Variance Lower Bound and Asymptotic Normality of Scrambled Geometric Nets

Kinjal Basu

Relevance Sciences, LinkedIn

Joint work with Rajarshi Mukherjee

15th August, 2016

Overview

- Introduction
- Scrambled Geometric Nets
- 3 Lower Bound on Variance
- 4 Asymptotic Normality

The Problem

- Numerical integration
- Domain of interest : $\mathcal{X}^s = \prod_{j=1}^s \mathcal{X}^{(j)}$, where each $\mathcal{X}^{(j)} \subset \mathbb{R}^d$.

The Problem

- Numerical integration
- Domain of interest : $\mathcal{X}^s = \prod_{j=1}^s \mathcal{X}^{(j)}$, where each $\mathcal{X}^{(j)} \subset \mathbb{R}^d$.
- To estimate

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

The Problem

- Numerical integration
- Domain of interest : $\mathcal{X}^s = \prod_{j=1}^s \mathcal{X}^{(j)}$, where each $\mathcal{X}^{(j)} \subset \mathbb{R}^d$.
- To estimate

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

by an equal weight rule

$$\hat{\mu}_n = \frac{1}{n} \sum_{i=1}^n f(\mathbf{x}_i),\tag{1}$$

where x_i are the points generated by QMC or RQMC methods.

• Need to construct a confidence interval.

- Need to construct a confidence interval.
- Asymptotic Distribution.

- Need to construct a confidence interval.
- Asymptotic Distribution.
- Upper bound from Basu and Owen (2015).

- Need to construct a confidence interval.
- Asymptotic Distribution.
- Upper bound from Basu and Owen (2015).
- Matching lower bound for the variance.

• Start with a (t, m, s)-net in base b in $[0, 1)^s$.

- Start with a (t, m, s)-net in base b in $[0, 1)^s$.
- Introduce randomization via Scrambling Algorithm to get $u_i \in [0,1)^s$.

- Start with a (t, m, s)-net in base b in $[0, 1)^s$.
- Introduce randomization via Scrambling Algorithm to get $u_i \in [0,1)^s$.
- Apply a mapping ϕ such that

$$\mathbf{x}_i = \phi(\mathbf{u}_i) \in \mathcal{X}^s$$

(Scrambled geometric net)

- Start with a (t, m, s)-net in base b in $[0, 1)^s$.
- Introduce randomization via Scrambling Algorithm to get $u_i \in [0,1)^s$.
- Apply a mapping ϕ such that

$$\mathbf{x}_i = \phi(\mathbf{u}_i) \in \mathcal{X}^s$$

(Scrambled geometric net)

• Equal weight rule

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

- Start with a (t, m, s)-net in base b in $[0, 1)^s$.
- Introduce randomization via Scrambling Algorithm to get $u_i \in [0,1)^s$.
- ullet Apply a mapping ϕ such that

$$\mathbf{x}_i = \phi(\mathbf{u}_i) \in \mathcal{X}^s$$

(Scrambled geometric net)

• Equal weight rule

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

Most interesting case: triangles, spherical triangles and discs.

Previous Results

Lemma 1 (B. and Owen (2015b))

 $\hat{\mu}_n$ is unbiased for μ .

Previous Results

Lemma 1 (B. and Owen (2015b))

 $\hat{\mu}_n$ is unbiased for μ .

Theorem 1 (B. and Owen (2015b))

There exists a constant C > 0 such that

$$\operatorname{Var}(\hat{\mu}_n) \leq C \frac{(\log n)^{s-1}}{n^{1+2/d}},$$

under certain smoothness conditions on f and a sphericity constraint on the partitioning of \mathcal{X}^s .

• Point set is a scrambled (0, m, s) geometric net in base b.

• Point set is a scrambled (0, m, s) geometric net in base b.

Theorem 2. (B. and Mukherjee (2016))

If $f \in \mathcal{F}_s$ and the partitioning of \mathcal{X}^s satisfies an eigenvalue condition, then there exists a positive constant c such that

$$\operatorname{Var}(\hat{\mu}_n) \geqslant c \frac{(\log n)^{s-1}}{n^{1+2/d}}.$$
 (2)

• Point set is a scrambled (0, m, s) geometric net in base b.

Theorem 2. (B. and Mukherjee (2016))

If $f \in \mathcal{F}_s$ and the partitioning of \mathcal{X}^s satisfies an eigenvalue condition, then there exists a positive constant c such that

$$\operatorname{Var}(\hat{\mu}_n) \geqslant c \frac{(\log n)^{s-1}}{n^{1+2/d}}.$$
 (2)

Define,

$$W = \frac{\hat{\mu}_n - \mu}{\sqrt{\operatorname{Var}(\hat{\mu}_n)}}.$$

• Point set is a scrambled (0, m, s) geometric net in base b.

Theorem 2. (B. and Mukherjee (2016))

If $f \in \mathcal{F}_s$ and the partitioning of \mathcal{X}^s satisfies an eigenvalue condition, then there exists a positive constant c such that

$$\operatorname{Var}(\hat{\mu}_n) \geqslant c \frac{(\log n)^{s-1}}{n^{1+2/d}}.$$
 (2)

Define,

$$W = \frac{\hat{\mu}_n - \mu}{\sqrt{\operatorname{Var}(\hat{\mu}_n)}}.$$

Theorem 3. (B. and Mukherjee (2016))

Let $b \geqslant \max(s, d, 2)$, $f \in \mathcal{F}_s$ and if (2) holds, then $W \to \mathcal{N}(0, 1)$ in distribution as $n \to \infty$.

Overview

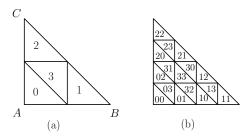
- Introduction
- Scrambled Geometric Nets
- 3 Lower Bound on Variance
- 4 Asymptotic Normality

• Set of $n = b^m$ points on the domain \mathcal{X}^s .

- Set of $n = b^m$ points on the domain \mathcal{X}^s .
- Fix a equal volume recursive partition in base b of the domain.

- Set of $n = b^m$ points on the domain \mathcal{X}^s .
- Fix a equal volume recursive partition in base b of the domain.
- Put a point x_i uniformly at random within a cell of volume $1/b^m$.

- Set of $n = b^m$ points on the domain \mathcal{X}^s .
- Fix a equal volume recursive partition in base b of the domain.
- Put a point x_i uniformly at random within a cell of volume $1/b^m$.
- For example on T^2 using base b = 4,



Splits on the Triangle

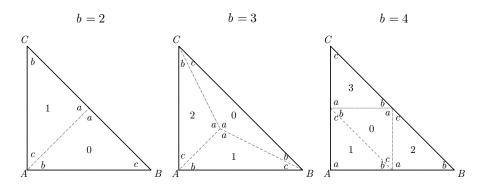


Figure: Splits of a triangle \mathcal{X} for bases b=2, 3 and 4. The subtriangles \mathcal{X}_j are labeled by the digit $j\in\mathbb{Z}_b$.

Recursive Splits on the Triangle

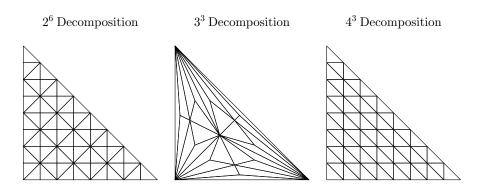


Figure: The base b splits from previous figure carried out to k=6 or 3 or 4 levels.

Splitting on the Disc

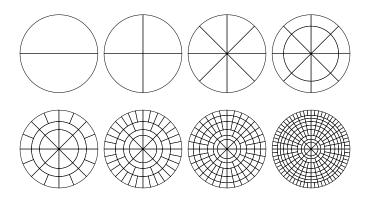


Figure: A recursive binary equal area splitting of the unit disk, keeping the aspect ratio close to unity.

Overview

- Introduction
- 2 Scrambled Geometric Nets
- 3 Lower Bound on Variance
- 4 Asymptotic Normality

Form of Variance

• Using Multiresolution Analysis of $L^2(\mathcal{X}^s)$,

$$\operatorname{Var}(\hat{\mu}_n) = \mathbb{E}\left(\left[\frac{1}{n}\sum_{i=1}^n (f(\mathbf{x}_i) - \mu)\right]^2\right)$$
$$= \frac{1}{n}\sum_{|u|>0}\sum_{\kappa|u} \Gamma_{u,\kappa}\sigma_{u,\kappa}^2.$$

Form of Variance

• Using Multiresolution Analysis of $L^2(\mathcal{X}^s)$,

$$\operatorname{Var}(\hat{\mu}_n) = \mathbb{E}\left(\left[\frac{1}{n}\sum_{i=1}^n (f(\mathbf{x}_i) - \mu)\right]^2\right)$$
$$= \frac{1}{n}\sum_{|u|>0}\sum_{\kappa|u} \Gamma_{u,\kappa}\sigma_{u,\kappa}^2.$$

where

$$\sigma_{u,\kappa}^2 = \sum_{\tau} \sum_{\gamma,\gamma'} \langle f, \psi_{u\kappa\tau\gamma} \rangle \langle f, \psi_{u\kappa\tau\gamma'} \rangle \prod_{j \in u} \left(\mathbb{1}_{c_j = c_j'} - \frac{1}{b} \right).$$

Main Theorem on Lower Bound

Theorem 2: B. and Mukherjee (2016)

If $f \in \mathcal{F}_s$ and an eigenvalue condition holds for the partitioning of the domain, then there exists a positive constant c such that

$$\operatorname{Var}(\hat{\mu}_n) \geqslant c \frac{(\log n)^{s-1}}{n^{1+2/d}},$$

for all sufficiently large n.

Smooth class of functions \mathcal{F}_s

Smooth class of functions \mathcal{F}_s

Definition

A real-valued function f on \mathcal{X}^s is smooth if for all $u \subseteq s$,

$$\|\nabla^u f(\mathbf{x}) - \nabla^u f(\mathbf{x}^*)\| \le B \|\mathbf{x} - \mathbf{x}^*\|^{\beta}$$

for some finite $B \ge 0$ and $\beta \in (0,1]$ for all $\mathbf{x}, \mathbf{x}^* \in \mathcal{X}^s$.

Smooth class of functions \mathcal{F}_s

Definition

A real-valued function f on \mathcal{X}^s is smooth if for all $u \subseteq s$,

$$\|\nabla^u f(\mathbf{x}) - \nabla^u f(\mathbf{x}^*)\| \le B \|\mathbf{x} - \mathbf{x}^*\|^{\beta}$$

for some finite $B \ge 0$ and $\beta \in (0,1]$ for all $\mathbf{x}, \mathbf{x}^* \in \mathcal{X}^s$.

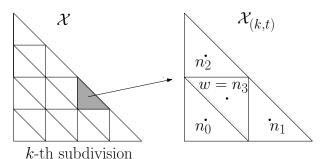
Definition

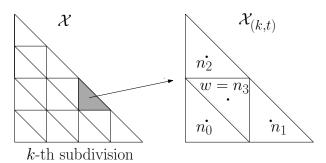
Define \mathcal{F}_s as the class of all smooth functions f on \mathcal{X}^s such that for all $u \subseteq s$,

$$\left\| \int_{\mathcal{V}^s} \nabla^u f(\mathbf{x}) \, \mathrm{d}\mathbf{x} \right\|^2 > 0.$$

Remember that,

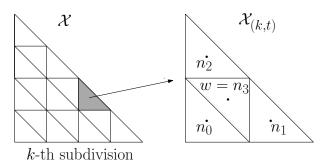
$$\sigma_{u,\kappa}^2 = \sum_{\tau} \sum_{\gamma,\gamma'} \langle f, \psi_{u\kappa\tau\gamma} \rangle \langle f, \psi_{u\kappa\tau\gamma'} \rangle \prod_{i \in u} \left(\mathbb{1}_{c_i = c_i'} - \frac{1}{b} \right).$$





• Define,

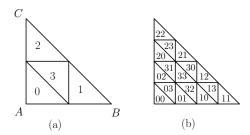
$$A^{(k,t)} = \sum_{c=0}^{b-1} (\boldsymbol{n}_c - \boldsymbol{w}) (\boldsymbol{n}_c - \boldsymbol{w})^T$$

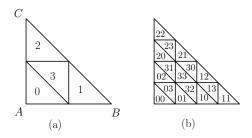


• Define,

$$A^{(k,t)} = \sum_{c=0}^{b-1} (\boldsymbol{n}_c - \boldsymbol{w}) (\boldsymbol{n}_c - \boldsymbol{w})^T$$

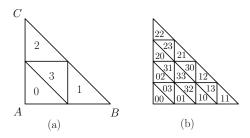
• $\lambda_1\left(A^{(k,t)}\right) \geq \tilde{c}b^{-2k/d}$ for some $\tilde{c}>0$.





• Using the above subdivision,

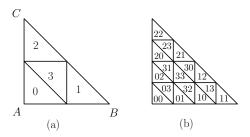
$$A^{(k,t)} = \frac{b^{-k}}{6} \begin{bmatrix} 2 & -1 \\ -1 & 2 \end{bmatrix}$$



• Using the above subdivision,

$$A^{(k,t)} = \frac{b^{-k}}{6} \begin{bmatrix} 2 & -1 \\ -1 & 2 \end{bmatrix}$$

• Thus, $\lambda_1\left(A^{(k,t)}\right) = b^{-k}/6$

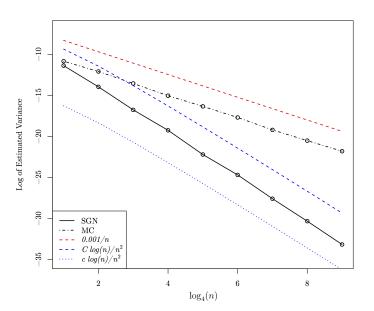


Using the above subdivision,

$$A^{(k,t)} = \frac{b^{-k}}{6} \begin{bmatrix} 2 & -1 \\ -1 & 2 \end{bmatrix}$$

- Thus, $\lambda_1(A^{(k,t)}) = b^{-k}/6$
- If $\mathcal{X}=[0,1]$, then $A^{(k,t)}=b^{-2k}\left(\frac{b^2-1}{12b}\right)$.

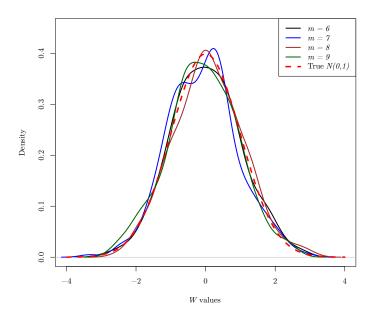
$f(\mathbf{x}, \mathbf{y}) = x_1 x_2^2 - y_1^3 y_2^4 \text{ on } T^2 \times T^2$



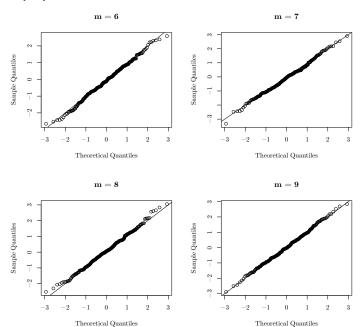
Overview

- Introduction
- 2 Scrambled Geometric Nets
- 3 Lower Bound on Variance
- Asymptotic Normality

Example continued



Normal Q-Q Plots



•
$$W = (\hat{\mu}_n - \mu)/\sqrt{Var(\hat{\mu}_n)}$$

- $W = (\hat{\mu}_n \mu)/\sqrt{Var(\hat{\mu}_n)}$
- ullet Create a $ilde{W}$ satisfying $W- ilde{W}=o_p(1)$

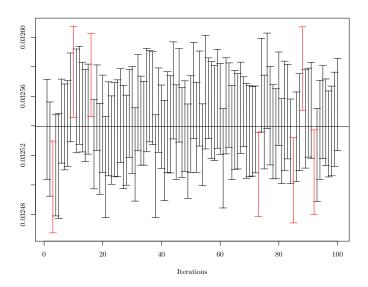
- $W = (\hat{\mu}_n \mu)/\sqrt{Var(\hat{\mu}_n)}$
- ullet Create a $ilde{W}$ satisfying $W- ilde{W}=o_p(1)$
- ullet Create an exchangeable pair $(ilde{W}, ilde{W}^*)$

- $W = (\hat{\mu}_n \mu)/\sqrt{Var(\hat{\mu}_n)}$
- ullet Create a $ilde{W}$ satisfying $W- ilde{W}=o_p(1)$
- ullet Create an exchangeable pair $(ilde{W}, ilde{W}^*)$
- Based on Exchangeable Pair technique of Stein's Method, show that $\tilde{W} \to \mathcal{N}(0,1)$ in distribution as $m \to \infty$.

- $W = (\hat{\mu}_n \mu)/\sqrt{Var(\hat{\mu}_n)}$
- ullet Create a $ilde{W}$ satisfying $W- ilde{W}=o_p(1)$
- ullet Create an exchangeable pair $(ilde{W}, ilde{W}^*)$
- Based on Exchangeable Pair technique of Stein's Method, show that $\tilde{W} \to \mathcal{N}(0,1)$ in distribution as $m \to \infty$.
- Use Slutsky's Theorem.

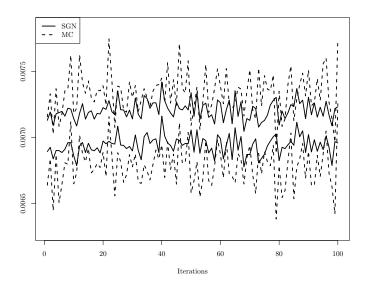
Confidence Intervals

• $f(x,y) = x_1x_2^2 - y_1^3y_2^4$ on $T^2 \times T^2$



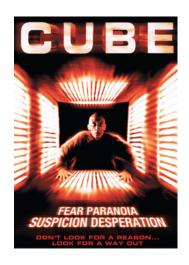
Confidence Intervals

• $f(x, y) = x_1x_2y_1y_2 \exp(x_1x_2y_1y_2)$ on $T^2 \times T^2$

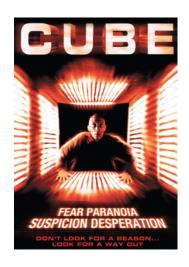


• There are good variance bounds for the estimator $\hat{\mu}_n$ for large n.

- There are good variance bounds for the estimator $\hat{\mu}_n$ for large n.
- Asymptotically accurate confidence sets can be easily constructed.



- There are good variance bounds for the estimator $\hat{\mu}_n$ for large n.
- Asymptotically accurate confidence sets can be easily constructed.



- There are good variance bounds for the estimator $\hat{\mu}_n$ for large n.
- Asymptotically accurate confidence sets can be easily constructed.
- QMC Methods can give us a way out of the Cube.

Thank you

- The organizers
- Co-author Rajarshi Mukherjee
- Art Owen
- NSF Grant DMS-1407397

References:

- Basu, K and Mukherjee, R. (2016) Asymptotic normality of scrambled geometric net quadrature. *The Annals of Statistics.* To Appear.
- Basu, K and Owen, A. (2015) Scrambled geometric net integration over general product spaces. Foundations of Computational Mathematics. In Press.