# QMC beyond the cube

Art B. Owen, Stanford University

based on joint work with

Kinjal Basu, LinkedIn

# Kinjal Basu

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# QMC

Estimate $\mu = \int_{[0,1]^d} f(\boldsymbol{x})\,\mathrm{d}\boldsymbol{x}$ by $\hat{\mu} = \frac{1}{n}\sum_{i=1}^n f(\boldsymbol{x}_i)$

## Koksma-Hlawka

$$|\hat{\mu} - \mu| \leqslant D_n^*(\boldsymbol{x}_1, \dots, \boldsymbol{x}_n) \times \|f\|_{\mathrm{HK}}$$

Discrepancy is with respect to **axis-oriented** boxes $[\boldsymbol{0}, \boldsymbol{a}]$ or $[\boldsymbol{a}, \boldsymbol{b}]$

Variation is based on **axis-oriented** differences of differences.

# Non-cubic domains

$$\mu = \int_\Omega f(\boldsymbol{x})\,\mathrm{d}\boldsymbol{x}$$

Triangle Simplex Cylinder

Disk Sphere Ball Spherical triangle

## What axes?

For discrepancy and variation

## Cartesian products

$$\Omega = \prod_{j=1}^{s} \Omega_j, \quad \Omega_j \subset \mathbb{R}^{d_j}$$

Disk $\times$ Sphere $\times$ Sphere $\times$ Interval $\times \cdots \times$ Spherical triangle

# The cube

"You'll never get out of the cube."

The Cube (Jim Henson, 1969) is a surreal film about being stuck in a cube.

Image from wikipedia

# General measures

$D_n^*(\cdot;\mu) = D_n^*(\boldsymbol{x}_1,\dots,\boldsymbol{x}_n;\mu)$ is star discrepancy wrt measure $\mu$

## Theorem from ‘Gates of Hell’ paper

Aistleitner, Bilyk & Nikolov (2016), For any normalized measure $\mu$ on $\mathbb{R}^d$ there exist points with $D_n^*(\cdot;\mu) \leqslant \log(n)^{d-1/2}/n$

## Refs from GoH paper

- Aistleitner & Dick (2015)

  discrepancy and Koksma-Hlawka for general signed measures.
- Aistleitner & Dick (2014) For any normalized measure $\mu$ on $[0,1]^d$,
  $$D_n^*(\cdot;\mu) \leqslant 63\sqrt{d}\big(2+\log_2(n)^{(3d+1)/2}\big)/n.$$
- Beck (1984) had $\log(n)^{2d}$ .
- Götz (2002) first Koksma-Hlawka for general measures.

# QMC sampling

We emphasize **constructions**

1) Measure preserving maps from $[0, 1]^d$ onto $\Omega$, and

2) Direct constructions, e.g., by recursively partitioning $\Omega$.

# Existence proofs

For users, they are frustrating.

- Constructions say how to do something.

  Yes! You can do this.

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  No! You can't do that.

- Existence proofs show that non-existence proofs don't exist.

  Maybe! Keep looking.

However

They can be interesting, elegant or deep.

(And may hint at constructions.)

# Non-cubic domains

We want

$$\mu = \int_\Omega f(\boldsymbol{x})\,\mathrm{d}\boldsymbol{x}, \quad \text{bounded } \Omega \subset \mathbb{R}^d, \quad \mathbf{vol}(\Omega) = 1$$

## Transformations

For measure preserving $\tau : [0,1]^s \to \Omega$

$$\hat{\mu} = \frac{1}{n}\sum_{i=1}^{n} (f \circ \tau)(\boldsymbol{x}_i), \quad \boldsymbol{x}_i \in [0,1]^s$$

But $f \circ \tau$ might not be well behaved. No problem for MC; challenge for QMC.

## Choices for $\tau$

Devroye (1986), Fang & Wang (1994), Pillards & Cools (2005)

# The triangle

## Brandolini, Colzani, Gigante & Travaglini (2013)

- define a 'trapezoid discrepancy' in the simplex and a variation
- prove a Koksma-Hlawka inequality

but gave no constructions of points with vanishing discrepancy.

## Pillards & Cools (2005)

- lots of measure preserving mappings
- get variation & discrepancy & Koksma-Hlawka

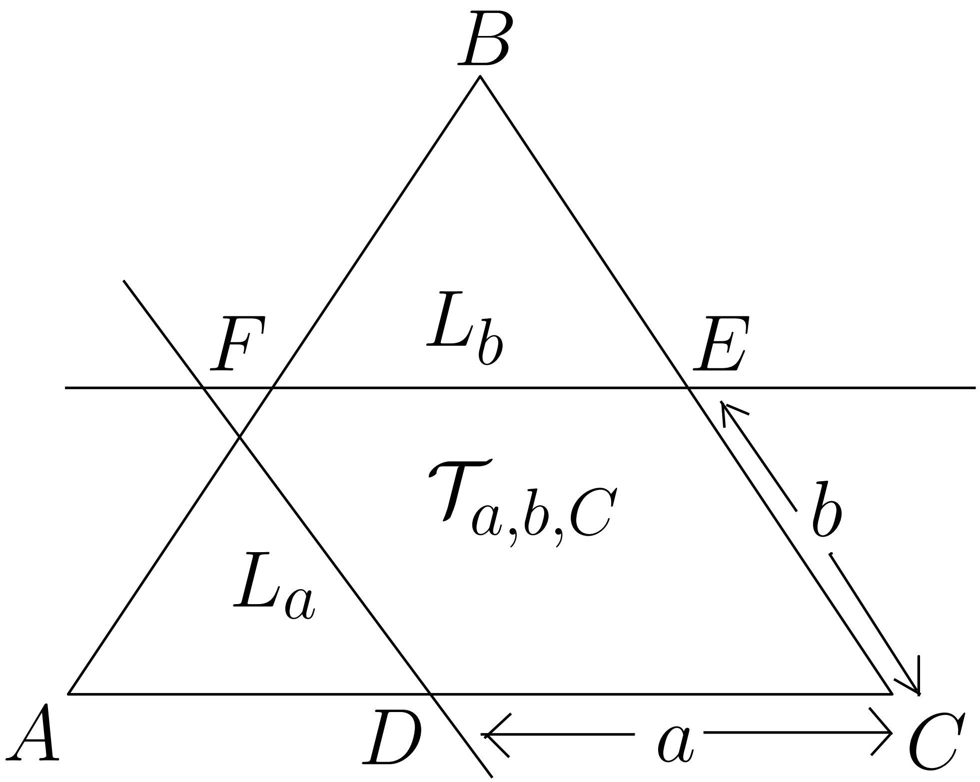
but gave no conditions for vanishing discrepancy of transformed points.

## Chen & Travaglini (2013)

prove existence of point sets with vanishing trapezoid discrepancy for the triangle

# Trapezoid discrepancy

Brandolini et al. (2013,2014)




$\Omega = \triangle(A, B, C)$

Discrepancy for $\mathcal{T}_{a,b,C} \cap \Omega$

$\sup$ over trapezoids

Corresponding variation

Elegant argument $\cdots$

$\cdots$ extends to simplices

# Triangular van der Corput

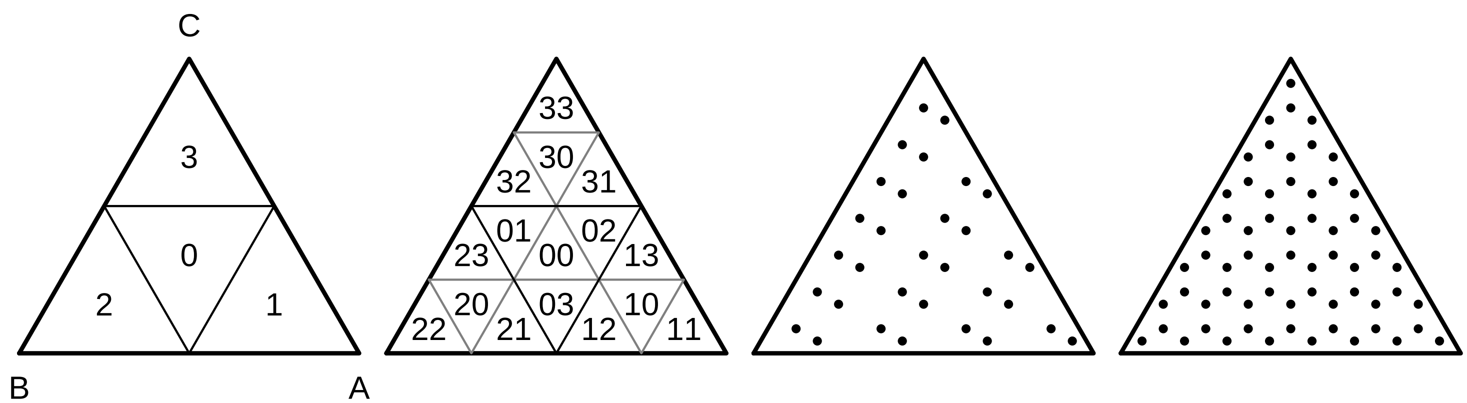
For $i$'th point in $T = \triangle(A,B,C)$, write

$$i = \sum_{k=1}^{K_i} d_{k,i} 4^{k-1}, \quad d_{k,i} \in \{0,1,2,3\}$$

Split $T$ into $4$ congruent sub-triangles, $T(0), T(1), T(2), T(3)$

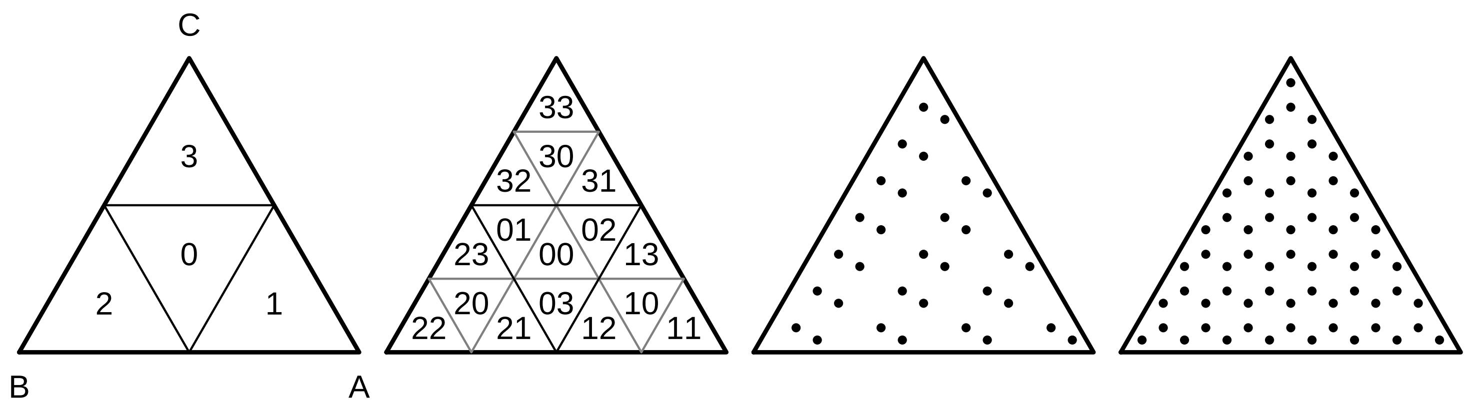
Place $\boldsymbol{x}_i$ in $T(d_{1,i})$

Recurse




Basu & O (2015)

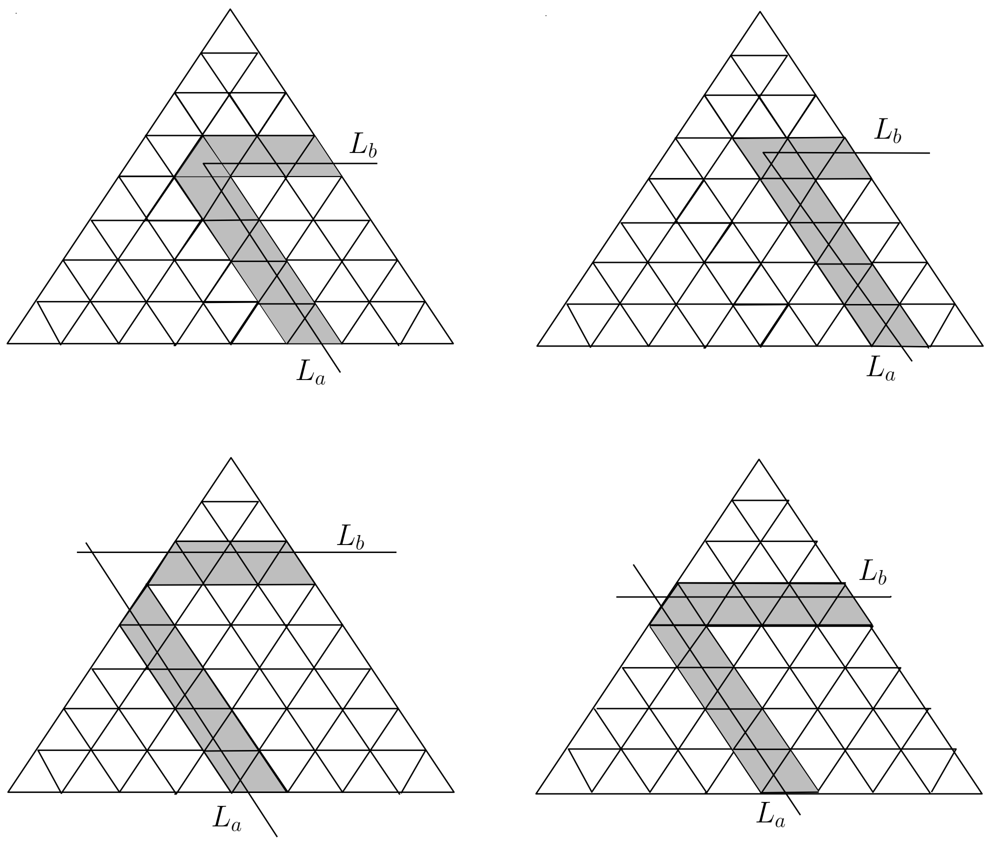
# Construction continued




## Corners of the subtriangle

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

# For $n = 4^k$




- $n$ subtriangles, $1$ point each
- all discrepancy from within shaded triangles
- enumerate all possibilities
- upright vs inverted are different

# Results

Let $D_n^P$ be (anchored) parallelogram discrepancy.

First $n = 4^k$ points

$$D_n^P = \begin{cases} \frac{7}{9}, & n = 1 \\ \frac{2}{3\sqrt{n}} - \frac{1}{9n} & \text{else} \end{cases}$$

Any consecutive $n = 4^k$ points

$$D_n^P \leqslant \frac{2}{\sqrt{n}} - \frac{1}{n}$$

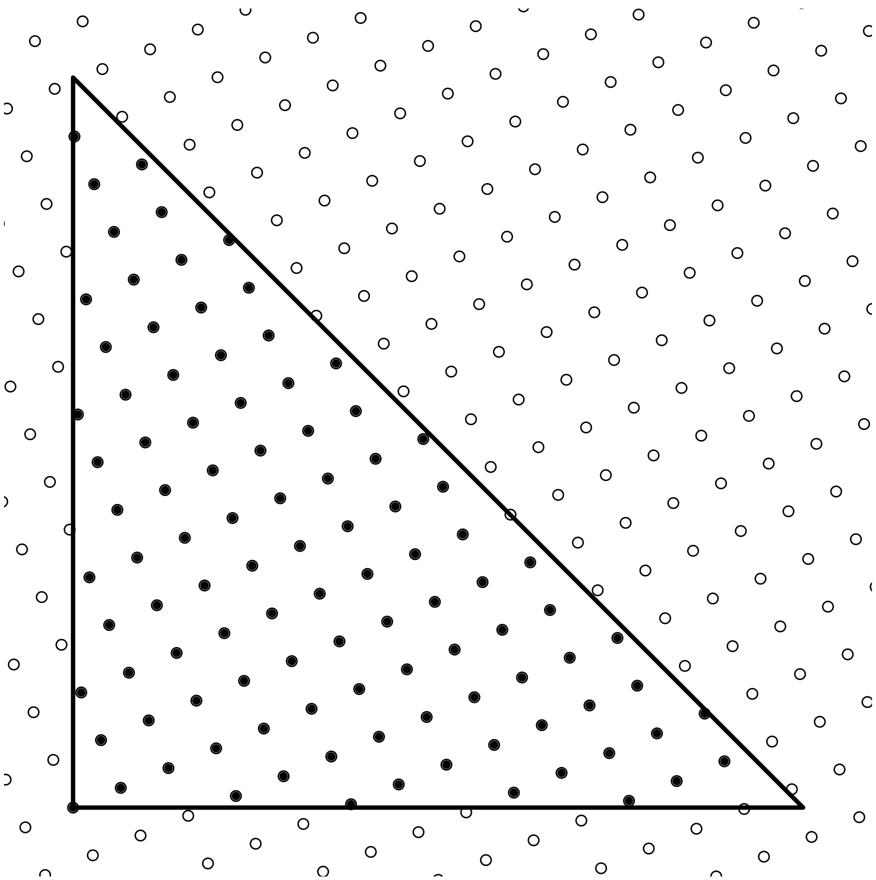
First $n$ points

$$D_n^P \leqslant \frac{12}{\sqrt{n}}$$

Basu & O (2015)

# Kronecker lattice in the triangle

Basu & O (2015)



1) Place a square grid in $\mathbb{R}^2$
2) Rotate it $\alpha$ radians
3) Intersect with right triangle
4) Linear map to desired $\triangle$

Critical: choose good $\alpha$

# Kronecker continued

$\theta \in \mathbb{R}$ is **badly approximable** if there exists $c > 0$ with

$$\mathbf{dist}(n\theta, \mathbb{Z}) > c/n, \quad \forall n \in \mathbb{N}$$

**Quadratic irrationals** $\theta = (a + b\sqrt{c})/d$ are badly approximable.

Here $a, b, c, d \in \mathbb{Z}, \quad b, d \neq 0,$ square free $c > 1$

Chen & Travaglini (2007) There exist points with

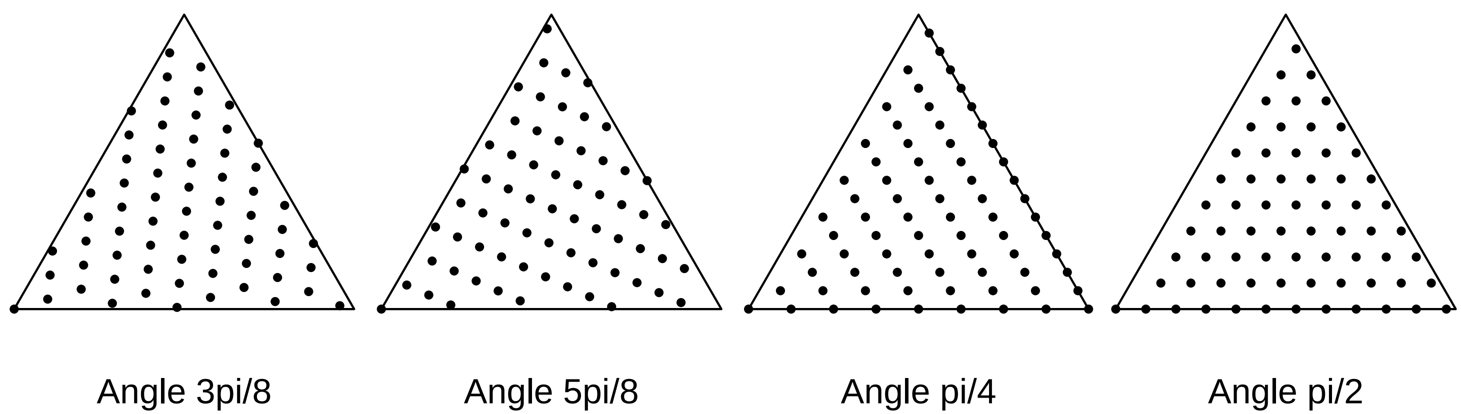
Polygon discrepancy $= O(\log(n)/n)$

Basu & O (2015) Here they are for trapezoids: rotate a grid by $\alpha$ radians where $\tan(\alpha)$ is a quadratic irrational.

E.g., for $\alpha = 3\pi/8, \quad \tan(\alpha) = 1 + \sqrt{2}$

# Triangular Kronecker

Triangular lattice points




$\checkmark$ $\checkmark$ $X$ $X$

A grid with a ‘Kronecker rotation’ gets $D_n^P = O(\log(n)/n)$. Basu & O (2015)

This is the best possible rate. Chen & Travaglini (2013)

## Generalization

Hexagon $=$ six triangles, et cetera

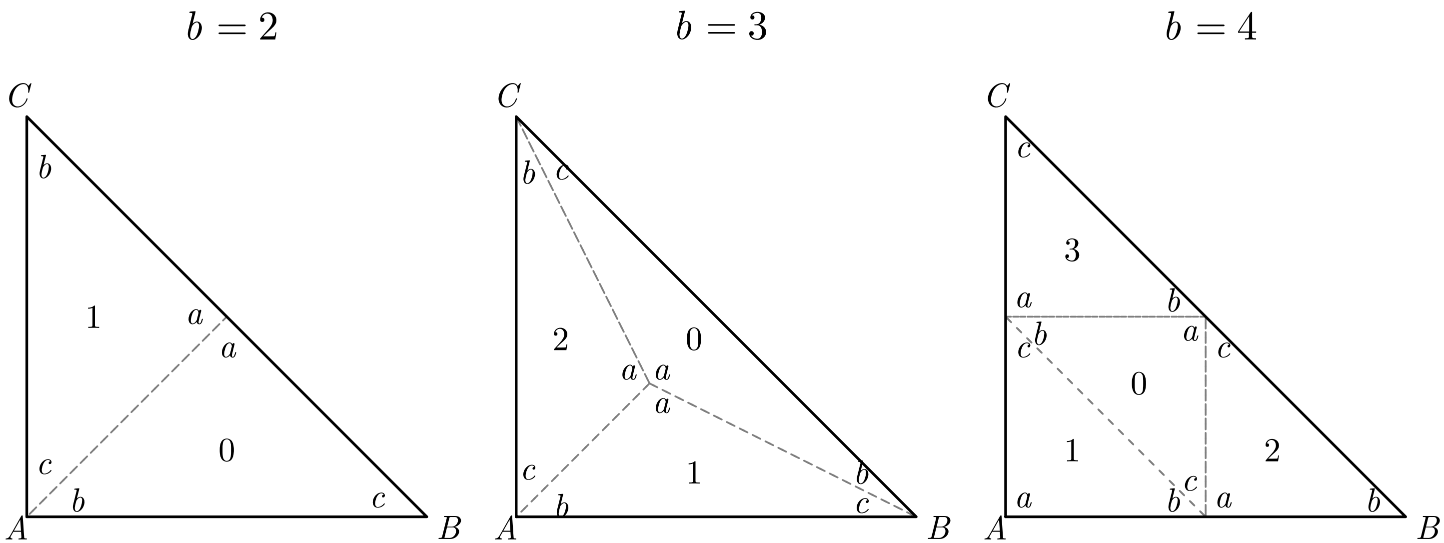
Very unlikely to generalize to higher dimensional simplices or Cartesian products of simplices. (D. Bilyk personal communication)

# Geometric van der Corput

Map $i = 1, 2, 3, \ldots$ into $\boldsymbol{x}_i \in \Omega$.

- replace triangle by more general set $\Omega$
- split $\Omega$ into $b$ equal volumes
- recursively

# Splits of a triangle

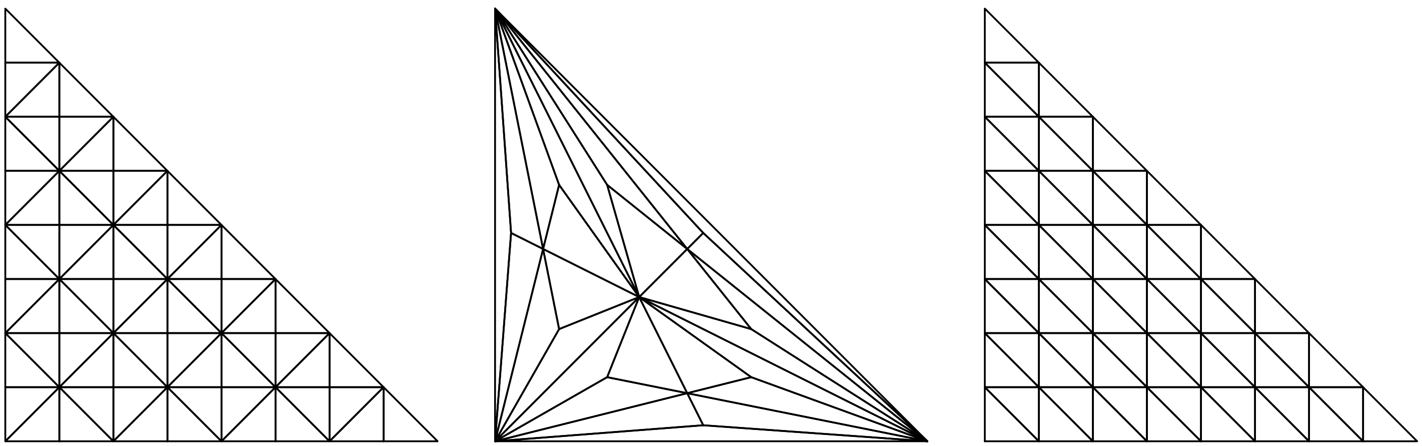



The triangle can be recursively split $2$-fold, $3$-fold or $4$-fold.

This allows digital constructions in those bases.

# Not all splits work well

$2^6$ Decomposition $3^3$ Decomposition $4^3$ Decomposition



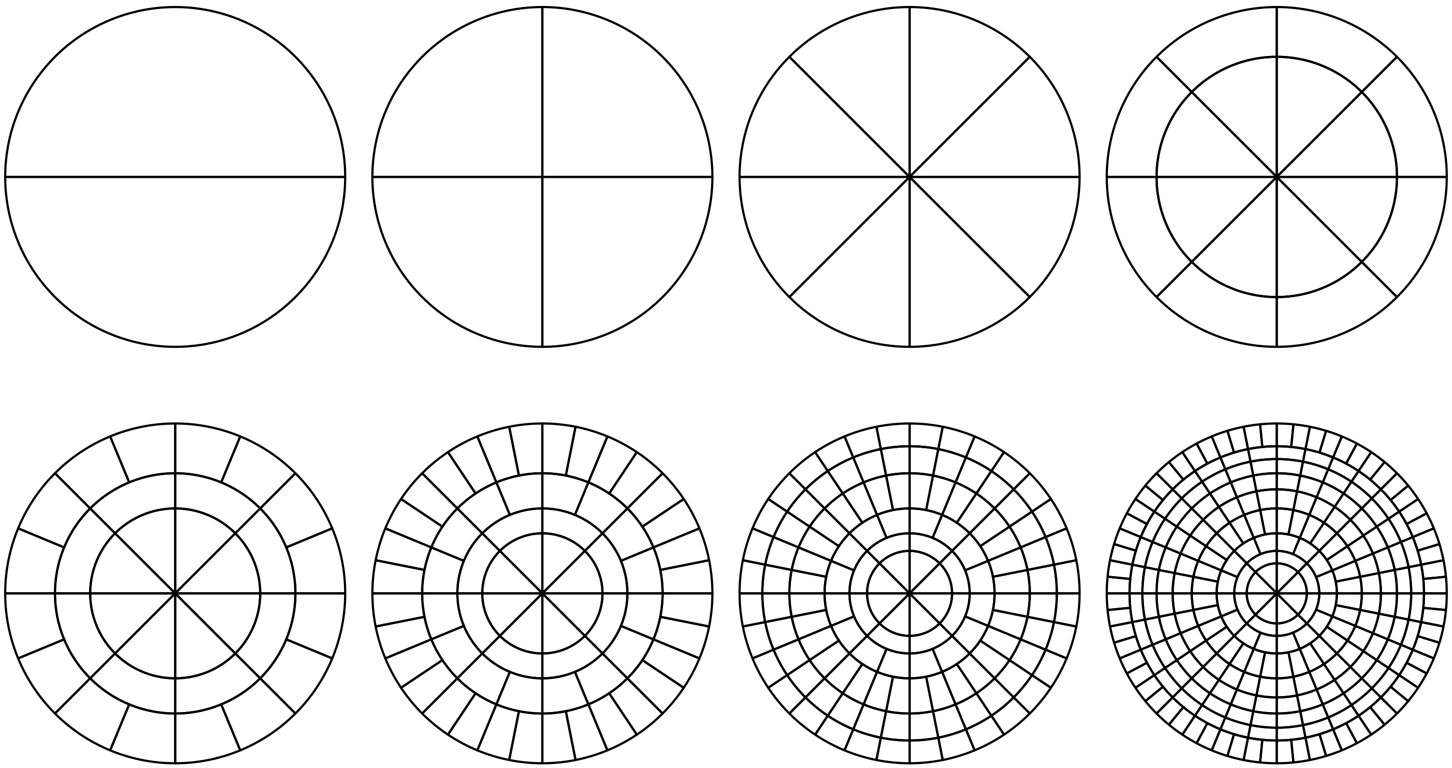
The base $3$ split leads to very unfavorable aspect ratios.

The regions do not 'converge nicely' to a point.

E.g., Stromberg (1994) defines 'converge nicely'

(Bounded aspect ratios.)

# Splits don't have to be congruent



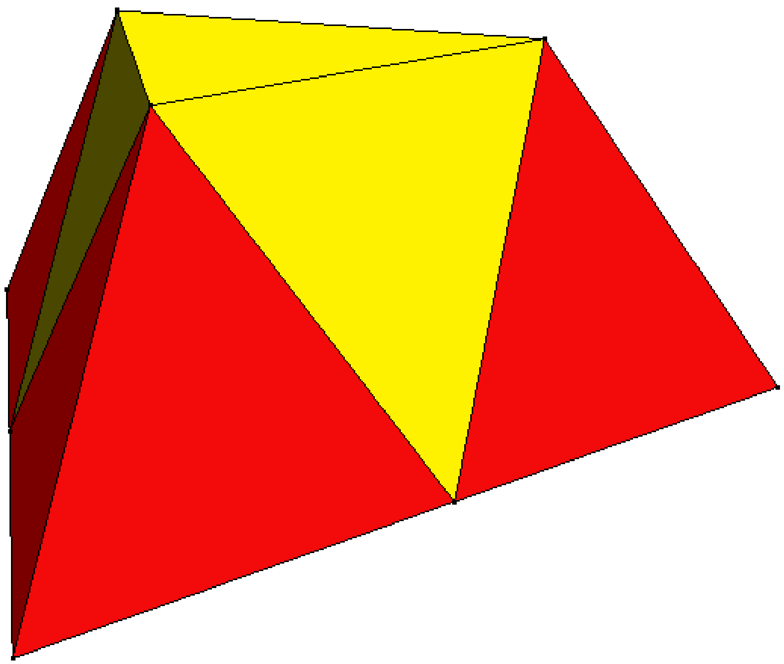
- Mix 'arc splits' and 'radial splits' to keep aspect ratio bounded
- Not a global alternation; different cells get different splits

Basu & O (2015)

See Beckers & Beckers (2012) for non-recursive splits

# Tetrahedron

- chop off $4$ tetrahedral corners
- remaining volume makes $4$ more



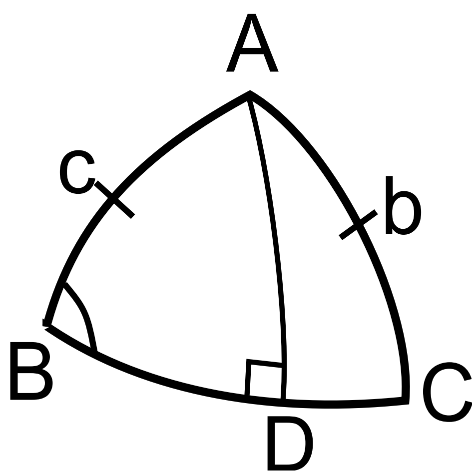
- but they're not congruent to first $4$
- binary splits may be better (split a longest edge)

Image: By Tomruen - Own work, CC BY-SA 3.0, `wikipedia`

# Spherical triangles

- $4$ way split at arc midpoints $\cdots$ not equal area
- $4$ way equal area split of Song, Kimerling, Sahr (2002) uses 'small circle' boundaries, not great circles
- binary splits may be better $\cdots$ use first step in Arvo (1995)

More about Arvo




Arvo shows how to pick $D$ so

$$\frac{\mathbf{vol}(ABD)}{\mathbf{vol}(ABC)} = u$$

We can use $u = 1/2$.

Image by Peter Mercator - Own work, CC BY-SA 3.0, Wikipedia

# Geometric nets

We want points in $\Omega^s$ for $\Omega \subset \mathbb{R}^d$

E.g., light path

$$\text{camera} \to \triangle \to \triangle \to \triangle \to \cdots \to \triangle \to \text{light source}$$

## Use digital nets

A $(t, m, s)$-net, $b = 4$ or $b = 2$, puts $\boldsymbol{x}_i \in \triangle^s$ (componentwise)

## Use other partitions

Other $b$-fold equal area recursive partitions can be used for $\Omega \neq \triangle$

## Scramble the nets

Unbiasedness and error cancellation benefits under smoothness.

# More generally

$$\Omega = \prod_{j=1}^{s} \Omega_j, \quad \Omega_j \subset \mathbb{R}^{d_j}$$

$\tau_j : [0,1] \to \Omega_j$ digital map, base $b$

Take $\boldsymbol{u}_i = (u_{i1}, \ldots, u_{is}) \in [0,1]^s$,
$(t,m,s)$-net or $(t,s)$-sequence in base $b$.

Componentwise map: $\boldsymbol{x}_i = \tau(\boldsymbol{u}_i)$

$$\boldsymbol{x}_i = (x_{i1}, \ldots, x_{is})$$

$$x_{ij} = \tau_j(u_{ij})$$

# Scrambled geometric nets

Take $\mathbf{vol}(\Omega_j) = 1$ and $\Omega = \prod_{j=1}^{s} \Omega_j$ and let

$$\mu = \int_{\Omega} f(\boldsymbol{x})\,\mathrm{d}\boldsymbol{x}, \qquad \hat{\mu} = \frac{1}{n}\sum_{i=1}^{n} f(\boldsymbol{x}_i)$$

where $\boldsymbol{x}_i$ are scrambled geometric nets.

For $f \in L^2(\Omega)$

$$\mathbb{E}(\hat{\mu}) = \mu \qquad \mathrm{Var}(\hat{\mu}) = o\Bigl(\frac{1}{n}\Bigr) \qquad \mathrm{Var}(\hat{\mu}) \leqslant \Gamma \times \frac{\sigma^2}{n}$$

where $\sigma^2 = \int_{\Omega}(f(\boldsymbol{x}) - \mu)^2\,\mathrm{d}\boldsymbol{x}$, and
$\Gamma$ is the largest gain coefficient of the $(t, m, s)$-net

E.g., $t = 0$ implies $\Gamma \leqslant \exp(1) \doteq 2.718$

# Convergence rates

$\mu = \int_{\Omega} f(\boldsymbol{x})\,\mathrm{d}\boldsymbol{x}, \quad \Omega \subset \mathbb{R}^D, \quad D = \sum_{j=1}^{s} d_j,$ e.g., $D = s \times d$.

For smooth $f$, nested uniform scrambled nets and nice partitions

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

Basu & O (2015)

## Two kinds of smooth

1) $\partial^{1:D} f$ continuous and all $\Omega_j$ Sobol' extensible (defined next)

2) $f \in C^D(\Omega)$ (using the Whitney extension)

# Sobol' extension

It begins with the fundamental theorem of calculus (FTC)

$$f(x) = f(c) + \int_c^x f'(y)\,\mathrm{d}y$$

## Dimension $D$, e.g., $D = d \times s$

$f(\boldsymbol{x}) = f(\boldsymbol{c})$ plus $2^D - 1$ integrated partial derivatives along all 'lower faces'


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

## Hybrid points

For $\boldsymbol{x}, \boldsymbol{y} \in \mathbb{R}^D$ and $u \subset \{1, 2, \dots, D\}$ the point $\boldsymbol{z} = \boldsymbol{x}_u{:}\boldsymbol{y}_{-u}$ has $z_j = x_j$ for $j \in u$ and $x_j = y_j$ for $j \notin u$.

# Sobol' extensible region

For $\boldsymbol{x}, \boldsymbol{c} \in \mathbb{R}^D$ define $\mathbf{rect}[\boldsymbol{c}, \boldsymbol{x}] = \prod_{j=1}^{D} [c_j \wedge x_j, c_j \vee x_j]$

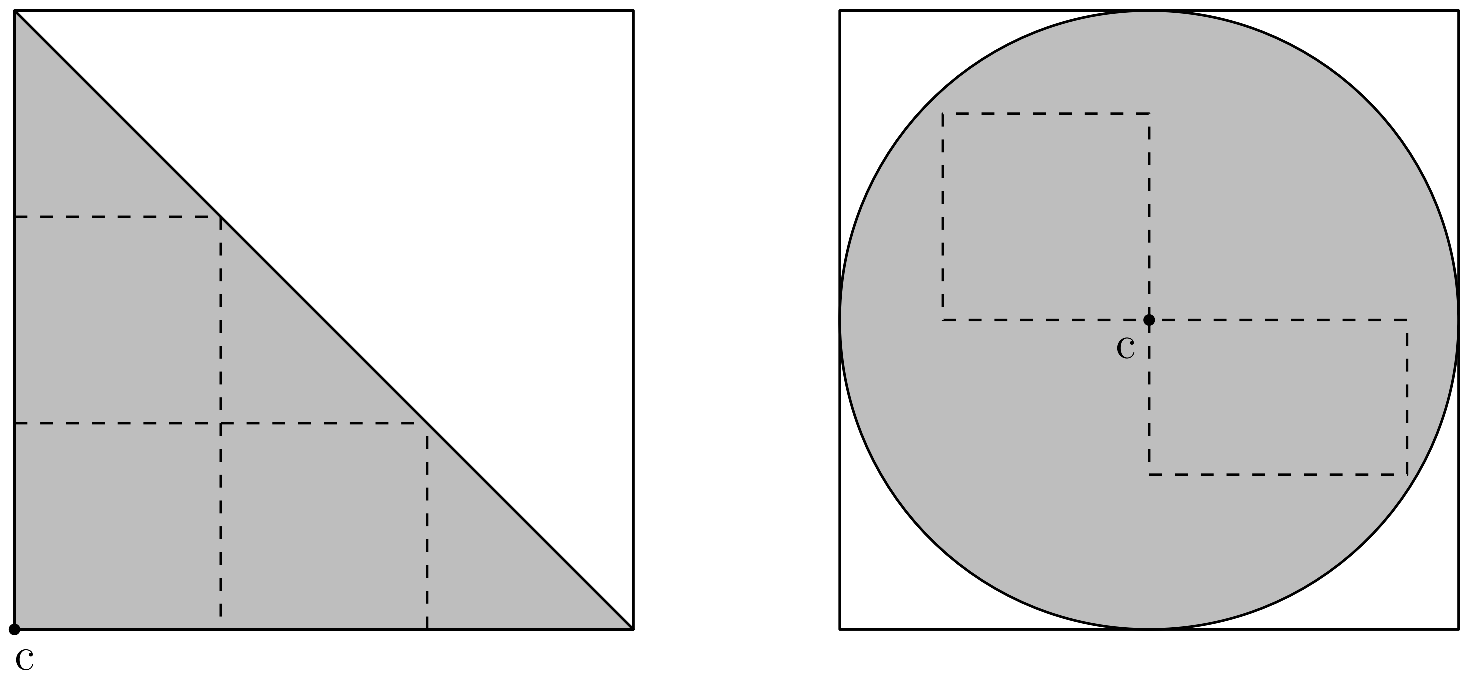

Rectangular hull, bounding box

## Definition

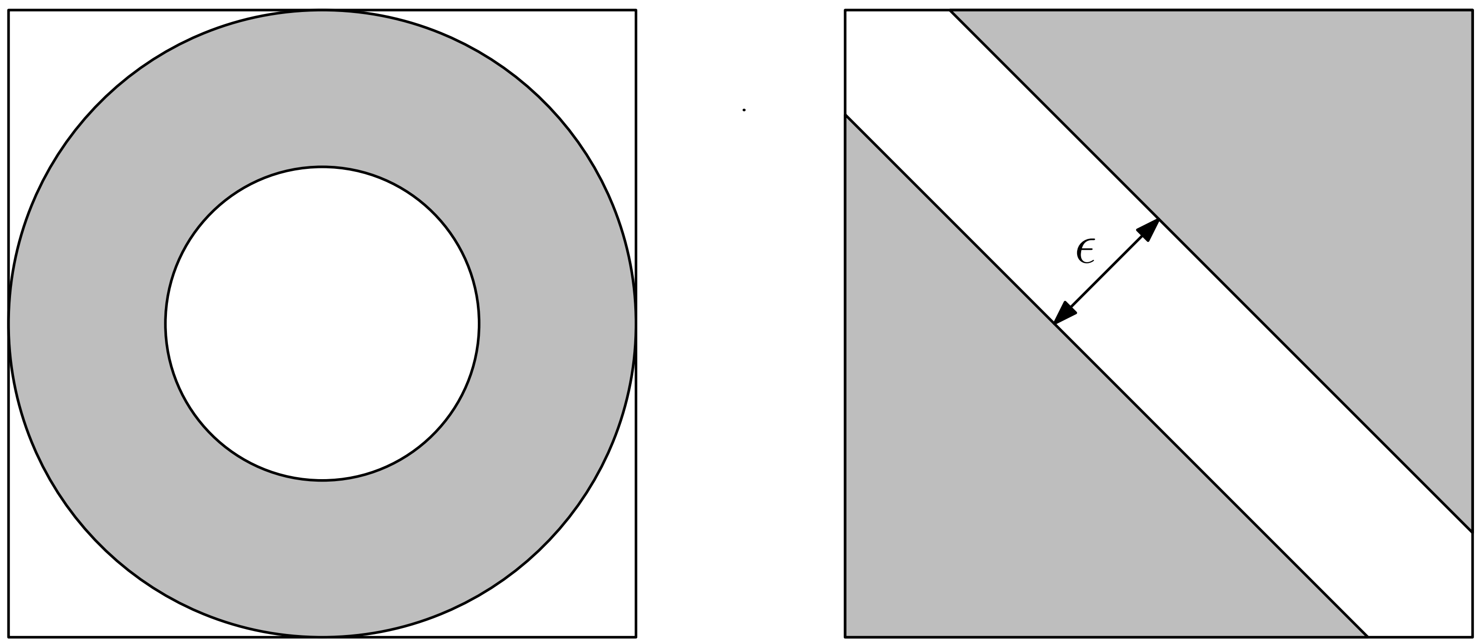
$\Omega \subset \mathbb{R}^d$ is Sobol' extensible with anchor $\boldsymbol{c} \in \mathbb{R}^D$ if

$$\boldsymbol{x} \in \Omega \implies \mathbf{rect}[\boldsymbol{c}, \boldsymbol{x}] \subset \Omega$$

# Sobol' extensible



# Non-Sobol' extensible




No place to put the anchor $\boldsymbol{c}$

# Sobol' extension

Let $\Omega \subset \mathbb{R}^D$ be Sobol' extensible with anchor $\boldsymbol{c}$ and let $\partial^{1:D} f$ be continuous.

Then the Sobol' extension of $f$ is

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

$$\text{vs.} \quad f(\boldsymbol{x}) = \sum_{u \subseteq 1:D} \int_{[\boldsymbol{c}_u, \boldsymbol{x}_u]} \partial^u f(\boldsymbol{c}_{-u}{:}\boldsymbol{y}_u) \, \mathrm{d}\boldsymbol{y}_u \qquad \text{(FTC)}$$

## Properties

$\widetilde{f}(\boldsymbol{x}) = f(\boldsymbol{x})$ for $\boldsymbol{x} \in \Omega$

Low variation

$\partial^{1:D} \widetilde{f}$ not necessarily continuous

but $\widetilde{f}$ satisfies the FTC

# Conditions

1) $\Omega \subset \mathbb{R}^d$ bounded and Sobol' extensible
2) $\boldsymbol{x}_i$ a geometric net, bounded 'gain' coefs
3) nice convergent splits
4) $f \in L^2(\Omega^s)$
5) $\partial^{1:s} f$ continuous

## Conclusion

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

as $n = b^m \to \infty$. Basu & O (2015)

## Challenge:

showing Haar wavelet coefficients decay
via Sobol' (or Whitney) extension from $\Omega$ to $\mathbb{R}^d$

# Dimension $D = ds$

$$\mathrm{Var}(\hat{\mu}) = O\Bigl(\frac{(\log n)^{s-1}}{n^{1+2/d}}\Bigr) \qquad \text{RMSE} = O\Bigl(\frac{(\log n)^{(s-1)/2}}{n^{1/2+1/d}}\Bigr)$$

## Comparisons

1) Better than MC rate for all $s$, $d$
2) Rate sensitive to $d$, not very sensitive to $s$
3) Better than QMC rate for BVHK on $[0,1]^D$ when $d = 2$ (just barely)
   $(\log(n))^{(s-1)/2}$ vs $(\log(n))^{ds-1}$
   Often $f \circ \tau \notin \mathrm{BVHK}$
4) (Barely) better than Kronecker $\triangle$ for $d = 2$ and $s = 1$ (was $\log(n)/n$)

## Note

$$g(\boldsymbol{x}) = 1_{\boldsymbol{x}\in\mathbf{rect}\Omega} \times f(\boldsymbol{x}), \quad \text{usually not BVHK}$$

# Followups to geometric nets

- maybe higher order nets would help Dick, Baldeaux
- geometric Halton sequences
- deterministic nets

## Central limit theorem

Basu & Mukerjee (2016) building on Loh (2003)

# Transformations

Let $\tau$ transform $\mathbf{U}[0,1]^m$ into $\mathbf{U}(\Omega)$.

$$\int_\Omega f(\boldsymbol{x})\,\mathrm{d}\boldsymbol{x} = \int_{[0,1]^m} (f\circ\tau)(\boldsymbol{u})\,\mathrm{d}\boldsymbol{u}$$

We want $f\circ\tau \in$ BVHK for QMC and mixed partials in $L^2$ for RQMC

## BVHK compositions

For $f\circ\tau : \mathbb{R}\to\mathbb{R}\to\mathbb{R}$:

$f\in$ Lipschitz, $\tau\in$ BV $\implies$ $f\circ\tau\in$ BV. Josephy (1981)

No such simple rule in higher dimensions.

Variation is bounded via integrated absolute mixed partials.

So we study derivatives of $f(\tau(\boldsymbol{u}))$.

# Faà di Bruno

Derivatives of composite functions, $\mathbb{R} \to \mathbb{R} \to \mathbb{R}$

Faà di Bruno (1855,1857), Arbogast (1800)

$$\begin{aligned} h(x) &= f(g(x)) \\ h'(x) &= f'(g(x))g'(x) \\ h''(x) &= f''(g(x))g'(x)^2 + f'(g(x))g''(x) \\ h'''(x) &= f'''(g(x))g'(x)^3 + 3f''(g(x))g'(x)g''(x) + f'(g(x))g'''(x) \end{aligned}$$

Our map is

$$\mathbb{R}^D \to \mathbb{R}^d \to \mathbb{R}$$

which has many more terms

Constantine & Savits (1996) give a general Faà di Bruno theorem

Basu & O (2016) simplify it for

$$\partial^u (f \circ \tau), u \subseteq \{1, \dots, D\}$$

i.e., differentiate at most once wrt each $x_j$

Allows tests of BVHK.

# Some mappings

The following mappings work well for MC, but not QMC

## Triangle $\mathbb{T}^2 \subset \mathbb{R}^3$

$$\boldsymbol{u} \in [0,1]^3, \quad x_j = \tau_j(\boldsymbol{u}) = \frac{\log(u_j)}{\sum_{i=1}^3 \log(u_i)} \quad \boldsymbol{x} \sim \mathbf{U}(\mathbb{T}^2)$$

Even $x_j(\boldsymbol{u}) \notin \mathrm{BVHK}([0,1]^3)$.

## Sphere $\mathbb{S}^{d-1} \subset \mathbb{R}^d$

$$x_j = \tau_j(\boldsymbol{u}) = \frac{\Phi^{-1}(u_j)}{\sqrt{\sum_{i=1}^d \Phi^{-1}(u_i)^2}}, \quad \boldsymbol{x} \sim \mathbf{U}(\mathbb{S}^{d-1})$$

Again, $x_j(\boldsymbol{u}) \notin \mathrm{BVHK}([0,1]^d)$.

# BVHK compositions

For $\boldsymbol{u} \in [0,1]^D$ and

$$f(\tau_1(\boldsymbol{u}), \dots, \tau_d(\boldsymbol{u}))$$

If these hold

1) $\partial^v \tau_j(\boldsymbol{u}_v{:}\mathbf{1}_{-v}) \in L^{p_j}([0,1]^{|v|}), \quad p_j \in [1,\infty] \quad v \subseteq \{1,2,\dots,D\}$
2) $\sum_{j=1}^d 1/p_j \leqslant 1$
3) $f \in C^{(d)}(\mathbb{R}^d)$

Then

$$f \circ \tau \in \mathrm{BVHK}$$

# RQMC smooth

1) $\partial^v \tau_j \in L^{p_j}([0,1]^D)$, $p_j \in [2,\infty]$, and
2) $\sum_{j=1}^d 1/p_j \leqslant 1/2$
3) $f \in C^{(d)}(\mathbb{R}^d)$

make $f \circ \tau$ smooth enough for RMSE$= O(n^{-3/2+\epsilon})$ under RQMC.

$f \in C^{(d)}$ can be weakened if $p_j$ are increased

# Fang & Wang (1993)

Three mappings to a simplex, one to the sphere, and one to a ball.

## Example

$$A_d = \{(x_1, \ldots, x_d) \mid 0 \leqslant x_1 \leqslant x_2 \leqslant \cdots \leqslant x_d \leqslant 1\}$$

## Transformation

$$\begin{aligned}
x_1 &= \tau_1(\boldsymbol{u}) = u_1 \\
x_2 &= \tau_2(\boldsymbol{u}) = u_1 \times u_2^{1/2} \\
x_3 &= \tau_3(\boldsymbol{u}) = u_1 \times u_2^{1/2} \times u_3^{1/3} \\
&\vdots \\
x_d &= \tau_d(\boldsymbol{u}) = u_1 \times u_2^{1/2} \times u_3^{1/3} \times \cdots \times u_d^{1/d}
\end{aligned}$$

# Results

All five Fang & Wang mappings $\tau$ are in BVHK.

So composing with $f$ has a chance.

None of them yield $\tau$ with mixed partials in $L^2$.

# Smoother mappings

Importance sampling from $[0, 1]^d$ to $\mathbb{T}^d$ (simplex) can yield RQMC smoothness.

The Jacobian exhibits a 'dimension' effect.

Effective sample size decays like $(8/9)^d$.

Basu & O (2016)

## Conclusion

The unit cube seems to be a relatively easy space to sample.

Despite GoH conjecture that it is the hardest.

# Thanks

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