if for every infinite sequence $a_1, a_2, a_3, \dots \in \mathbb{Z}_b$, the cells $\mathcal{X}_{a_1,a_2,\dots a_K}$ converges a point as $K \to \infty$. That point is denoted $\lim_{K\to\infty} \mathcal{X}_{a_1,a_2,\dots,a_K}$.

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$\phi(x) = \lim_{K\to\infty} \mathcal{X}_{x_1,x_2,\dots,x_K}$ where x has the base b representation $0.x_1x_2\dots$.

Splitting on the Disc

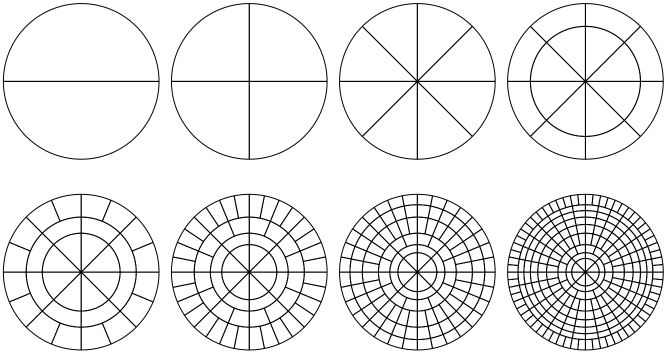

Figure: A recursive binary equal area splitting of the unit disk, keeping the aspect ratio close to unity.

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- For $\boldsymbol{a} = (a_1,\ldots,a_s) \in [0,1)^s$, we apply nested uniform scramble component-wise.
- A nested uniform scramble of $\boldsymbol{a}_1,\ldots,\boldsymbol{a}_n \in [0,1)^s$ applies the same set of permutations to the digits of all n of those points.

Scrambled Geometric nets in $\mathcal{X}^s$ via splitting

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Scrambled Geometric nets in $\mathcal{X}^s$ via splitting

- For $s \geq 1$, let $\boldsymbol{a}_i$ be (t, m, s)-net in base b
- Let $\boldsymbol{u}_i \in [0, 1]^s$ - nested uniform scrambling.
- $x_{ij} = \phi(u_{ij})$ for $j = 1, \dots, s$. Then $\boldsymbol{x}_i \in \mathcal{X}^s$ and we use

$$\hat{\mu} = \frac{1}{n} \sum_{i=1}^{n} f(\boldsymbol{x}_i).$$

[Niederreiter (1992), Dick and Pillichshammer (2010), Owen (1995).]

Overview

Results

Theorem 1

Let $\boldsymbol{u}_1, \dots, \boldsymbol{u}_n$ be a nested uniform scramble of a (t, m, s)-net in base $b \geq 2$ and let $\boldsymbol{x}_i = \phi(\boldsymbol{u}_i)$ componentwise. Then for any $f \in L^2(\mathcal{X}^{1:s})$,

$$\mathbb{E}(\hat{\mu}) = \mu$$

$$\mathrm{Var}(\hat{\mu}) = o\left(\frac{1}{n}\right)$$

as $n \to \infty$.

Results

Theorem 2

Under the conditions of Theorem 1

$$\mathrm{Var}(\hat{\mu}) \le b^t \left(\frac{b+1}{b-1}\right)^{s-1} \frac{\sigma^2}{n},$$

where $\sigma^2 = \mathrm{Var}(f(\boldsymbol{x}))$ for $\boldsymbol{x} \sim \mathbf{U}(\mathcal{X}^{1:s})$. If $t = 0$, then $\mathrm{Var}(\hat{\mu}) \le e\sigma^2/n \doteq 2.718\sigma^2/n$.

Main Theorem

Theorem : B. and Owen (2015b)

Let $\boldsymbol{u}_1, \ldots, \boldsymbol{u}_n$ be the points of a randomized (t, m, s)-net in base b. Let $\boldsymbol{x}_i = \phi(\boldsymbol{u}_i) \in \mathcal{X}^{1:s}$ for $i = 1, \ldots, n$ where ϕ is the componentwise application of the transformation from convergent recursive splits in base b. Then for a smooth f on $\mathcal{X}^{1:s}$,

$$\mathrm{Var}(\hat{\mu}) = O\left(\frac{(\log n)^{s-1}}{n^{1+2/d}}\right).$$

Sobol' Extensible $\mathcal{X}$

- A closed set $\mathcal{X} \subseteq \mathbb{R}^m$ with non-empty interior is said to be *Sobol' extensible* if there exists a point $\boldsymbol{c} \in \mathcal{X}$ such that $\boldsymbol{z} \in \mathcal{X}$ implies $\mathrm{rect}[\boldsymbol{c}, \boldsymbol{z}] \subseteq \mathcal{X}$. The point $\boldsymbol{c}$ is called the anchor.

Sobol Extensible $\mathcal{X}$

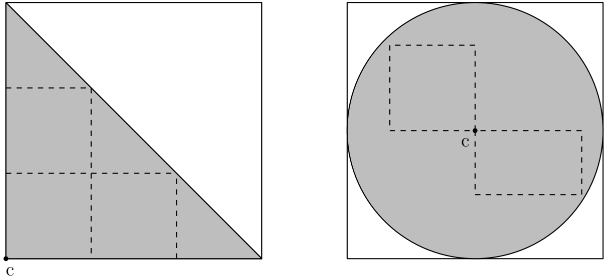

Figure: Sobol' extensible regions. At left, $\mathcal{X}$ is the triangle with vertices $(0,0)$, $(0,\sqrt{2})$, $(\sqrt{2},0)$ and the anchor is $\boldsymbol{c} = (0,0)$. At right, $\mathcal{X}$ is a circular disk centered its anchor $\boldsymbol{c}$. The dashed lines depict some rectangular hulls joining selected points to the anchor.

Non Sobol Extensible $\mathcal{X}$

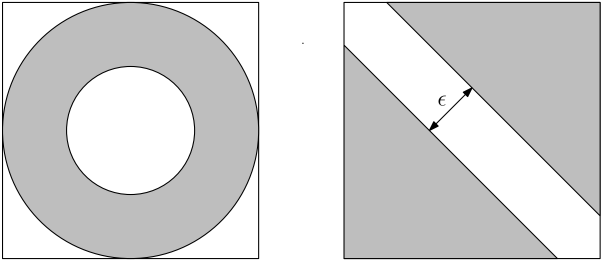

Figure: Non-Sobol' extensible regions. At left, $\mathcal{X}$ is an annular region centered at the origin. At right, $\mathcal{X}$ is the unit square exclusive of an ϵ-wide strip centered on the diagonal.

Smoothness Condition

- Let $\mathcal{X} \subseteq \mathbb{R}^m$ for $m \in \mathbb{N}$ be Sobol extensible. The function $f : \mathcal{X} \to \mathbb{R}$ is said to be smooth if $\partial^{1:m} f$ is continuous on $\mathcal{X}$.

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- For general $\mathcal{X}$, f is said to be smooth if $f \in C^m(\mathcal{X})$.

Overview

Proof Idea of Main Theorem

- If $\mathbb{X}$ is convergent and $f \in L^2(\mathcal{X})$ then,

$$f(\boldsymbol{x}) = \langle f, \varphi \rangle \varphi(\boldsymbol{x}) + \sum_{k=1}^{\infty} \sum_{t=0}^{b^k-1} \sum_{c=0}^{b-1} \langle f, \psi_{ktc} \rangle \psi_{ktc}(\boldsymbol{x}).$$

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- ψ_{ktc} are Haar wavelets in base b.

Proof Idea of Main Theorem

- Multiresolution of $L^2(\mathcal{X}^{1:s})$ is

$$\begin{aligned} f(\boldsymbol{x}) &= \sum_{u\subseteq 1:s}\sum_{\kappa|u}\sum_{\tau|u,\kappa}\sum_{\gamma|u}\langle\psi_{u\kappa\tau\gamma}, f\rangle\psi_{u\kappa\tau\gamma}(\boldsymbol{x}) \\ &= \mu + \sum_{|u|>0}\sum_{\kappa|u}\sum_{\tau|u,\kappa}\sum_{\gamma|u}\langle\psi_{u\kappa\tau\gamma}, f\rangle\psi_{u\kappa\tau\gamma}(\boldsymbol{x}). \end{aligned}$$

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- $\psi_{u\kappa\tau\gamma}$ are tensor products of Haar wavelets in base b.

Variance expression

- $$\mathrm{Var}(\hat{\mu}) = \mathbb{E}\Bigg(\frac{1}{n^2} \sum_{i=1}^{n} \sum_{i'=1}^{n} \sum_{|u|>0} \sum_{\kappa|u} \sum_{\tau|u,\kappa} \sum_{\gamma|u} \sum_{|u'|>0} \sum_{\kappa'|u'} \sum_{\tau'|u',\kappa'} \sum_{\gamma'|u'} \langle f, \psi_{u\kappa\tau\gamma}\rangle \langle f, \psi_{u'\kappa'\tau'\gamma'}\rangle \psi_{u\kappa\tau\gamma}(\boldsymbol{x}_i) \psi_{u'\kappa'\tau'\gamma'}(\boldsymbol{x}_{i'}) \Bigg).$$

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- $$\mathrm{Var}(\hat{\mu}) = \sum_{|u|>0}\sum_{\kappa|u}\mathrm{Var}\Bigg(\frac{1}{n}\sum_{i=1}^{n}\nu_{u\kappa}(\boldsymbol{x}_i)\Bigg),$$

  where $\nu_{u\kappa}(\boldsymbol{x}) = \sum_{\tau|u,\kappa}\sum_{\gamma|u}\langle f,\psi_{u\kappa\tau\gamma}\rangle\psi_{u\kappa\tau\gamma}(\boldsymbol{x})$ with $\nu_{\emptyset,()} = \mu$.

Simplification of Variance expression

- $\sigma^2_{u\kappa} = \int_{\mathcal{X}^{1:s}} \nu^2_{u\kappa}(x)\,\mathrm{d}\boldsymbol{x}$.
- The multiresolution-based ANOVA decomposition is

$$\sigma^2 = \int_{\mathcal{X}^{1:s}} (f(\boldsymbol{x}) - \mu)^2\,\mathrm{d}\boldsymbol{x} = \sum_{|u|>0} \sum_{\kappa|u} \sigma^2_{u\kappa}$$

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- From the equidistribution properties of $\boldsymbol{a}_i$

$$\begin{aligned}\mathrm{Var}(\hat{\mu}) &= \frac{1}{n} \sum_{|u|>0} \sum_{\kappa|u} \Gamma_{u,\kappa} \sigma^2_{u\kappa} \\ &\le \frac{b^t}{n} \left(\frac{b+1}{b-1}\right)^s \sum_{|u|>0} \sum_{|\kappa|+|u|>m-t} \sigma^2_{u\kappa}.\end{aligned}$$

Proof Idea Continued

- Bound $\sigma^2_{u\kappa}$.

$$\begin{aligned}
\sigma^2_{u\kappa} &= \int_{\mathcal{X}^{1:s}} \nu^2_{u\kappa}(\boldsymbol{x})\,\mathrm{d}\boldsymbol{x} \\
&= \sum_{\tau|u,\kappa}\sum_{\gamma,\gamma'|u} \langle f, \psi_{u\kappa\tau\gamma}\rangle\langle f, \psi_{u\kappa\tau\gamma'}\rangle \int_{\mathcal{X}^{1:s}} \psi_{u\kappa\tau\gamma}(\boldsymbol{x})\psi_{u\kappa\tau\gamma'}(\boldsymbol{x})\,\mathrm{d}\boldsymbol{x} \\
&= \sum_{\tau|u,\kappa}\sum_{\gamma,\gamma'|u} \langle f, \psi_{u\kappa\tau\gamma}\rangle\langle f, \psi_{u\kappa\tau\gamma'}\rangle \prod_{j\in u}(1_{\gamma_j=\gamma'_j} - b^{-1})
\end{aligned}$$

- Bound $|\langle f, \psi_{u\kappa\tau\gamma}\rangle|$

Proof Idea Continued

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- The coefficients $|\langle f, \psi_{u\kappa\tau\gamma}\rangle|$ decay quickly.
- Extend the region from $\mathcal{X}^s$ to a bounding box
- Extend the integrand to that bounding box.
- Sobol's low variance extension given by

$$\tilde{f}(\boldsymbol{x}) = \sum_{u \subseteq 1:m} \int_{[\boldsymbol{c}_u, \boldsymbol{x}_u]} \partial^u f(\boldsymbol{c}_{-u}{:}\boldsymbol{y}_u) 1_{\boldsymbol{c}_{-u}:\boldsymbol{y}_u \in \mathcal{X}} \, \mathrm{d}\boldsymbol{y}_u$$

- Whitney extension requiring extra smoothness.

Summary

- RQMC available for $\mathcal{X}^s$ and $\mathcal{X} \subset \mathbb{R}^d$
- Root mean squared error of $O(n^{-1/2-1/d}(\log(n))^{(s-1)/2})$.
- We can extend it to unequal d_j by taking $d = \max_{j\in 1:s} d_j$.
- QMC and composition mapping, $O(n^{-1}\log(n)^{sd-1})$
- Advantage for $d = 1$ and 2
- Convergence guarantee as well as error estimates.
- Given additional smoothness perhaps higher order nets would work.

[Dick and Baldeaux (2009)]

Thank you!

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