On Confidence Intervals for Randomized Quasi-Monte Carlo Estimators

Bruno Tuffin
(based on joint works with P. L'Ecuyer, M. Nakayama and A. Owen)

Inria

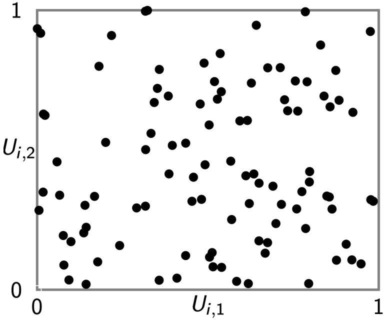
Atelier d'évaluation de performance, 2024

Review: Monte Carlo (MC)

- MC: **random sampling** to estimate $\mu = \mathbb{E}[\,h(U)\,]$ with $U \sim \mathcal{U}[0,1]^s$

$$\widehat{\mu}_n^{\mathrm{MC}} = \frac{1}{n}\sum_{i=1}^{n} h(U_i)$$

- $U_1, U_2, \ldots, U_n$ i.i.d. $\mathcal{U}[0,1]^s$



Review: MC — Error Estimation Easy, But Slow Convergence

- MC estimator: $\widehat{\mu}_n^{\mathrm{MC}} = \frac{1}{n}\sum_{i=1}^{n} h(U_i)$
- **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 $100\gamma\%$ confidence interval (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)**:

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

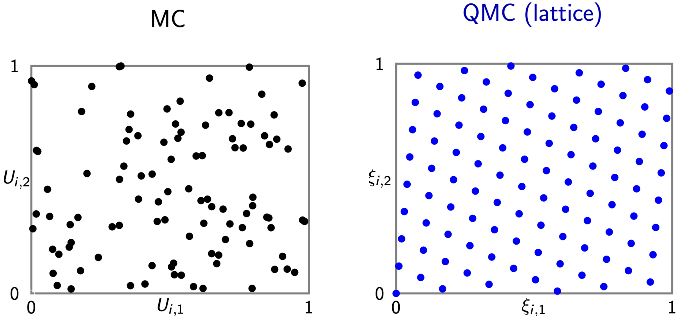
- Root mean-squared error: $\mathrm{RMSE}\left[\,\widehat{\mu}_n^{\mathrm{MC}}\,\right] = \frac{\psi}{\sqrt{n}}$

Review: Quasi-Monte Carlo (QMC)

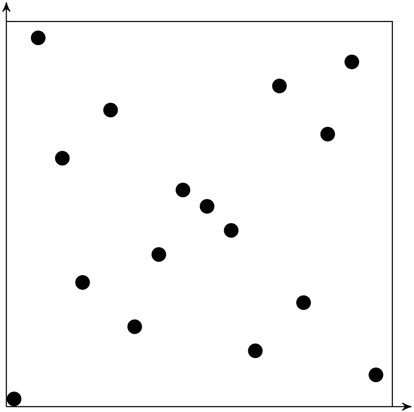
- QMC: **deterministic points** to estimate $\mu = \mathbb{E}[h(U)]$

$$\widehat{\mu}_n^{Q} = \frac{1}{n}\sum_{i=1}^{n} h(\xi_i)$$

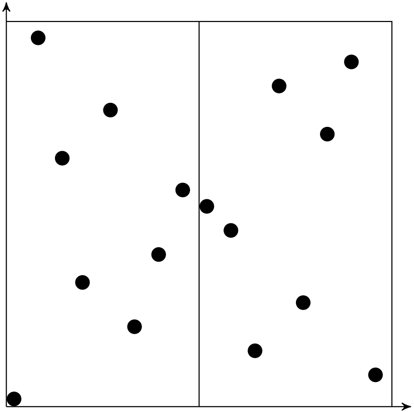
- **Low-discrepancy sequence** $\Xi = (\xi_i : i = 1, 2, \ldots)$
  - Ξ is deterministic and evenly fill $[0,1]^s$
  - **lattices** (e.g., Korobov, . . .), **Digital nets/sequences** (e.g., Sobel', Faure, . . .)



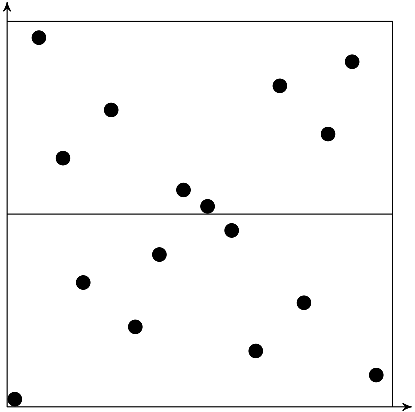
Example: 16 points of a Digital Net in base 2, in dimension $s = 2$



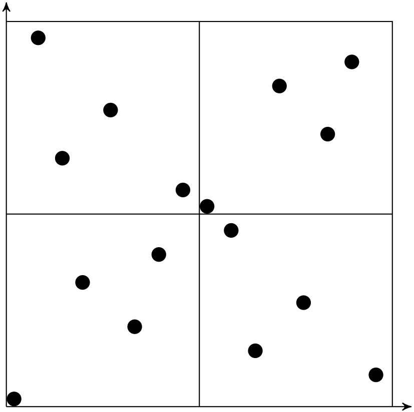
Example: 16 points of a Digital Net in base 2, in dimension $s = 2$



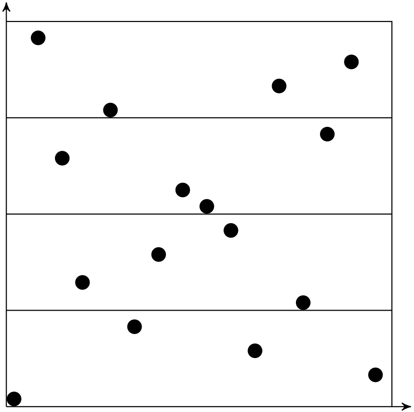
Example: 16 points of a Digital Net in base 2, in dimension $s = 2$



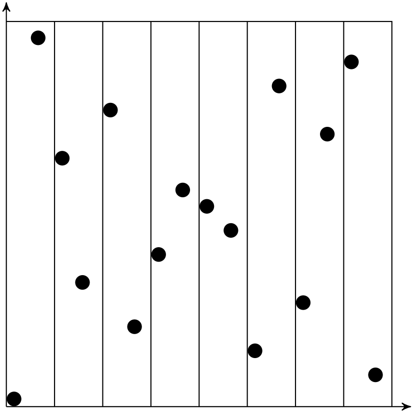
Example: 16 points of a Digital Net in base 2, in dimension $s = 2$



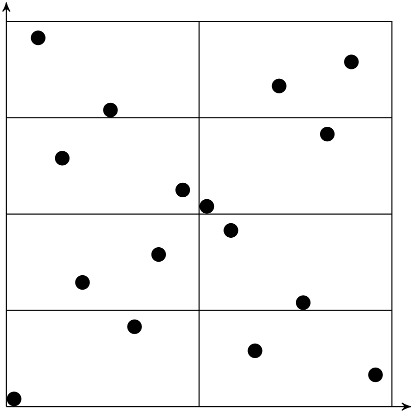
Example: 16 points of a Digital Net in base 2, in dimension $s = 2$



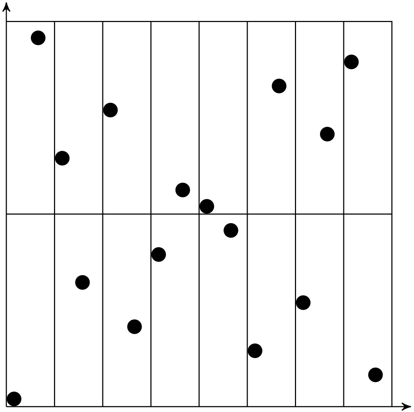
Example: 16 points of a Digital Net in base 2, in dimension $s = 2$



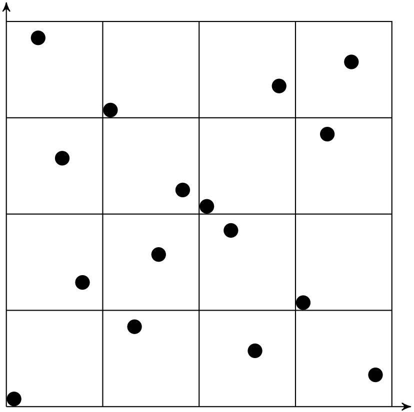
Example: 16 points of a Digital Net in base 2, in dimension $s = 2$



Example: 16 points of a Digital Net in base 2, in dimension $s = 2$



Example: 16 points of a Digital Net in base 2, in dimension $s = 2$



Review: QMC — Fast Convergence, But Error Estimation Difficult

- 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 $V_{\mathrm{HK}}(h) \in [0, \infty]$: "roughness" of h
  - Star-discrepancy $D_n^*(\Xi) \in [0, 1]$: 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 $\Theta(n^{-1/2})$

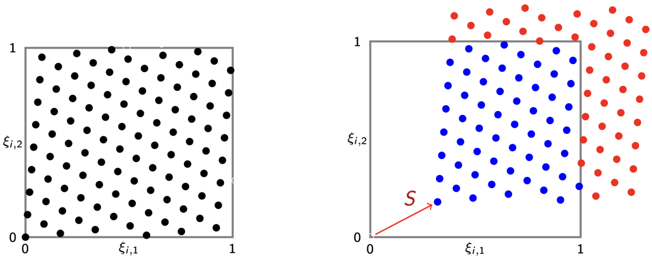
$$|\,\widehat{\mu}_n^{\mathrm{Q}} - \mu\,| \approx O\left(n^{-1}\right).$$

    - 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 $\mu = \mathbb{E}[h(U)]$

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

  - $X_{n,1}, X_{n,2}, \ldots, X_{n,r_n}$ i.i.d.: estimate $\sigma^2_{m_n} \equiv \text{Var}[X_{n,1}]$ typically $o(m_n^{-1})$ (even $O(m_n^{-2}(\ln m_n)^{2s})$ if BVHK) by

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

- Approx γ-level CI for μ

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

  - $X_{n,1}, X_{n,2}, \ldots, X_{n,r_n}$ i.i.d., but distn of each $X_{n,j}$ depends on n: Triangular array.

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, Munger, T. 2010]
- **Goal:** Sufficient conditions to ensure CLT and AVCI (as $n \to \infty$).

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, Munger, T. 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.

RQMC CLT

Theorem

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

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

under **either**

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

or

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

- $\sigma^2_{m_n} = \mathbb{E}[(X_{n,1}-\mu)^2]$ = variance of estimator $X_{n,1}$ from single randomization of m_n points.

RQMC Asymptotically Valid CI (AVCI)

- Recall **Lyapounov condition:**

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

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

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

Theorem

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

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

and **AVCI**

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

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

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

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

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

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

$$c < c_k(\alpha_*)$$

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

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

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

Corollaries Ensuring CLT or AVCI

Corollary

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

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

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

$$c < 1 \equiv c_3(\alpha_*),$$

and optimal $RMSE \approx \Theta(n^{-v_3(\alpha_*)})$ *as* $n \to \infty$ *with*

$$v_3(\alpha_*) \equiv \alpha_*.$$

If (1) *holds for* $b' = 2,$ *then* **AVCI** *holds for* $c < c_3(\alpha_*)$*, and RMSE rate exponent is* $v_3(\alpha_*)$.

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

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

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

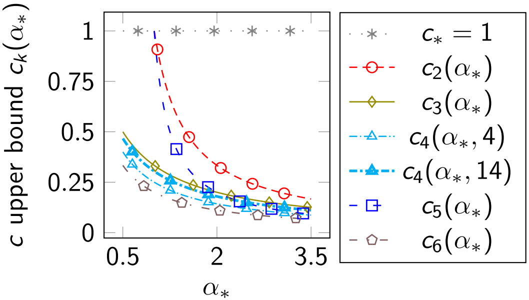
- **Assumption 1**: $(m_n, r_n) = (n^c, n^{1-c})$, $c \in (0,1)$
- Corollary k: $c < c_k(\alpha_*)$
- $\sigma_{m_n} \approx \Theta(\,m_n^{-\alpha_*}\,)$, $\alpha_* > 1/2$

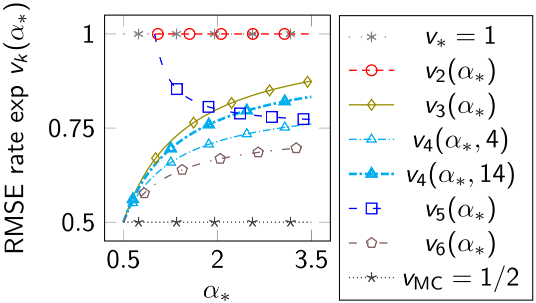
Corollaries CLT or AVCI: Tradeoffs

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 ($b>0$)	$\frac{1}{2\alpha_*(1+\frac{2}{b})+1}$	$\in \left(0, \frac{1}{2}\right)$	$\frac{2\alpha_*(1+\frac{1}{b})}{2\alpha_*(1+\frac{2}{b})+1}$	$> \frac{1}{2}$
5	**AVCI**	3.A (BVHK)	$\frac{1}{4\alpha_*-3}$	$>$	$\frac{3\alpha_*-2}{4\alpha_*-3}$	$>$
6	**AVCI**	3.C ($b=2$)	$\frac{1}{4\alpha_*+1}$	$\in \left(0, \frac{1}{3}\right)$	$\frac{3\alpha_*}{4\alpha_*+1}$	$> \frac{1}{2}$

- 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 $\approx \Theta(n^{-v_k(\alpha_*)})$.

Conditions Ensuring CLT or AVCI: Tradeoffs





- All $c_k(\alpha_*) \downarrow$ as $\alpha_* \uparrow$
  - Corollary k: $c < c_k(\alpha_*)$ in $(m_n, r_n) = (n^c, n^{1-c})$.
  - $\sigma_{m_n} \approx \Theta(m_n^{-\alpha_*})$, $\alpha_* > 1/2$ $(\geq 1$ 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.

Bootstrap

- *Percentile bootstrap*
  - From RQMC values $y_1, \ldots, y_R$, bootstrap values $y_1^*, \ldots, y_R^*$ sampled indep. (with replacement)
  - Take $\bar{y}^* = (1/R) \sum_{r=1}^{R} y_r^*$
  - Repeat this resampling B times independently, getting $\bar{y}^{*b}$ for $b = 1, \ldots, B$.
  - Sorting yields $\bar{y}^{*(1)} \leq \bar{y}^{*(2)} \leq \cdots \leq \bar{y}^{*(B)}$.
  - Confidence interval endpoints are quantiles

$$\left(\bar{y}^{*(\lfloor B\alpha/2 \rfloor)}, \bar{y}^{*(\lceil B(1-\alpha)/2 \rceil)}\right).$$

Bootstrap

- *Percentile bootstrap*
  - From RQMC values $y_1, \ldots, y_R$, bootstrap values $y_1^*, \ldots, y_R^*$ sampled indep. (with replacement)
  - Take $\bar{y}^* = (1/R)\sum_{r=1}^{R} y_r^*$
  - Repeat this resampling B times independently, getting $\bar{y}^{*b}$ for $b = 1, \ldots, B$.
  - Sorting yields $\bar{y}^{*(1)} \le \bar{y}^{*(2)} \le \cdots \le \bar{y}^{*(B)}$.
  - Confidence interval endpoints are quantiles

$$\left(\bar{y}^{*(\lfloor B\alpha/2 \rfloor)}, \bar{y}^{*(\lceil B(1-\alpha)/2 \rceil)}\right).$$

- *Bootstrap t*
  - Recommended (for RQMC) without much analysis (Owen 2023)
  - Reasoning: distribution of the t statistic $\sqrt{R}(\bar{y} - \mu)/S$ well approximated by the sample distribution of a bootstrapped t statistic $\sqrt{R}(\bar{y}^* - \bar{y})/S^*$ (S^* is the standard deviation of $y_1^*, \ldots, y_R^*$).
  - Take B independent bootstrap t values t^{*b} ($b = 1, \ldots, B$), sort them, and then let t_L^* and t_U^* be the $\alpha/2$ and $1 - \alpha/2$ quantiles of the t^{*b} values.
  - With B large enough, $\Pr\left(t_L^* \le \sqrt{R}\frac{\bar{y}^* - \bar{y}}{S^*} \le t_U^*\right) \approx 1 - \alpha$.
  - Then if we reason that $\Pr\left(t_L^* \le \sqrt{R}(\bar{y} - \mu)/S \le t_U^*\right) \approx 1 - \alpha$, we take

$$\left(n\bar{y} - St_U^* R^{-1/2}, \bar{y} - St_L^* R^{-1/2}\right).$$

Bootstrap t properties (Hall 88)

- Highly accurate for estimating the mean, asymptotically and for small sample sizes
- Coverage error $\mathcal{O}(1/R)$
- With γ skewness and κ kurtosis, coverage error

$$\begin{aligned}
\text{Normal theory:} \quad & (1/R)\varphi(z^{1-\alpha/2})\left[\ \ 0.14\kappa - 2.12\gamma^2 - 3.35\right] + \mathcal{O}(1/R^2),\\
\text{Percentile:} \quad & (1/R)\varphi(z^{1-\alpha/2})\left[-0.72\kappa - 0.37\gamma^2 - 3.35\right] + \mathcal{O}(1/R^2),\\
\text{Bootstrap } t\text{:} \quad & (1/R)\varphi(z^{1-\alpha/2})\left[-2.84\kappa + 4.25\gamma^2 \qquad\quad\right] + \mathcal{O}(1/R^2).
\end{aligned}$$

- The bootstrap t has an advantage in missing the -3.35 component that the others have.
- It has a large positive coefficient for γ^2 (extra coverage for skewed data) where the others have negative coefficients.
- The asymptotics predict that the bootstrap t will undercover when κ is large and $\gamma = 0$.
- For R different values y_r, one can show that $\Pr(S^* = 0) = R^{1-R}$, not negligible for $R = 5$ as we consider.

Selected functions and set of experiments

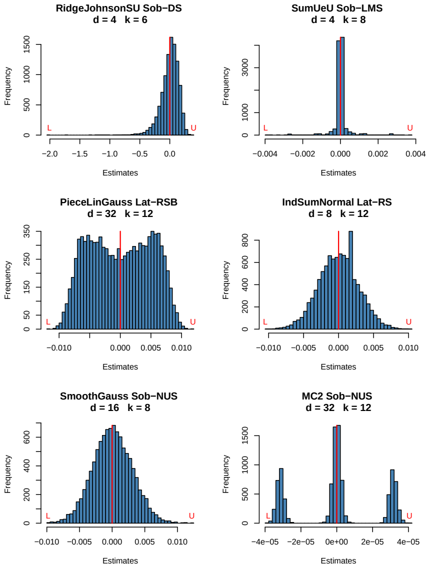
- Five types of RQMC point sets Lat-RS, Lat-RSB, Sob-DS, Sob-LMS, Sob-NUS
- Each with $n = 2^k$ points for $k = 6, 8, 10, 12, 14$, and in $d = 4, 8, 16, 32$ dimensions.
- Selected functions:
  1. SumUeU (smooth, additive): $f(\boldsymbol{u}) = -d + \sum_{j=1}^{d} u_j \exp(u_j)$.
  2. MC2 (smooth): $f(\boldsymbol{u}) = -1 + (d - 1/2)^d \prod_{j=1}^{d} (x_j - 1/2)$.
  3. PieceLinGauss (piecewise linear and continuous and Gaussian inputs): $f(\boldsymbol{u}) = \max\left(d^{-1/2} \sum_{j=1}^{d} \Phi^{-1}(u_j) - \tau, 0\right) - \varphi(\tau) + \tau\Phi(-\tau)$.
  4. IndSumNormal (discontinuous, infinite variation): $f(\boldsymbol{u}) = -\Phi(1) + \mathbb{I}\{d^{-1/2} \sum_{j=1}^{d} \Phi^{-1}(u_j) \geq 1\}$,
  5. SmoothGaus (smooth and bounded and monotone): $f(\boldsymbol{u}) = -\Phi(1/\sqrt{2}) + \Phi(1 + d^{-1/2} \sum_{j=1}^{d} \Phi^{-1}(u_j))$.
  6. RidgeJohnsonSU (heavy-tailed): $f(\boldsymbol{u}) = -\eta + F^{-1}(d^{-1/2} \sum_{j=1}^{s} u_j)$ where F is the CDF of the Johnson's SU distribution with skewness -5.66 and kurtosis 96.8 (for any d) making it heavy tailed.
- Bootstrap with $B = 1000$.

Results

- Experiments
  - 2400 tasks: 6 integrands, 5 RQMC methods, 4 dimensions, 5 RQMC sample sizes and 4 values of the replication size R (5, 10, 20, 30).
  - From each time 10^3 replicated confidence intervals at 95%, we judged any method that attained less than 92.7% coverage to have failed.
- Results
  - The percentile method failed 1698 (70.75%) of those tasks
    - ★ Not well suited to very small sample sizes
    - ★ Not well regarded for setting confidence intervals for the mean.
  - The bootstrap t method failed 81 times
    - ★ 74 for Sob-LMS on SumUeU (44 times) or MC2 (30 times); spiky histograms, see next slide
    - ★ Interval of infinite length if $S^* = 0$: 21 times for IndSumNormal with $R = 5$. Discrete distribution, fewer than 2^k different values.
  - The plain Student t confidence interval method failed only 3 times.
    - ★ Fails only when $R = 5$ (bootstrap t has coverage higher than 95% then)
    - ★ Coverage higher than 97% 81 times (SumUeU and MC2)...
    - ★ ... kurtosis of the RQMC points diverges to infinity as n increases.

(Pan & Owen 2023)

Histograms (mostly unusual ones)

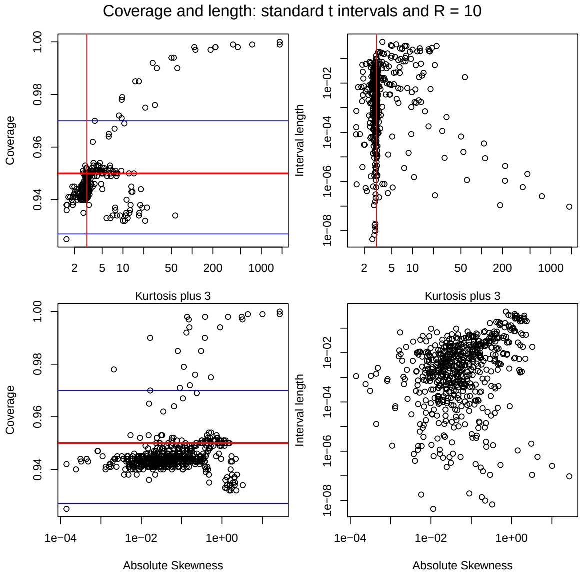


- RidgeJohnsonSU: negatively skewed (other RQMC methods too)
- SumUeU (and MC2): "spike plus outliers"

- PieceLinGauss: bimodal (often for LAT+baker)
- IndSumNormal: Gaussian plus a spike near one value

- SmoothGauss: roughly Gaussian, as most of those in the data set
- MC2 Sob-NUS: untypical for NUS (more frequent for LMS).

Coverage experiments (versus skewness and kurtosis, $R = 10$)



- Some examples high kurtosis, none with extreme skewness
- Standard CI known to have robust coverage in response to kurtosis but vulnerable to skewness.
- Kurtosis brings above nominal coverage for the standard t intervals
- interval length decreasing with extreme kurtosis (Sob-LMS with SumUeU and MC2)
- Small R: rare outliers, confidence intervals are extremely short and cover the true mean often enough.

Conclusions

- CLT for RQMC provided (but only sufficient conditions on the respective growth of RQMC points and number of randomizations)
- On comparison with bootstrap: Plain normal theory two-sided confidence intervals for RQMC performed best overall.
- Surprising as the bootstrap t method had much better coverage in the literature.
- Standard normal theory intervals known to underperform bootstrap t for one-sided intervals ($O(1/\sqrt{n})$ vs $O(1/n)$). Symmetry ubiquitous property of RQMC estimates, advantage disappears.

Thank you!

- M.K. Nakayama, B. Tuffin. Sufficient Conditions for Central Limit Theorems and Confidence Intervals for Randomized Quasi-Monte Carlo Methods. *ACM Transactions on Modeling and Computer Simulation*,Volume 34 Issue 3, 2024.
- P. L'Ecuyer, M. K Nakayama, A. B Owen, B. Tuffin. Confidence Intervals for Randomized Quasi-Monte Carlo Estimators. *Proceedings of the 2023 Winter Simulation Conference*, San Antonio, USA, December 2023.