Low-discrepancy quadrature in the triangle

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Overview

Introduction

- Problem : Numerical Integration over triangular domain using quasi-Monte Carlo (QMC) sampling.
- QMC in $[0,1]^d$.

$$\mu = \int_{[0,1]^d} f(x)dx \qquad \hat{\mu}_n = \frac{1}{n}\sum_{i=1}^{n} f(x_i)$$

- Koksma-Hlawka inequality

$$|\hat{\mu}_n - \mu| \leqslant D_n^*(x_1,\dots,x_n) \times V_{HK}(f)$$

- Recent work relating to general spaces by Aistleitner et al., (2012), Brandolini et. al (2013)

Motivation

- Need in computer graphics, genetic experimental studies, etc.
- Mapping by special functions/transformation from $[0,1]^d$ Pillards and Cools (2005).
- Several notions of discrepancy on the triangle/simplex but no explicit constructions. Pillards and Cools (2005), Brandolini et. al (2013).
- Two constructions - van der Corput sequence and hybrid of lattice and Kronecker construction.

General Notions of Discrepancy

- The signed discrepancy of $\mathcal{P}$ at the measurable set $S \subseteq \Omega \subset \mathbb{R}^d$ is

$$\delta_N(S; \mathcal{P}, \Omega) = \mathbf{vol}(S \cap \Omega)/\mathbf{vol}(\Omega) - A_N(S; \mathcal{P})/N.$$

- The absolute discrepancy of points $\mathcal{P}$ for a class $\mathcal{S}$ of measurable subsets of Ω is

$$D_N(\mathcal{S}; \mathcal{P}, \Omega) = \sup_{S \in \mathcal{S}} D_N(S; \mathcal{P}, \Omega),$$

  where

$$D_N(S; \mathcal{P}, \Omega) = |\delta_N(S; \mathcal{P}, \Omega)|.$$

- Standard QMC works with $\Omega = [0,1)^d$ and takes for $\mathcal{S}$ the set of anchored boxes $[0, \mathbf{a})$ with $\mathbf{a} \in [0,1)^d$.

Discrepancy due to Brandolini et al. (2013)

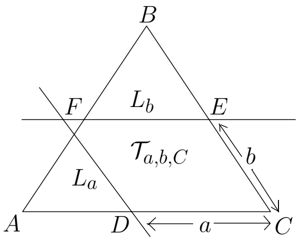
- $\mathcal{S}_C = \{\mathcal{T}_{a,b,C} \mid 0 < a < \|A - C\|, 0 < b < \|B - C\|\}$
- The parallelogram discrepancy of points $\mathcal{P}$ for $\Omega = \Delta(A, B, C)$ is

$$D_N^P(\mathcal{P}; \Omega) = D_N(\mathcal{S}_P; \mathcal{P}, \Omega)$$

for

$$\mathcal{S}_P = \mathcal{S}_A \cup \mathcal{S}_B \cup \mathcal{S}_C.$$

Figure : The construction of the parallelogram $\mathcal{T}_{a,b,C} = CDFE$



Discrepancy due to Pillards and Cools (2005)

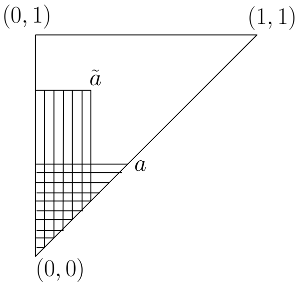
- $\Omega = \Delta((0,0)^\mathsf{T},(0,1)^\mathsf{T},(1,1)^\mathsf{T})$
- Their discrepancy

$$D_N^{PC}(\mathcal{P};\Omega) = D_N(\mathcal{S}_I,\mathcal{P},\Omega)$$

where

$$\mathcal{S}_I = \{[0,\mathbf{a}) \mid \mathbf{a} \in [0,1)^2\}.$$

Figure : Star Discrepancy on the Simplex



Relationship between the discrepancies

Lemma 1

Let T_{PC} be the triangle from Pillards and Cools and for $N \geqslant 1$, let $\mathcal{P}$ be the list of points $\mathbf{x}_1, \ldots, \mathbf{x}_N \in T_{PC}$. Then

$$D_N^{PC}(\mathcal{P}, T_{PC}) \leqslant 2D_N^{P}(\mathcal{P}, T_{PC})$$

Proof

- $[0, a_1) \times [0, a_2) = [0, a_1) \times [0, 1) - [0, a_1) \times [a_2, 1)$
- Taking C to be the vertex $(0, 1)^{\mathsf{T}}$ of T_{PC},
- $D_N^{PC}(\mathcal{P}; T_{PC}) \leqslant 2D_N(\mathcal{S}_C, \mathcal{P}, T_{PC}) \leqslant 2D_N^{P}(\mathcal{P}, T_{PC})$.

Triangular van der Corput construction

- van der Corput sampling of $[0,1]$ the integer $n = \sum_{k \geqslant 1} d_k b^{k-1}$ in base $b \geqslant 2$ is mapped to $x_n = \sum_{k \geqslant 1} d_k b^{-k}$.
- Points $x_1, \dots, x_n \in [0,1)$ have a discrepancy of $O(\log(n)/n)$.
- Our situation : 4-ary expansion.

Triangular van der Corput construction

- $n \geqslant 0$ in a base 4 representation $n = \sum_{k \geqslant 1} d_k 4^{k-1}$ where $d_k \in \{0, 1, 2, 3\}$

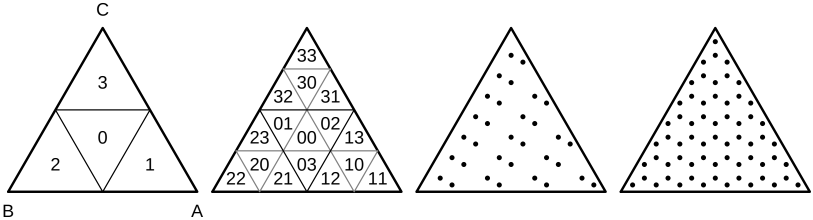


Figure : A labeled subdivision of $\Delta(A, B, C)$ into 4 and then 16 congruent subtriangles. Next are the first 32 triangular van der Corput points followed by the first 64. The integer labels come from the base 4 expansion.

Triangular van der Corput construction

- Computation : $T = \Delta(A, B, C)$

$$T(d) = \begin{cases} \Delta\left(\frac{B+C}{2}, \frac{A+C}{2}, \frac{A+B}{2}\right), & d = 0 \\ \Delta\left(A, \frac{A+B}{2}, \frac{A+C}{2}\right), & d = 1 \\ \Delta\left(\frac{B+A}{2}, B, \frac{B+C}{2}\right), & d = 2 \\ \Delta\left(\frac{C+A}{2}, \frac{C+B}{2}, C\right), & d = 3. \end{cases}$$

- This construction defines an infinite sequence of $f_T(i) \in T$ for integers $i \geqslant 0$.
- For an n point rule, take $\mathbf{x}_i = f_T(i-1)$ for $i = 1, \ldots, n$.

Discrepancy Results

Theorem 1

For an integer $k \geqslant 0$ and non-degenerate triangle $\Omega = \Delta(A, B, C)$, let $\mathcal{P}$ consist of $\mathbf{x}_i = f_\Omega(i-1)$ for $i = 1, \ldots, N = 4^k$. Then

$$D_N^P(\mathcal{P}; \Omega) = \begin{cases} \frac{7}{9}, & N = 1 \\ \frac{2}{3\sqrt{N}} - \frac{1}{9N}, & \text{else.} \end{cases}$$

Discrepancy Results

Theorem 2

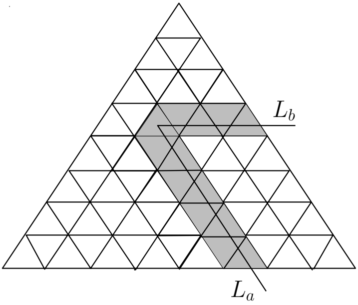
Let Ω be a nondegenerate triangle, and let $\mathcal{P}$ contain points $\mathbf{x}_i = f_\Omega(s+i-1)$, $i = 1, \ldots, N = 4^k$, for a starting integer $s \geqslant 1$ and an integer $k \geqslant 0$. Then

$$D_N^P(\mathcal{P};\Omega) \leq \frac{2}{\sqrt{N}} - \frac{1}{N}.$$

Proof of Theorem 2

Proof

- A set $S \in \mathcal{S}_C$ can be written $S = \mathcal{T}_{a,b,C} \cap \Omega$.
- Let T_j be the interiors of the subtriangles of Ω for $j = 1, \ldots, N$ and then let $T_0 = \Omega \setminus \cup_{j=1}^{N} T_j$.
- $S_j = S \cap T_j$, $j = 0, 1, \ldots, N$.



Proof of Theorem 2

- $\delta_N(S) = \sum_{j=0}^{N} \delta_N(S_j)$.
- $\delta_N(S_0) = 0$.
- If the boundary of $\mathcal{T}_{a,b,C}$ does not touch S_j for $1 \leqslant j \leqslant N$ then $\delta_N(S_j) = 0$ too. Otherwise $-1/N \leqslant \delta_N(S_j) \leqslant 1/N$.
- $D_N(S;\mathcal{P}) \leqslant m/N$ where m is the number of subtriangles touching a boundary line of $\mathcal{T}_{a,b,C}$.
- $m \leqslant 2\sqrt{N} - 1$
- $D_N(\mathcal{S}_C;\mathcal{P}) \leqslant (2\sqrt{N} - 1)/N$

Discrepancy Results

Theorem 3

Let Ω be a non-degenerate triangle and, for integer $N \geqslant 1$, let $\mathcal{P} = (\mathbf{x}_1, \dots, \mathbf{x}_N)$, where $\mathbf{x}_i = f_\Omega(i-1)$. Then

$$D_N^P(\mathcal{P}; \Omega) \leqslant 12/\sqrt{N}.$$

Proof:

- Let $N = \sum_{j=0}^k a_j 4^j$ for some k, with $a_k \neq 0$.
- Let $\mathcal{P}_j^l$ denote a set of 4^j consecutive points from $\mathcal{P}$, for $l = 1, \dots, a_j$ and $j \leqslant k$. These $\mathcal{P}_j^l$ can be chosen to partition the N points $\mathbf{x}_i$. Fix any $S \in \mathcal{S}_P$.

Proof of Theorem 3

- Now,

$$\delta_N(S;\mathcal{P}) = \frac{1}{N}\sum_{j=0}^{k}\sum_{l=1}^{a_j} 4^j \delta(S;\mathcal{P}_j^l).$$

- Therefore from Theorem 2,

$$D_N(S;\mathcal{P}) = |\delta_N(S;\mathcal{P})| \leqslant \frac{1}{N}\sum_{j=0}^{k}\sum_{l=1}^{a_j} 4^j\left(\frac{2}{2^j} - \frac{1}{4^j}\right) \leqslant \frac{1}{N}\sum_{j=0}^{k} a_j(2^{j+1}-1)$$

$$\leqslant \frac{3}{N}(2(2^{k+1}-1)-(k+1)) \leqslant \frac{12\times 2^k}{N}$$

and then $k \leqslant \log_4(N)$, gives $D_N(S;\mathcal{P}) \leqslant 12/\sqrt{N}$.

- Taking the supremum over $S \in \mathcal{S}_P$ yields the result.

Triangular Kronecker Lattice

- We use Theorem 1 of Chen and Travalini (2007)
- This construction yields parallel discrepancy of $O(\log N/N)$

Definition 1

A real number θ is said to be *badly approximable* if there exists a constant $c > 0$ such that $n||n\theta|| > c$ for every natural number $n \in \mathbb{N}$ and $||\cdot||$ denotes the distance from the nearest integer.

Definition 2

Let a, b, c and d be integers with $b \neq 0$, $d \neq 0$ and $c > 0$, where c is not a perfect square. Then $\theta = (a + b\sqrt{c})/d$ is a *quadratic irrational number*.

Triangular Kronecker Lattice

- Let $\Theta = \{\theta_1, \dots, \theta_k\}$ be a set of $k \geqslant 1$ angles in $[0, 2\pi)$.
- Then let $\mathcal{A}(\Theta)$ be the set of convex polygonal subsets of $[0,1]^2$ whose sides make an angle of θ_i with respect to the horizontal axis.

Theorem 1 (Chen and Travaglini (2007))

There exists a constant $C_\Theta < \infty$ such that for any integer $N > 1$ there exists a list $\mathcal{P} = (\mathbf{x}_1, \dots, \mathbf{x}_N)$ of points in $[0,1]^2$ with

$$D_N(\mathcal{A}(\Theta); \mathcal{P}, [0,1]^2) < C_\Theta \log(N)/N.$$

Triangular Kronecker Lattice

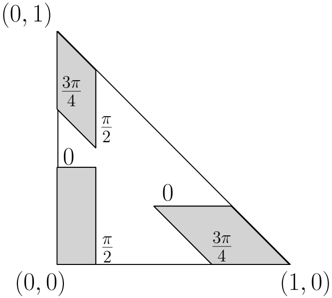
Lemma 2 (Davenport)

Suppose that the angles $\theta_1, \dots, \theta_k \in [0, 2\pi)$ are fixed. Then there exists $\alpha \in [0, 2\pi)$ such that $\tan(\alpha)$,$\tan(\alpha - \pi/2)$, $\tan(\alpha - \theta_1)$,... $\tan(\alpha - \theta_k)$ are all finite and badly approximable.

Triangular Kronecker Lattice

- $R = \Delta((0,0)^\mathsf{T}, (0,1)^\mathsf{T}, (1,0)^\mathsf{T})$.
- $\Theta = \{0, \pi/2, 3\pi/4\}$

Figure : Set of Angles for Kronecker Construction



Triangular Kronecker Lattice

Lemma 3

Let α be an angle for which $\tan(\alpha)$ is a quadratic irrational number. Then $\tan(\alpha)$, $\tan(\alpha - \pi/2)$ and $\tan(\alpha - 3\pi/4)$ are all finite and badly approximable.

- $\tan(3\pi/8) = 1 + \sqrt{2}$.
- $\tan(5\pi/8) = -1 - \sqrt{2}$.

Triangular Kronecker Lattice

Theorem 4

Let $N > 1$ be an integer and let R defined above be the triangle. Let $\alpha \in (0, 2\pi)$ be an angle for which $\tan(\alpha)$ is a quadratic irrational. Let $\mathcal{P}_1$ be the points of the lattice $(2N)^{-1/2}\mathbb{Z}^2$ rotated anticlockwise by angle α. Let $\mathcal{P}_2$ be the points of $\mathcal{P}_1$ that lie in R. If $\mathcal{P}_2$ has more than N points, let $\mathcal{P}_3$ be any N points from $\mathcal{P}_2$, or if $\mathcal{P}_2$ has fewer than N points, let $\mathcal{P}_3$ be a list of N points in R including all those of $\mathcal{P}_2$. Then there is a constant C with

$$D^P(\mathcal{P}_3; R) < C\log(N)/N.$$

Triangular Kronecker Lattice

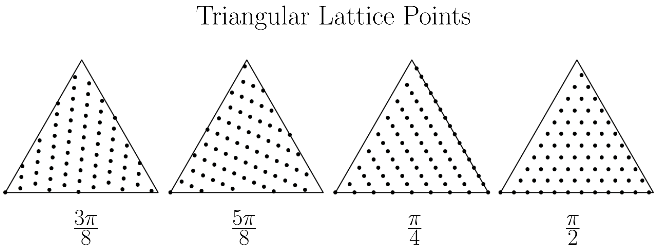
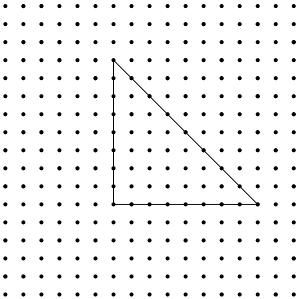


Figure : Triangular lattice points for target $N = 64$. Domain is an equilateral triangle. Angles $3\pi/8$ and $5\pi/8$ have badly approximable tangents. Angles $\pi/4$ and $\pi/2$ have integer and infinite tangents respectively and do not satisfy the conditions for discrepancy $O(\log(N)/N)$.

Construction Algorithm

Given a target sample size N, an angle α such as $3\pi/8$ satisfying Lemma 3. and a target triangle $\Delta(A, B, C)$,

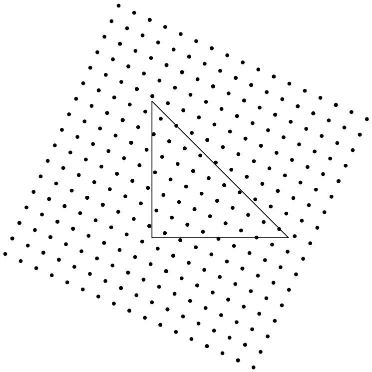
- Take integer grid $\mathbb{Z}^2$



Construction Algorithm

Given a target sample size N, an angle α such as $3\pi/8$ satisfying Lemma 3. and a target triangle $\Delta(A, B, C)$,

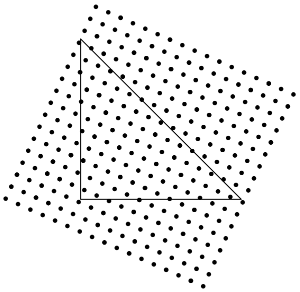
- Take integer grid $\mathbb{Z}^2$
- Rotate anti clockwise by α



Construction Algorithm

Given a target sample size N, an angle α such as $3\pi/8$ satisfying Lemma 3. and a target triangle $\Delta(A, B, C)$,

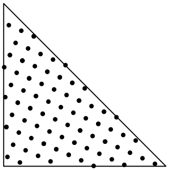
- Take integer grid $\mathbb{Z}^2$
- Rotate anti clockwise by α
- Shrink by $\sqrt{2N}$



Construction Algorithm

Given a target sample size N, an angle α such as $3\pi/8$ satisfying Lemma 3. and a target triangle $\Delta(A, B, C)$,

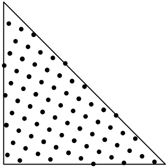
- Take integer grid $\mathbb{Z}^2$
- Rotate anti clockwise by α
- Shrink by $\sqrt{2N}$
- Remove points not in the triangle.



Construction Algorithm

Given a target sample size N, an angle α such as $3\pi/8$ satisfying Lemma 3. and a target triangle $\Delta(A, B, C)$,

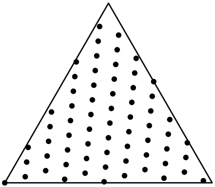
- Take integer grid $\mathbb{Z}^2$
- Rotate anti clockwise by α
- Shrink by $\sqrt{2N}$
- Remove points not in the triangle.
- (Optionally) add/subtract points to get exactly N points



Construction Algorithm

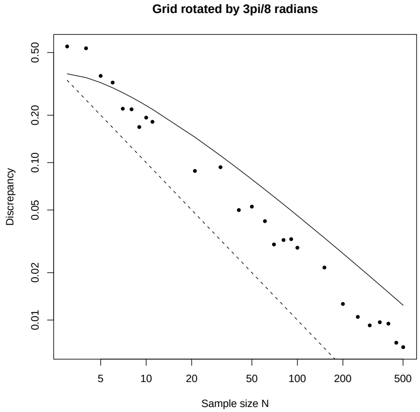
Given a target sample size N, an angle α such as $3\pi/8$ satisfying Lemma 3. and a target triangle $\Delta(A, B, C)$,

- Take integer grid $\mathbb{Z}^2$
- Rotate anti clockwise by α
- Shrink by $\sqrt{2N}$
- Remove points not in the triangle.
- (Optionally) add/subtract points to get exactly N points
- Linearly map R onto the desired triangle $\Delta(A, B, C)$



Triangular Kronecker Lattice

Parallel discrepancy of triangular lattice points for angle $\alpha = 3\pi/8$ and various targets N. The number of points was always N or $N+1$. The dashed reference line is $1/N$. The solid line is $\log(N)/N$.

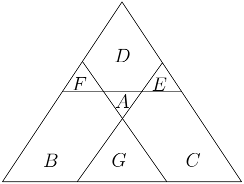


Preliminaries

Lemma 4

Let T be a triangle and $\mathcal{P}$ a list of $N \geqslant 1$ points in T, having parallel discrepancy $D_N^P(\mathcal{P}; T)$. Let S be a subtriangle of T with sides parallel to those of T. Then $D_N(S; \mathcal{P}) \leqslant 6 D_N^P(\mathcal{P}; T)$.

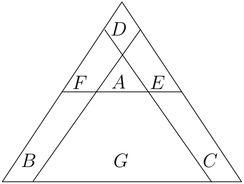
Proof of Lemma 4



- For inverted subtriangle A

$$
\begin{aligned}
& \delta(AB)+\delta(AC)+\delta(AD)-\delta(ABDF)-\delta(ACDE)-\delta(ACGB) \\
&= -\delta(B)-\delta(C)-\delta(D)-\delta(E)-\delta(F)-\delta(G) \\
&= \delta(A),
\end{aligned}
$$

Proof of Lemma 4



- For upright subtriangle A

$$
\begin{aligned}
&\delta(ABFG) + \delta(ADEF) + \delta(ACEG) + \delta(B) + \delta(C) + \delta(D) \\
&= 3\delta(A) + 2\delta(B) + 2\delta(C) + 2\delta(D) + 2\delta(E) + 2\delta(F) + 2\delta(G) \\
&= \delta(A).
\end{aligned}
$$

Consistency Theorem

Theorem 5

Let f be a Riemann integrable function on a nondegenerate triangle Ω, and let $\mathcal{P}_N = (\mathbf{x}_{N,1}, \mathbf{x}_{N,2}, \dots, \mathbf{x}_{N,N})$ for $\mathbf{x}_{N,i} \in \Omega$. If $\lim_{N\to\infty} D_N^P(\mathcal{P};\Omega) = 0$, then

$$\lim_{N\to\infty} \frac{\mathbf{vol}(\Omega)}{N} \sum_{i=1}^{N} f(\mathbf{x}_{N,i}) = \int_\Omega f(\mathbf{x})\,\mathrm{d}\mathbf{x}.$$

Conclusion

- The Kronecker construction attains a lower discrepancy than the van der Corput construction.
- van der Corput construction is extensible and the digits in it can be randomized.
- If f is continuously differentiable, then for $N = 4^k$, the randomization in Owen (1995) will give root mean square error $O(1/N)$

Future Work

- Generalization to tetrahedrons, spherical triangles
- Working with higher order integrals.

Conclusion

Thank you. Questions?