Sufficient Conditions for Central Limit Theorems for Randomized Quasi-Monte Carlo

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Motivation

- Estimate μ and provide **computable measure of error**, where

$$\mu = \int_{[0,1]^s} h(u)\, du = \mathbb{E}[\, h(U) \,], \qquad U \sim \mathcal{U}[0,1]^s$$

- Monte Carlo (MC), Quasi-Monte Carlo (QMC), Randomized QMC (RQMC)

Method	Key Idea	Error Estimation	Convergence
MC	Random points in $[0,1]^s$	Conf. Interval (CI)	Slow
QMC	Deterministic points in $[0,1]^s$	Difficult	Fast
RQMC	i.i.d. randomizations of QMC points	**CI**	Fast

- RQMC CI validity relies on **CLT: not proven for many RQMC settings.**
- **Goal:** General conditions for broad range of RQMC settings to ensure
  - Central limit theorem (CLT)
  - **Asymptotically valid CI (AVCI)**

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Review: Monte Carlo (MC)

- MC: **random sampling** to estimate $\mu = \mathbb{E}[\, h(U) \,]$

$$\widehat{\mu}_n^{\mathrm{MC}} = \tfrac{1}{n} \textstyle\sum_{i=1}^{n} h(U_i), \qquad U_1, U_2, \ldots, U_n \text{ i.i.d. } \mathcal{U}[0,1]^s$$

- **CLT**: If $\psi^2 \equiv \mathrm{Var}[\, h(U) \,] \in (0, \infty)$, then [Billingsley 1995]

$$\sqrt{\frac{n}{\psi^2}} \left[\widehat{\mu}_n^{\mathrm{MC}} - \mu \right] \Rightarrow \mathcal{N}(0,1) \quad \text{as } n \to \infty$$

  - Approximate $100\gamma\%$ **CI** for μ:

$$I_{n,\gamma}^{\mathrm{MC}} \equiv \left[\widehat{\mu}_n^{\mathrm{MC}} \pm z_\gamma \frac{\widehat{\psi}_n}{\sqrt{n}} \right]$$

    - $\widehat{\psi}_n^2 = \frac{1}{n-1} \sum_{i=1} \left[h(U_i) - \widehat{\mu}_n^{\mathrm{MC}} \right]^2$ and $\Phi(z_\gamma) = 1 - (1-\gamma)/2$.

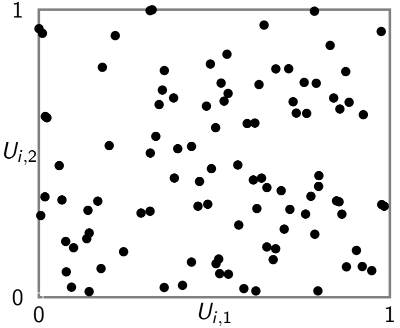
  - **Asymptotically valid CI (AVCI)**:

$$\mathbb{P}(\, \mu \in I_{n,\gamma}^{\mathrm{MC}} \,) \to \gamma, \quad \text{as } n \to \infty$$

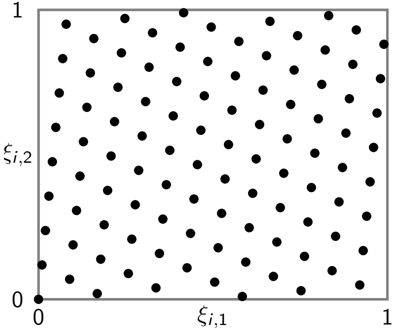
  - Root mean-squared error: $\mathrm{RMSE}\left[\widehat{\mu}_n^{\mathrm{MC}} \right] = \frac{\psi}{\sqrt{n}}$

- Replace i.i.d. $U_1, U_2, \ldots$ with **low-discrepancy sequence** $\Xi = (\xi_i : i = 1, 2, \ldots)$
  - Ξ is deterministic and evenly fill $[0,1]^s$
  - **lattices** (e.g., Korobov, ...), **Digital nets/sequences** (e.g., Sobel', Faure, ...)

MC



QMC (lattice)



Review: Quasi-Monte Carlo (QMC)

- QMC: **deterministic points** to estimate $\mu = \mathbb{E}[\, h(U) \,]$

$$\widehat{\mu}_n^{\mathrm{Q}} = \frac{1}{n} \sum_{i=1}^{n} h(\xi_i), \qquad \Xi = (\xi_i : i = 1, 2, \ldots)$$

- **Koksma-Hlawka (K-H) inequality** [Niederreiter 1992]: for each $n > 1$,

$$|\, \widehat{\mu}_n^{\mathrm{Q}} - \mu \,| \le V_{\mathrm{HK}}(h)\, D_n^*(\Xi)$$

  - Hardy-Krause variation $V_{\mathrm{HK}}(h)$: "roughness" of h
  - Star-discrepancy $D_n^*(\Xi)$: how unevenly first n points of Ξ fill $[0,1]^s$

$$D_n^*(\Xi) = O\left(n^{-1}(\ln n)^s\right) \approx O\left(n^{-1}\right), \quad n \to \infty.$$

  - If $V_{\mathrm{HK}}(h) < \infty$ (BVHK), then K-H bound shrinks at faster rate than MC rate $\Theta(n^{-1/2})$

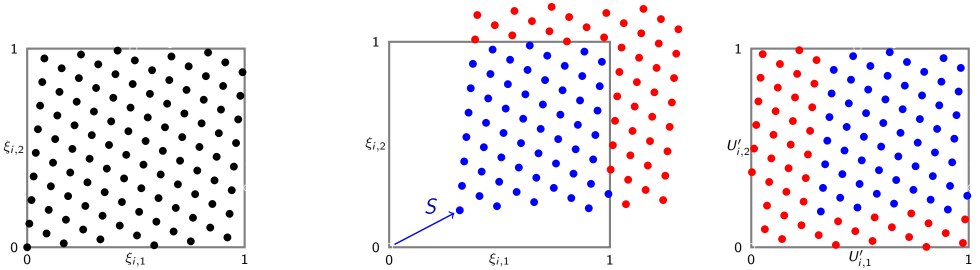
$$|\, \widehat{\mu}_n^{\mathrm{Q}} - \mu \,| \approx O\left(n^{-1}\right).$$

    - BVHK: "bounded variation in sense of Hardy and Krause"
  - **But K-H bound not practical**
    - Difficult to compute, often $V_{\mathrm{HK}}(h) = \infty$, often very loose, ...

Review: Randomized Quasi-Monte Carlo (RQMC)

- i.i.d. randomizations of $\Xi = (\xi_i : i \geq 1)$, each yielding $\Xi' = (U_i' : i \geq 1)$
  - Each $U_i' \sim \mathcal{U}[0,1]^s$
  - Ξ' retains low-discrepancy properties of Ξ
- **Lattice:** random shift [Cranley & Patterson 1976]

QMC (lattice): Ξ $\qquad$ $\Xi + S, \quad S \sim \mathcal{U}[0,1]^s$ $\qquad$ $\Xi' = (\Xi + S) \mod 1$



- **Digital net:** nested scrambling [Owen 1995], digital shift [L'Ecuyer & Lemieux 2002], ...

Review: Randomized Quasi-Monte Carlo (RQMC)

- RQMC computation budget of n evaluations of h (as for MC)
  - allocation (m_n, r_n) with $m_n \times r_n \approx n$
  - $r_n = \#$ i.i.d. randomizations
  - $m_n = \#$ points used from jth randomized sequence $\Xi'_j = (U'_{i,j} : i \geq 1)$, $j = 1, 2, \ldots, r_n$
- RQMC: $r_n \geq 2$ i.i.d. **randomizations** to estimate $\mu = \mathbb{E}[\, h(U)\,]$

$$\widehat{\mu}^{\mathrm{RQ}}_{m_n,r_n} = \frac{1}{r_n} \sum_{j=1}^{r_n} X_{n,j}, \quad \text{where} \quad X_{n,j} = \frac{1}{m_n} \sum_{i=1}^{m_n} h(U'_{i,j})$$

  - $X_{n,1}, X_{n,2}, \ldots, X_{n,r_n}$ i.i.d.: estimate $\sigma^2_{m_n} \equiv \mathrm{Var}[X_{n,1}]$ by

$$\widehat{\sigma}^2_{m_n,r_n} = \frac{1}{r_n - 1} \sum_{j=1}^{r_n} \left(X_{n,j} - \widehat{\mu}^{\mathrm{RQ}}_{m_n,r_n} \right)^2 .$$

- Approx γ-level CI for μ

$$I^{\mathrm{RQ}}_{m_n,r_n,\gamma} \equiv \left[\widehat{\mu}^{\mathrm{RQ}}_{m_n,r_n} \pm z_\gamma \frac{\widehat{\sigma}_{m_n,r_n}}{\sqrt{r_n}} \right]$$

How to choose RQMC Allocation (m_n, r_n) with $m_n \times r_n \approx n$?

- **Heuristic:** For given budget n, choose r_n small and $m_n \approx n/r_n$ large to exploit QMC.
  - CI: $I^{\mathrm{RQ}}_{m_n,r_n,\gamma} \equiv \left[\widehat{\mu}^{\mathrm{RQ}}_{m_n,r_n} \pm z_\gamma \frac{\widehat{\sigma}_{m_n,r_n}}{\sqrt{r_n}} \right]$
  - $r_n = \#$ i.i.d. randomizations
  - $m_n = \#$ points used from each randomized sequence
- But heuristic lacks rigorous justification.
- AVCI relies on **CLT: not established for many RQMC settings**.
  - Nested scrambling of digital nets: CLT as $m_n = n \to \infty$, **fixed** $r_n = 1$ [Loh 2003]
  - Randomly shifted lattices: **no** CLT as $m_n = n/r_n \to \infty$, **fixed** $r_n \geq 1$ [L'Ecuyer et al. 2010]
- **Goal:** Sufficient conditions to ensure CLT and AVCI (as $n \to \infty$).
- **Assumption 1.** "Simple allocation": $(m_n, r_n) = (n^c, n^{1-c})$ for constant $c \in (0, 1)$.
  - **Main Issue:** How to choose c?
  - More general allocation (m_n, r_n): $r_n \to \infty$ with $m_n \times r_n \approx n$ as $n \to \infty$.
- **Assumption 2.** $\sigma^2_{m_n} \equiv \mathrm{Var}[X_{n,1}] > 0$ for all n large enough.

How to choose RQMC Allocation (m_n, r_n) with $m_n \times r_n \approx n$?

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RQMC CLT

Theorem 1

If Assumptions 1 and 2 hold, then RQMC estimator $\widehat{\mu}^{RQ}_{m_n,r_n}$ *satisfies* **CLT**

$$\sqrt{\frac{r_n}{\sigma^2_{m_n}}}\left[\widehat{\mu}^{RQ}_{m_n,r_n} - \mu\right] \Rightarrow \mathcal{N}(0,1), \quad as \;\; n \to \infty$$

under **either**

Lindeberg condition: $$\frac{\mathbb{E}\Big[(X_{n,1}-\mu)^2 \,;\, |X_{n,1}-\mu| > t\sqrt{r_n\,\sigma^2_{m_n}}\Big]}{\mathbb{E}\Big[(X_{n,1}-\mu)^2\Big]} \to 0, \quad as \;\; n \to \infty, \;\; \forall t > 0;$$

or

Lyapounov condition: $$\frac{\mathbb{E}\Big[|X_{n,1}-\mu|^{2+b'}\Big]}{r_n^{b'/2}\sigma^{2+b'}_{m_n}} \to 0, \quad as \;\; n \to \infty, \;\; \textit{for some } b' > 0.$$

- $\sigma^2_{m_n} = \mathbb{E}[\,(X_{n,1}-\mu)^2\,]$

RQMC Asymptotically Valid CI (AVCI)

- Recall **Lyapounov condition:**

$$\frac{\mathbb{E}\left[\left|X_{n,1}-\mu\right|^{2+b'}\right]}{r_n^{b'/2}\sigma_{m_n}^{2+b'}} \to 0, \quad \text{as } n\to\infty, \text{ for some } b'>0.$$

- $\widehat{\sigma}^2_{m_n,r_n} = \frac{1}{r_n-1}\sum_{j=1}^{r_n}\left(X_{n,j}-\widehat{\mu}^{\mathrm{RQ}}_{m_n,r_n}\right)^2$ is unbiased estimator of $\sigma^2_{m_n} = \mathrm{Var}[X_{n,1}]$.
- Approx. γ-level CI for μ

$$I^{\mathrm{RQ}}_{m_n,r_n,\gamma} = \left[\widehat{\mu}^{\mathrm{RQ}}_{m_n,r_n} \pm z_\gamma \frac{\widehat{\sigma}_{m_n,r_n}}{\sqrt{r_n}}\right]$$

Theorem 2

If Assumptions 1 and 2 hold, along with Lyapounov condition for $b'=2$, then **CLT**

$$\sqrt{\frac{r_n}{\widehat{\sigma}^2_{m_n,r_n}}}\left[\widehat{\mu}^{RQ}_{m_n,r_n}-\mu\right] \Rightarrow \mathcal{N}(0,1), \quad \text{as} \quad n\to\infty$$

and **AVCI**

$$P(\mu\in I^{RQ}_{m_n,r_n,\gamma}) \to \gamma, \quad \text{as} \quad n\to\infty.$$

Corollaries Ensuring CLT or AVCI

- For estimator $X_{n,1}$ from **single** randomization of m_n points,

$$\sigma_{m_n} \equiv \sqrt{\mathrm{Var}[X_{n,1}]} \approx \Theta(m_n^{-\alpha_*}) \quad \text{as} \quad m_n \to \infty, \quad \text{where} \quad \alpha_* \equiv -\lim_{m_n \to \infty} \frac{\ln(\sigma_{m_n})}{\ln(m_n)} > \frac{1}{2}$$

  - $\alpha_* \geq 1$ when $V_{\mathrm{HK}}(h) < \infty$ (BVHK).

- Under Assumption 1 $[\ (m_n, r_n) = (n^c, n^{1-c}),\ \ c \in (0,1)\ ]$,

$$\boxed{\mathrm{RMSE}\left[\widehat{\mu}^{\mathrm{RQ}}_{m_n,r_n}\right] = \frac{\sigma_{m_n}}{\sqrt{r_n}} \approx \Theta\left(n^{-v(\alpha_*,c)}\right)} \text{ as } n \to \infty, \text{ with } \boxed{v(\alpha_*, c) \equiv c\left[\alpha_* - \tfrac{1}{2}\right] + \tfrac{1}{2}.}$$

- Corollary $k = 1, 2, \ldots, 6$: ensure CLT or AVCI under constraint

$$\boxed{c < c_k(\alpha_*)}$$

  - $c_k(\alpha_*) \in (0,1]$, sometimes $c_k(\alpha_*) = 1$.
  - Optimal RMSE: take $c < c_k(\alpha_*)$ with $c \approx c_k(\alpha_*)$

$$\boxed{\mathrm{RMSE}\left[\widehat{\mu}^{\mathrm{RQ}}_{m_n,r_n}\right] \approx \Theta\left(n^{-v_k(\alpha_*)}\right)} \text{ as } n \to \infty, \text{ with } \boxed{v_k(\alpha_*, c) \equiv c_k(\alpha_*)\left[\alpha_* - \tfrac{1}{2}\right] + \tfrac{1}{2} > \tfrac{1}{2}}$$

$\Longrightarrow$ **RQMC better than MC.**

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$\Longrightarrow$ **RQMC better than MC.**

Corollaries Ensuring CLT or AVCI

Corollary 1

Suppose that Assumptions 1 and 2 hold, and $\exists\ b' > 0$ *and* $k_1 \in (0, \infty)$ *such that*

$$\frac{\mathbb{E}\left[\,|X_{n,1} - \mu|^{2+b'}\,\right]}{\sigma_{m_n}^{2+b'}} \leq k_1 \quad \forall\ m_n \ \textit{ sufficiently large.} \tag{1}$$

Then **CLT** *holds for allocation* $(m_n, r_n) = (n^c, n^{1-c})$ *with any*

$$c < 1 \equiv c_1(\alpha_*),$$

and optimal $RMSE \approx \Theta(n^{-v_1(\alpha_*)})$ *as* $n \to \infty$ *with*

$$v_1(\alpha_*) \equiv \alpha_*.$$

If (1) *holds for* $b' = 2,$ *then* **AVCI** *holds for* $c < c_1(\alpha_*)$, *and RMSE rate exponent is* $v_1(\alpha_*)$.

- CLT/AVCI with $r_n \to \infty$ since $c < 1$.
- RMSE rate same as $\sigma_{m_n} \approx \Theta(m_n^{-\alpha_*})$ for **single** randomization of $m_n = n$ points.

Corollaries Ensuring CLT or AVCI: Tradeoffs

Instead of condition (1), impose alternative conditions on integrand h

- **Assumption 3.A**: $V_{\mathrm{HK}}(h) < \infty$ (BVHK)
- **Assumption 3.B**: h is bounded
- **Assumption 3.C**: $\mathbb{E}[\,|h(U) - \mu|^{2+b}\,] < \infty$ for some $b > 0$, where $U \sim \mathcal{U}[0,1]^s$.

Proposition 1

- *Assumption 3.A* $\Longrightarrow$ *3.B* $\Longrightarrow$ *3.C,*
  leading to successively smaller $c_k(\alpha_*)$ for Corollaries k (next slide).
- *Under Assumption 3.x, for $c_k(\alpha_*)$ ensuring CLT and $c_{k'}(\alpha_*)$ ensuring AVCI,*

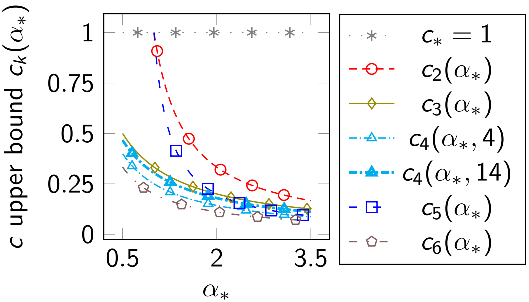
$$c_k(\alpha_*) \;\geq\; c_{k'}(\alpha_*) \qquad (\text{often} >).$$

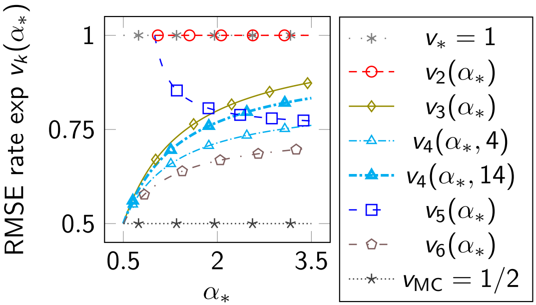
- **Assumption 1**: $(m_n, r_n) = (n^c, n^{1-c})$, $c \in (0,1)$
- Corollary k: $c < c_k(\alpha_*)$
- $\sigma_{m_n} \approx \Theta(\, m_n^{-\alpha_*} \,)$, $\alpha_* > 1/2$

Corollaries CLT or AVCI: Tradeoffs

Cor. k	Ensures	Assumption on h	c upper bd $c_k(\alpha_*)$		RMSE rate exp $v_k(\alpha_*)$	
2	**CLT**	3.A (BVHK)	$\frac{1}{2\alpha_*-1}$	$>$	1	$>$
3	**CLT**	3.B (h bdd)	$\frac{1}{2\alpha_*+1}$	$>$	$\frac{2\alpha_*}{2\alpha_*+1}$	$>$
4	**CLT**	3.C ($b > 0$)	$\frac{1}{2\alpha_*(1+\frac{2}{b})+1}$	$\in \ (0, \frac{1}{2})$	$\frac{2\alpha_*(1+\frac{1}{b})}{2\alpha_*(1+\frac{2}{b})+1}$	$> \ \frac{1}{2}$
5	**AVCI**	3.A (BVHK)	$\frac{1}{4\alpha_*-3}$	$>$	$\frac{3\alpha_*-2}{4\alpha_*-3}$	$>$
6	**AVCI**	3.C ($b = 2$)	$\frac{1}{4\alpha_*+1}$	$\in \ (0, \frac{1}{3})$	$\frac{3\alpha_*}{4\alpha_*+1}$	$> \ \frac{1}{2}$

- 3.A $\implies$ 3.B $\implies$ 3.C
  - **Assumption 3.A**: $V_{\mathrm{HK}}(h) < \infty$ (BVHK: $\implies \alpha_* \geq 1$)
  - **Assumption 3.B**: h is bounded.
  - **Assumption 3.C**: $\mathbb{E}[\,|h(U) - \mu|^{2+b}] < \infty$ for some $b > 0$, where $U \sim \mathcal{U}[0,1]^s$.
- Comparisons for fixed $\alpha_* > 1/2$
  - $(m_n, r_n) = (n^c, n^{1-c})$, $c < c_k(\alpha_*)$, opt RMSE $\approx \Theta(n^{-v_k(\alpha_*)})$.





- All $c_k(\alpha_*) \downarrow$ as $\alpha_* \uparrow$
  - Corollary k: $c < c_k(\alpha_*)$ in $(m_n, r_n) = (n^c, n^{1-c})$.
  - $\sigma_{m_n} \approx \Theta(m_n^{-\alpha_*})$, $\alpha_* > 1/2$ (≥ 1 BVHK)
- Most $v_k(\alpha_*) \uparrow$ as $\alpha_* \uparrow$
  - Optimal RMSE $\approx \Theta(n^{-v_k(\alpha_*)})$, $n \to \infty$
  - Larger α_* usually yields better RQMC performance.

Concluding Remarks

- Sufficient conditions for RQMC CLT and AVCI for $\mu = \mathbb{E}[\,h(U)\,]$
  - Corollary k: $c < c_k(\alpha_*)$ for allocation $(m_n, r_n) = (n^c, n^{1-c})$.
  - Tradeoffs: Weaker conditions on integrand h
    $\longrightarrow$ stronger restrictions on c.
  - AVCI imposes (often strictly) stronger restrictions on c than CLT.
  - RMSE: RQMC outperforms MC.
- Current work
  - Estimate $c_k(\alpha_*)$.
  - Weaker conditions.
  - CLT and AVCI for biased estimators, e.g., quantiles.
  - Alternative CIs: Bootstrap-t, etc.

Thank you!