Sufficient Conditions for a Central Limit Theorem to Assess the Error of Randomized Quasi-Monte Carlo Methods

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ABSTRACT

Randomized quasi-Monte Carlo (RQMC) can produce an estimator of a mean (i.e., integral) with root-mean-square error that shrinks at a faster rate than Monte Carlo's. While RQMC is often employed to provide a confidence interval (CI) for the mean, this approach implicitly assumes that the RQMC estimator obeys a central limit theorem (CLT), which has not been established for most RQMC settings. To address this, we provide various conditions that ensure an RQMC CLT, as well as an asymptotically valid CI, and examine the tradeoffs in our restrictions. Our sufficient conditions, depending on the regularity of the integrand, generally require that the number of randomizations grows sufficiently fast relative to the number of points used from the low-discrepancy sequence.

1 INTRODUCTION

Analyzing a stochastic model frequently involves computing the mean performance μ. Often, μ can be expressed as an integral of a function h over an s-dimensional unit hypercube $[0,1]^s$ for some fixed $s \geq 1$. Such integrals for $s > 1$ are typically analytically intractable, leading to the use of numerical methods, including simulation. As these techniques incur error, we should give a measure of the error.

Monte Carlo (MC) estimates μ via random sampling (Asmussen and Glynn 2007). Repeatedly feeding *independent and identically distributed* (i.i.d.) uniformly distributed random vectors on $[0,1]^s$ into integrand h produces i.i.d. outputs, which are averaged to yield the MC estimator. The method affords simple error estimation through a *confidence interval* (CI). Based on a *central limit theorem* (CLT), a CI uses the sample variance to provide a computable (probabilistic) measure of the MC error. But as the sample size n (i.e., number of evaluations of h) grows, the CI and the MC estimator's *root-mean-square error* (RMSE) shrink at a slow rate $n^{-1/2}$; adding another digit of precision requires a 100-fold increase in n.

To obtain a more efficient estimator, *quasi-Monte Carlo* (QMC) replaces the i.i.d. uniforms driving the MC method with n *deterministic* points from a low-discrepancy sequence (e.g., a lattice or digital net), designed to more evenly fill $[0,1]^s$ than a typical random sample; see Niederreiter (1992) and Lemieux (2009). When the integrand h has bounded Hardy-Krause variation, the Koksma-Hlawka inequality (e.g., Section 2.2 of Niederreiter 1992) shows that the QMC error decreases as $O(n^{-1}(\ln n)^s)$ as $n \to \infty$, better than the rate at which MC's RMSE shrinks. While theoretically useful, the Koksma-Hlawka inequality has limited practical value as its bound is not easily computed and is often quite loose.

Randomized QMC (RQMC) suggests a way to obtain a computable error bound: randomize the QMC points $r \geq 2$ i.i.d. times and build a CI from the sample variance of the resulting r i.i.d. estimators; e.g., see Tuffin (2004), Section 6.2 of Lemieux (2009), and L'Ecuyer (2018). For a given (large) computation budget of n integrand evaluations, we specify the number m of points used from each randomized sequence so that $mr \approx n$. To choose such an allocation (m, r), a common rule of thumb recommends taking r small (e.g., $10 \leq r \leq 30$) so that m is correspondingly large to benefit from QMC's superior convergence rate.

The RQMC CI's validity implicitly assumes that the RQMC estimator obeys a Gaussian CLT. When $m \to \infty$ and r is fixed, Loh (2003) establishes a CLT that covers only a computationally prohibitive form of RQMC, limiting its practical use. But more generally, a Gaussian limit is not guaranteed; e.g., randomly shifting a lattice leads to non-normal limits (as $m \to \infty$ for fixed r) (L'Ecuyer et al. 2010). Thus, while intuitively appealing, the CI lacks rigorous theoretical justification for most RQMC methods.

Our paper addresses these shortcomings. We provide sufficient conditions on both h and (m, r) that ensure the RQMC estimator obeys a CLT, as well as an *asymptotically valid CI* (AVCI). We focus on the setting where both $m, r \to \infty$ since a Gaussian limit may not hold for fixed r. We will show tradeoffs in our restrictions on h and (m, r): more stringent limitations on h lead to looser constraints on (m, r). But in all cases, the RQMC RMSE shrinks faster than for the corresponding MC estimator with sample size $n = mr$.

The rest of the paper unfolds as follows. Section 2 builds our study's basic framework. We present general conditions that yield a CLT and AVCI in Sections 3 and 4, respectively. Section 5 provides simpler sufficient conditions for a CLT or AVCI, and gives graphical comparisons of the alternative restrictions. Concluding remarks are in Section 6. All formal proofs appear in Nakayama and Tuffin (2021).

2 NOTATION AND FRAMEWORK

For an integrand $h : [0, 1]^s \to \mathfrak{R}$ on the unit hypercube of fixed dimension $s \geq 1$, the goal is to compute

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

where random vector $U \sim \mathscr{U}[0, 1]^s$ with $\mathscr{U}[0, 1]^s$ denoting a uniform distribution on $[0, 1]^s$, $\sim$ means "is distributed as", and $\mathbb{E}$ represents the expectation operator. We can think of h as a (complicated) simulation program that transforms s i.i.d. 1-dimensional uniform random numbers into observations from specified input distributions, which are then used to produce an output of the random performance of a stochastic system, so μ is its mean. We next explain how to apply MC, QMC, and RQMC to estimate μ.

2.1 Monte Carlo

With MC, we generate n i.i.d. copies $U_1, U_2, \ldots, U_n$ of $U \sim \mathscr{U}[0, 1]^s$, and compute $\widehat{\mu}_n^{\text{MC}} = \sum_{i=1}^n h(U_i)/n$ as the MC estimator of μ. Let $\psi^2 \equiv \text{Var}[h(U)]$, with $\text{Var}[\cdot]$ the variance operator, and assume that $0 < \psi^2 < \infty$. The MC estimator is unbiased (i.e., $\mathbb{E}[\widehat{\mu}_n^{\text{MC}}] = \mu$), as are all the estimators of μ that we consider, so

$$\text{RMSE}\left[\widehat{\mu}_n^{\text{MC}}\right] = \frac{\psi}{\sqrt{n}}. \tag{1}$$

The MC estimator obeys a Gaussian CLT $\sqrt{n}[\widehat{\mu}_n^{\text{MC}} - \mu]/\psi \Rightarrow \mathscr{N}(0, 1)$ as $n \to \infty$ (Billingsley 1995, Theorem 27.1), where $\Rightarrow$ denotes convergence in distribution, and $\mathscr{N}(a, b^2)$ is a normal random variable with mean a and variance b^2. Let $\widehat{\psi}_n^2 = \sum_{i=1}^n [h(U_i) - \widehat{\mu}_n^{\text{MC}}]^2/(n-1)$ be the sample variance of the i.i.d. $h(U_i)$. For a desired confidence level $0 < \gamma < 1$, we can exploit the CLT to construct an approximate γ-level CI for μ as $I_{n,\gamma}^{\text{MC}} \equiv [\widehat{\mu}_n^{\text{MC}} \pm z_\gamma \widehat{\psi}_n / \sqrt{n}]$, where the critical point z_γ satisfies $\Phi(z_\gamma) = 1 - (1 - \gamma)/2$ and Φ is the $\mathscr{N}(0, 1)$ *cumulative distribution function* (CDF). Providing a probabilistic measure of the MC estimator's error, $I_{n,\gamma}^{\text{MC}}$ is an AVCI in the sense that $\lim_{n \to \infty} P(\mu \in I_{n,\gamma}^{\text{MC}}) = \gamma$ (Asmussen and Glynn 2007, p. 71).

2.2 Quasi-Monte Carlo

QMC replaces MC's i.i.d. uniforms with carefully placed *deterministic* points from a *low-discrepancy sequence* $\Xi = (\xi_i)_{i \geq 1}$, such as a *digital net* (e.g., a Sobol' sequence) or *lattice*; see, e.g., Chapters 3–5 of Niederreiter (1992). Using the first n points from Ξ leads to QMC approximating μ by $\widehat{\mu}_n^{\text{Q}} = \sum_{i=1}^n h(\xi_i)/n$. We can bound the error $|\widehat{\mu}_n^{\text{Q}} - \mu|$ via the *Koksma-Hlawka inequality* (Niederreiter 1992, Section 2.2):

$$|\widehat{\mu}_n^{\text{Q}} - \mu| \leq V_{\text{HK}}(h) D_n^*(\Xi) \tag{2}$$

for all $n > 1$, where $D_n^*(\Xi)$ is the star-discrepancy of the first n points in Ξ, and $V_{\text{HK}}(h)$ is the Hardy-Krause variation of the integrand h. In (2), $V_{\text{HK}}(h) \geq 0$ quantifies the "roughness" of h, and $D_n^*(\Xi) \in [0,1]$ measures the "nonuniformity" of Ξ. Low-discrepancy sequences often have

$$D_n^*(\Xi) = O(n^{-1}(\ln n)^s), \quad \text{as } n \to \infty, \tag{3}$$

where $f(n) = O(g(n))$ (resp., $f(n) = \Theta(g(n))$) as $n \to \infty$ for functions f and g means that there exist positive constants a_0, a_1, and n_0 such that $|f(n)| \leq a_1|g(n)|$ (resp., $a_0|g(n)| \leq |f(n)| \leq a_1|g(n)|$) for all $n \geq n_0$. Thus, if $V_{\text{HK}}(h) < \infty$, (2) and (3) imply that the QMC error shrinks as $O(n^{-1}(\ln n)^s)$ as $n \to \infty$, better than the $\Theta(n^{-1/2})$ rate at which MC's RMSE decreases. While theoretically useful, the bound in (2) has limited practical value as it is not easily computed and is often quite loose. There are other related error bounds (e.g., Hickernell 1998; Hickernell 2018; Lemieux 2006; Niederreiter 1992), but all suffer from the same issues.

2.3 Randomized Quasi-Monte Carlo

RQMC applies i.i.d. randomizations of the QMC sequence Ξ to produce i.i.d. estimators of μ, and builds an approximate CI via their sample variance. A randomization creates from Ξ another sequence $\Xi' \equiv (U_i')_{i \geq 1}$ that retains the low-discrepancy properties of Ξ. Each $U_i' \sim \mathscr{U}[0,1]^s$, but the points in Ξ' are *dependent*. RQMC employs such a randomization $r \geq 1$ i.i.d. times, and for each $j = 1, \ldots, r$, let $\Xi_j' \equiv (U_{i,j}')_{i \geq 1}$ be the jth randomized sequence. Given a computation budget of n integrand evaluations, we specify the number m of points to use from each Ξ_j' so that $mr \approx n$, leading to the RQMC estimator of μ as

$$\widehat{\mu}_{m,r}^{\text{RQ}} = \frac{1}{r} \sum_{j=1}^{r} X_j, \quad \text{where} \quad X_j = \frac{1}{m} \sum_{i=1}^{m} h(U_{i,j}'). \tag{4}$$

The X_j, $j = 1, \ldots, r$, are i.i.d., and let $\widehat{\sigma}_{m,r}^2 = \sum_{j=1}^{r}(X_j - \widehat{\mu}_{m,r}^{\text{RQ}})^2/(r-1)$ be their sample variance when $r \geq 2$. We then arrive at a possible γ-level CI $I_{m,r,\gamma}^{\text{RQ}} \equiv [\widehat{\mu}_{m,r}^{\text{RQ}} \pm z_\gamma \widehat{\sigma}_{m,r}]$ for μ.

The literature includes several methods to construct Ξ', including *scrambled digital nets* (Owen 1995; Owen 1997) and *digital shifts* (L'Ecuyer 2018). To simplify the discussion, we describe only one approach: *random shifts* (Cranley and Patterson 1976). Here, randomization j generates a single $U_j \sim \mathscr{U}[0,1]^s$ and adds it (modulo 1) to each point in Ξ, so the ith point in the jth randomized sequence Ξ_j' is $U_{i,j}' = \langle U_j + \xi_i \rangle$, where $\langle x \rangle$ is the modulo-1 operator applied to each coordinate of $x \in \mathfrak{R}^s$. The U_j across randomizations $j = 1, 2, \ldots, r$, are independent. It is easy to show that each $U_{i,j}' \sim \mathscr{U}[0,1]^s$, so $\widehat{\mu}_{m,r}^{\text{RQ}}$ and each X_j are unbiased estimators of μ. But for each randomization j, the sequence Ξ_j' has *dependent* points because they all share the same uniform U_j.

With random shifts, each randomized sequence Ξ_j' satisfies (Tuffin 1997, Theorem 2)

$$D_m^*(\Xi_j') \leq 4^s D_m^*(\Xi). \tag{5}$$

Thus, if $V_{\text{HK}}(h) < \infty$, the estimator X_j in (4) from a single randomization of m points satisfies $\text{RMSE}[X_j] = O(m^{-1}(\log m)^s)$ as $m \to \infty$, an improvement over the $\Theta(m^{-1/2})$ rate in (1) for MC using the same number m of integrand evaluations. Even faster convergence rates can be achieved for special classes of functions and specific sequences Ξ called *lattice rules* (Tuffin 1998; L'Ecuyer and Lemieux 2000).

Although intuitively appealing, the CI $I_{m,r,\gamma}^{\text{RQ}}$ in general lacks theoretical justification, as it implicitly relies on $\widehat{\mu}_{m,r}^{\text{RQ}}$ obeying a Gaussian CLT. For $m \to \infty$ with $r \geq 1$ fixed, Loh (2003) establishes an RQMC CLT that covers solely the case of fully nested scrambling of a digital net, which is computationally prohibitive, limiting its adoption by practitioners. For random shifts of a lattice, the RQMC estimator $\widehat{\mu}_{m,r}^{\text{RQ}}$ may not obey a Gaussian CLT as $m \to \infty$ for fixed $r \geq 1$, as shown by L'Ecuyer et al. (2010). Indeed, they prove that for $r = 1$, the limiting error distribution has simple non-Gaussian forms for dimension $s = 1$, and $s > 1$ generally leads to non-Gaussian limits with no such easy characterizations, so the same holds for any fixed $r \geq 1$. Thus, we see the need for general Gaussian CLTs for RQMC, which is our aim.

2.4 Assumptions and Preliminary Results

We want to study the asymptotic behavior of the RQMC estimator in (4) as the computation budget n for the number of integrand evaluations grows large. To do this, we take the number $m \equiv m_n \geq 1$ of points from the randomized sequence and the number $r \equiv r_n \geq 1$ of randomizations to be functions of n satisfying

Assumption 1.A $m_n r_n \leq n$ for each $n \geq 1$, with $m_n \to \infty$, $r_n \to \infty$, and $m_n r_n / n \to 1$ as $n \to \infty$.

Under Assumption 1.A, the RQMC estimator in (4) becomes

$$\widehat{\mu}_{m_n, r_n}^{\mathrm{RQ}} = \frac{1}{r_n} \sum_{j=1}^{r_n} X_{n,j}, \quad \text{where} \quad X_{n,j} = \frac{1}{m_n} \sum_{i=1}^{m_n} h(U'_{i,j}), \tag{6}$$

so $X_{n,j}$ averages h on the first m_n points of the jth randomized sequence. Our goal is to provide conditions on h and (m_n, r_n) that yield (as $n \to \infty$) a Gaussian CLT (Section 3) or AVCI (Section 4). Other papers (e.g., Glynn 1987; Damerdji 1994) adopt frameworks akin to Assumption 1.A to study MC methods for analyzing steady-state behavior via multiple replications or batching.

Assumption 1.A requires $r_n \to \infty$ because otherwise, the limiting error distribution may not be Gaussian, as noted at the end of Section 2.3. We simplify the discussion by further having $m_n \to \infty$ in Assumption 1.A, but this is not necessary; Nakayama and Tuffin (2021) also analyze the special case that $m_n \equiv m_0$ for a fixed $m_0 \geq 1$. Section 5 will adopt the following specialization of Assumption 1.A.

Assumption 1.B $m_n = n^c$ and $r_n = n^{1-c}$ with $c \in (0, 1)$.

We should define, e.g., $m_n = \lfloor n^c \rfloor$ and $r_n = \lfloor n^{1-c} \rfloor$ ($\lfloor \cdot \rfloor$ is the floor function) so that m_n and r_n are integers, but for simplicity, we ignore this technicality. Section 5 will determine constraints on h and $c \in (0, 1)$ that secure a CLT or AVCI, and in each case, the optimal such c that minimizes the rate at which $\mathrm{RMSE}[\widehat{\mu}_{m_n, r_n}^{\mathrm{RQ}}]$ shrinks as $n \to \infty$. Also, we will examine the tradeoffs in the conditions on h and c.

For a randomized sequence Ξ' constructed from scrambling or a digital shift of a digital net, or for a randomly shifted lattice rule, the randomization preserves the partitioning structure of the original sequence Ξ: a randomly shifted lattice is still a lattice, and scrambling or digitally shifting a digital net retains the original sequence's finer-grain properties (Owen 1995; Owen 1997; L'Ecuyer 2018). Moreover, these Ξ' obey similar discrepancy bounds as Ξ. Specifically, consider any low-discrepancy sequence Ξ for which (3) holds, so there exists some constant $0 < w_0 < \infty$ such that $D_m^*(\Xi) \leq w_0 m^{-1}(\ln m)^s$ for all $m > 1$. Then its random shift Ξ' satisfies $D_m^*(\Xi') \leq w_0' m^{-1}(\ln m)^s$ with $w_0' = 4^s w_0$ by (5), and scrambling or digital shifting digital nets yields analogous bounds. Thus, all of these randomizations fulfill the following assumption, which we use to analyze RQMC estimators when $V_{\mathrm{HK}}(h) < \infty$.

Assumption 2 For the RQMC method used, there exists a constant $0 < w_0' < \infty$ such that each randomized sequence Ξ' satisfies $D_m^*(\Xi') \leq w_0' m^{-1}(\ln m)^s$ for all $m > 1$, where w_0' depends on the RQMC method but not on the randomization's realization (e.g., of $U \sim \mathscr{U}[0, 1]^s$ in a random shift).

We often will further impose one of the following conditions on the integrand h. The conditions are presented in order of decreasing strength (see Proposition 1 below), and Section 5 will show that this leads to corresponding tradeoffs in our conditions on (m_n, r_n) to ensure a CLT or AVCI.

Assumption 3.A The integrand h is of bounded Hardy-Krause variation, i.e., $V_{\mathrm{HK}}(h) < \infty$.

Assumption 3.B The integrand h is bounded; i.e., $|h(u)| \leq t_0$ for all $u \in [0, 1]^s$ for some constant $t_0 < \infty$.

Assumption 3.C There exists $b > 0$ such that $\mathbb{E}\left[|h(U) - \mu|^{2+b}\right] < \infty$, where $U \sim \mathscr{U}[0, 1]^s$.

Limiting the roughness of h over $[0, 1]^s$, Assumption 3.A imposes substantial restrictions; it does not hold, e.g., in dimension $s \geq 2$ when h is an indicator function (so μ is a probability) with discontinuities not lining up with the coordinate axes (Owen and Rudolf 2020). In contrast, Assumption 3.C constrains the heaviness of the tails of the distribution of $h(U)$.

Proposition 1 Assumption 3.A is strictly stronger than Assumption 3.B, itself strictly stronger than Assumption 3.C.

Using different conditions on h, we next derive two bounds on absolute central moments of the estimator $X_{n,1}$ in (6) from a single randomization. The first lemma, for $V_{HK}(h) < \infty$ (Assumption 3.A), follows from Theorem 2 of Tuffin (1997); the second applies Minkowski's inequality (Billingsley 1995, eq. (5.40)) when Assumption 3.C holds for $2+b$ replaced by $q \geq 1$.

Lemma 1 Under Assumptions 1.A, 2, and 3.A, for any $q > 0$ and for all n such that $m_n > 1$,

$$\eta_{n,q} \equiv \mathbb{E}\left[|X_{n,1} - \mu|^q\right] \leq \mathbb{E}\left[(V_{HK}(h)D^*_{m_n}(\Xi'))^q\right] \leq \left(\frac{w'_0 V_{HK}(h)(\ln m_n)^s}{m_n}\right)^q < \infty. \tag{7}$$

Lemma 2 Under Assumption 1.A, for any $q \geq 1$, if $\mathbb{E}[|h(U) - \mu|^q] < \infty$ for $U \sim \mathscr{U}[0,1]^s$, then $\eta_{n,q} \leq \mathbb{E}[|h(U) - \mu|^q]$ for every n.

For a single randomization of m points, RQMC typically has $\sigma_m \equiv (\text{Var}[\sum_{i=1}^m h(U'_{i,1})/m])^{1/2} = O(m^{-\alpha})$ as $m \to \infty$ with $\alpha > 1/2$ (e.g., see (7) when $V_{HK}(h) < \infty$). This improves on MC's RMSE convergence rate, which satisfies $\text{RMSE}[\widehat{\mu}_m^{MC}] = \sqrt{\text{Var}[\widehat{\mu}_m^{MC}]} = \psi m^{-1/2}$ by (1). Assume the following limit exists:

$$\alpha_* = -\lim_{m \to \infty} \frac{\ln(\sigma_m)}{\ln(m)}, \tag{8}$$

so α_* is the constant such that σ_m decreases, as $m \to \infty$, at a rate (ignoring leading coefficients and lower-order terms) strictly faster than $m^{-\alpha_*+\varepsilon}$ and strictly slower than $m^{-\alpha_*-\varepsilon}$ for every $\varepsilon > 0$; i.e., $\sigma_m = o(m^{-\alpha_*+\varepsilon})$ and $\sigma_m = \omega(m^{-\alpha_*-\varepsilon})$ as $m \to \infty$ for any $\varepsilon > 0$, where $f(m) = o(g(m))$ as $m \to \infty$ means that $f(m)/g(m) \to 0$ as $m \to \infty$, and $f(m) = \omega(g(m))$ as $m \to \infty$ means that $f(m)/g(m) \to \infty$ as $n \to \infty$. By (7),

$$\alpha_* \geq 1 \quad \text{when } V_{HK}(h) < \infty, \tag{9}$$

as in Assumption 3.A, and more generally, as is typical of RQMC, we assume that

$$\alpha_* > \frac{1}{2}. \tag{10}$$

The value of α_* depends on the particular integrand h and the RQMC method applied, but not on how (m_n, r_n) or c are specified in Assumptions 1.A and 1.B.

For any randomized sequence $\Xi' = (U'_i)_{i \geq 1}$, let $E_m(\Xi') = \frac{1}{m}\sum_{i=1}^m h(U'_i) - \mu$ be the error of the estimator based on the first m points. Then define its exponential rate as

$$\alpha(\Xi') = -\lim_{m \to \infty} \frac{\ln(|E_m(\Xi')|)}{\ln(m)}, \tag{11}$$

assuming the limit always exists, and define the worst-case rate among all randomizations as

$$\alpha' = \inf_{\Xi'} \alpha(\Xi'). \tag{12}$$

Thus, for any randomized sequence Ξ', we see that $|E_m(\Xi')| = o(m^{-\alpha+\varepsilon})$ and $|E_m(\Xi')| = \omega(m^{-\alpha-\varepsilon})$ as $m \to \infty$ for each $\varepsilon > 0$, and $\alpha' \leq \alpha_*$ always holds.

Assumption 4 The convergence rate exponent α' of the worst-case error among all randomizations is the same as the standard deviation rate exponent α_*; i.e., $\alpha' = \alpha_*$.

Corollary 1 in Section 5.1 will later show that when Assumption 4 holds, the RQMC estimator $\widehat{\mu}_{m_n,r_n}^{RQ}$ will obey a CLT for $(m_n, r_n) = (n^c, n^{1-c})$ for *any* $c \in (0,1)$ (Assumption 1.B). However, establishing Assumption 4 in practice may be difficult, so much of our paper focuses on providing other more verifiable sufficient conditions that secure a CLT.

For a given total number n of integrand evaluations, RQMC papers often suggest choosing m_n as large as possible to gain from the fast convergence rate of QMC. But as noted at the end of Section 2.3, we still should specify r_n big enough to ensure a Gaussian CLT. Under Assumptions 1.B, 2 and 3.A, (7) implies

$$\text{RMSE}[\widehat{\mu}^{\text{RQ}}_{m_n,r_n}] \leq \frac{[w'_0 V_{\text{HK}}(h)(\ln m_n)^s/m_n]}{\sqrt{r_n}} = \Theta\left(\frac{(c\ln n)^s}{n^{(1+c)/2}}\right),$$

so larger c leads to faster convergence. While $c = 1$ minimizes the RMSE bound, a Gaussian CLT may not be guaranteed, as noted earlier at the end of Section 2.3.

3   GENERAL CONDITIONS FOR A CENTRAL LIMIT THEOREM

We next study limiting properties of $\widehat{\mu}^{\text{RQ}}_{m_n,r_n}$ in (6) as $n \to \infty$. The estimator averages $X_{n,1}, X_{n,2}, \ldots, X_{n,r_n}$, but their distribution changes with n, complicating the asymptotic analysis. To develop a theoretical framework for handling this under Assumption 1.A, note that $(X_{n,j})_{n=1,2,\ldots;j=1,2,\ldots,r_n}$ forms a *triangular array* (Billingsley 1995, p. 359), also called a *double array*. In a triangular array, the r_n variables within a row n are independent, but there may be dependence across rows. While the general formulation allows for the CDFs of the r_n variables within a row n to differ, RQMC actually has

$$X_{n,1}, X_{n,2}, \ldots, X_{n,r_n} \text{ are i.i.d., each with some distribution } F_n, \tag{13}$$

where F_n may change with n, as occurs in (6). To preclude trivialities, we impose another assumption, without which the exact result is eventually always returned by the RQMC estimator.

Assumption 5 $\sigma^2_{m_n} \equiv \text{Var}[X_{n,1}] > 0$ for all sufficiently large n.

The Lindeberg and Lyapounov CLTs (Billingsley 1995, Theorems 27.2 and 27.3) apply for the RQMC structure in (13). To set them up, write the variance of the sum of the r_n random variables in (13) as $s^2_n \equiv r_n \sigma^2_{m_n}$. Denote the CDF of $X_{n,j} - \mu$ by G_n, which does not depend on j by (13). Note that $\sigma^2_{m_n} = \int_{y \in \Re} y^2 \, dG_n(y)$, and let $\tau^2_n(t) = \int_{|y|>ts_n} y^2 \, dG_n(y)$ for $t > 0$. Then the RQMC estimator in (6) satisfies the following.

Theorem 1 If Assumptions 1.A and 5 hold and also the *Lindeberg condition*

$$\frac{\tau^2_n(t)}{\sigma^2_{m_n}} \to 0, \quad \text{as } n \to \infty, \ \forall t > 0, \tag{14}$$

then the RQMC estimator in (6) satisfies the CLT

$$\frac{\widehat{\mu}^{\text{RQ}}_{m_n,r_n} - \mu}{\sigma_{m_n}/\sqrt{r_n}} \Rightarrow \mathcal{N}(0,1), \quad \text{as } n \to \infty. \tag{15}$$

Also, (14) holds if, for some $b > 0$, $\mathbb{E}\left[|X_{n,1} - \mu|^{2+b}\right] < \infty$ for each n and the *Lyapounov condition* holds:

$$\frac{\mathbb{E}\left[|X_{n,1} - \mu|^{2+b}\right]}{r_n^{b/2} \sigma^{2+b}_{m_n}} \to 0, \quad \text{as } n \to \infty. \tag{16}$$

The Lindeberg condition (14) constrains the tail behavior of G_n. In the general setting of independent but not identically distributed $X_{n,j}$, $1 \leq j \leq r_n$, the analogous version of (14) (Billingsley 1995, eq. (27.8)) ensures that the contribution of any single $X_{n,j}$ to their sum's variance s^2_n is negligible for large n. We can show (Billingsley 1995, p. 361) that (14) is even necessary for the CLT (15) when (13) holds. Imposing restrictions on moments rather than tail properties, the Lyapounov condition (16) can sometimes be easier to apply than the Lindeberg condition (14). Section 5.1 will obtain sufficient conditions for (14) or (16) under Assumption 1.B to secure Theorem 1 for each of our Assumptions 3.A–3.C on the integrand h.

4   ASYMPTOTICALLY VALID CONFIDENCE INTERVAL

To build a CI from the CLT (15), suppose that $r_n \geq 2$, which Assumption 1.A ensures for all n large enough. As $X_{n,j}$, $j = 1, 2, \ldots, r_n$, are i.i.d. by (13), their sample variance $\widehat{\sigma}^2_{m_n, r_n} = \sum_{j=1}^{r_n} \left(X_{n,j} - \widehat{\mu}^{RQ}_{m_n, r_n} \right)^2 / (r_n - 1)$ provides an unbiased estimator of $\sigma^2_{m_n} = \text{Var}[X_{n,1}]$. For a given desired confidence level $\gamma \in (0,1)$, we get

$$I^{RQ}_{m_n, r_n, \gamma} \equiv \left[\widehat{\mu}^{RQ}_{m_n, r_n} \pm z_\gamma \widehat{\sigma}_{m_n, r_n} / \sqrt{r_n} \right] \tag{17}$$

as the RQMC CI for μ. The next result imposes conditions guaranteeing that $I^{RQ}_{m_n, r_n, \gamma}$ is an AVCI in the sense that (20) below holds.

Theorem 2 Suppose that Assumptions 1.A and 5 hold. Also, suppose that $\mathbb{E}\left[(X_{n,1} - \mu)^4 \right] < \infty$ and that

$$\frac{\mathbb{E}\left[(X_{n,1} - \mu)^4 \right]}{r_n \sigma^4_{m_n}} \to 0, \quad \text{as } n \to \infty. \tag{18}$$

Then

$$\frac{\widehat{\mu}^{RQ}_{m_n, r_n} - \mu}{\widehat{\sigma}_{m_n, r_n} / \sqrt{r_n}} \Rightarrow \mathcal{N}(0,1), \quad \text{as } n \to \infty, \tag{19}$$

and

$$\lim_{n \to \infty} P(\mu \in I^{RQ}_{m_n, r_n, \gamma}) = \gamma. \tag{20}$$

As (18) is the same as (16) for $b = 2$, Theorem 1 implies CLT (15), which is expressed in terms of the exact σ_{m_n}. But the left side of (19) instead uses the estimator $\widehat{\sigma}_{m_n, r_n}$. Theorem 2's conditions further ensure $\widehat{\sigma}_{m_n, r_n} / \sigma_{m_n} \Rightarrow 1$ as $n \to \infty$, so Slutsky's theorem (Billingsley 1995, p. 340) verifies (19), securing AVCI (20). Section 5.1 will provide sufficient conditions under Assumption 1.B that yield Theorem 2 for two of our conditions on the integrand h (Assumptions 3.A and 3.C).

5   ANALYSIS WHEN $(m_n, r_n) = (n^c, n^{1-c})$ (ASSUMPTION 1.B)

Assumption 1.B specializes Assumption 1.A by taking $(m_n, r_n) = (n^c, n^{1-c})$ for some $c \in (0,1)$. We next will determine the values of c that imply CLT (15) through Theorem 1 or that guarantee AVCI (20) via Theorem 2. For those c, we then find the ones leading to $\text{RMSE}[\widehat{\mu}^{RQ}_{m_n, r_n}]$ shrinking fastest as $n \to \infty$.

Under Assumption 1.B, we have that $m_n = n^c$ with $c \in (0,1)$, so (8) implies that

$$\sigma_{m_n} = \omega\left(n^{-c\alpha_* - \varepsilon} \right) \quad \text{and} \quad \sigma_{m_n} = o\left(n^{-c\alpha_* + \varepsilon} \right) \quad \text{as } n \to \infty, \text{ for all } \varepsilon > 0. \tag{21}$$

Taking $\varepsilon > 0$ arbitrarily small in (21) leads to $\sigma_{m_n} \approx \Theta(n^{-c\alpha_*})$ as $n \to \infty$. Thus, a combination of $r_n = n^{1-c}$ with (6) and (13) yields, for any $c \in (0,1)$,

$$\text{RMSE}\left[\widehat{\mu}^{RQ}_{m_n, r_n} \right] = \frac{\sigma_{m_n}}{\sqrt{r_n}} \approx \Theta\left(n^{-v(\alpha_*, c)} \right) \quad \text{as } n \to \infty, \quad \text{where } v(\alpha_*, c) \equiv c\left[\alpha_* - \frac{1}{2} \right] + \frac{1}{2}. \tag{22}$$

Our assumption (10) guarantees that $v(\alpha_*, c) > 1/2$ for $c \in (0,1)$. Hence, the convergence rate of RQMC's RMSE for *any* c in Assumption 1.B is better than $\text{RMSE}[\widehat{\mu}^{MC}_n] = \Theta(n^{-v_{MC}})$ as $n \to \infty$ for MC, where

$$v_{MC} \equiv \frac{1}{2} \tag{23}$$

by (1). For any fixed α_* satisfying (10), $v(\alpha_*, c)$ strictly increases in c by (22), so RQMC's RMSE shrinks faster for larger c. We thus want to determine how large c can be and still ensure CLT (15) or AVCI (20).

Section 5.1 will provide various corollaries of the CLT and AVCI theorem in Sections 3 and 4. Each such Corollary k will result in restricting c as

$$c < c_k(\alpha_*) \tag{24}$$

for some $0 < c_k(\alpha_*) \leq 1$ depending on the particular Corollary k. As we will see, most of the $c_k(\alpha_*)$ are strictly decreasing in α_*. Thus, as α_* increases, (24) further restricts the choices of c, thereby reducing the maximum allowable number of QMC points and increasing the minimum number of randomizations because $(m_n, r_n) = (n^c, n^{1-c})$. But by (8), larger α_* corresponds to a better convergence rate for the estimator based on a single randomization, so in some sense, securing a CLT or AVCI often entails hampering better QMC performance.

Because (22) implies that larger c leads to RMSE shrinking at a faster rate, the "optimal" c that maximizes the rate subject to the constraint (24) is $c = c_k(\alpha_*) - \delta$ for infinitesimally small $\delta > 0$. Accordingly, an analysis akin to the arguments applied to achieve (22) arrives at the optimal approximate rate:

$$\text{RMSE}[\widehat{\mu}_{m_n,r_n}^{\text{RQ}}] \approx \Theta\left(n^{-v_k(\alpha_*)}\right) \quad \text{as } n \to \infty, \tag{25}$$

where, for each Corollary k (and k') in Section 5.1, the exponent $v_k(\alpha_*)$ appears below in (26).

Proposition 2 Under Assumption 1.B and (10), the optimal approximate RMSE rate exponent in (25) is

$$v_k(\alpha_*) \equiv c_k(\alpha_*)\left(\alpha_* - \frac{1}{2}\right) + \frac{1}{2} > v_{\text{MC}} \tag{26}$$

for v_{MC} in (23), so RQMC outdoes MC. If $c_k(\alpha_*) = 1$ in (24), then $v_k(\alpha_*) = \alpha_*$. Also, for any k and k',

$$v_k(\alpha_*) > v_{k'}(\alpha_*) \quad \text{if and only if} \quad c_k(\alpha_*) > c_{k'}(\alpha_*). \tag{27}$$

When $c_k(\alpha_*) = 1$, (24) becomes the weakest possible constraint satisfying Assumption 1.B. In this case, Proposition 2 implies that $v_k(\alpha_*) = \alpha_*$, so the RMSE of the multiple-randomization RQMC estimator $\widehat{\mu}_{m_n,r_n}^{\text{RQ}}$ decreases at about the same rate as for a single randomization with full length $m = n$.

The next subsection will specialize $c_k(\alpha_*)$ in (24) and $v_k(\alpha_*)$ in (26) for various corollaries. Section 5.2 will compare the resulting values graphically.

5.1 Corollaries of Theorems 1 and 2

We first provide a corollary of Theorem 1 based on Assumption 4, which imposes constraints on both the integrand and RQMC sequence.

Corollary 1 Suppose that Assumptions 1.B, 4, and 5 hold. If $c < 1 \equiv c_1(\alpha_*)$, then the Lindeberg condition (14) and CLT (15) hold. Moreover, (25) and (26) have $v_k(\alpha_*) = v_1(\alpha_*) \equiv \alpha_*$.

Under Assumption 4 (the worst-case error and the standard deviation decrease at the same exponential rate), Corollary 1 secures a CLT for $(m_n, r_n) = (n^{1-\varepsilon}, n^{\varepsilon})$ with $\varepsilon > 0$ as small as we wish. Thus, although $r_n \to \infty$ is needed, choosing $\varepsilon > 0$ small allows taking a large number $m_n = n^{1-\varepsilon}$ of points from the low-discrepancy sequence, which enables exploiting QMC's superior convergence rates.

As establishing Assumption 4 may be difficult in practice, we next provide other conditions that are more readily verifiable to ensure CLT (15). We give corollaries corresponding to each of our restrictions on the integrand h in Assumptions 3.A–3.C, which are in decreasing order of strength (Proposition 1). We first specialize (16) of Theorem 1 to establish a CLT when $V_{\text{HK}}(h) < \infty$, which enables using Lemma 1.

Corollary 2 Suppose that Assumptions 1.B, 2, 3.A ($V_{\text{HK}}(h) < \infty$), and 5 hold. Also, suppose that for some constant $\lambda \in (0,1)$,

$$c < \frac{1-\lambda}{2\alpha_* - 1 - \lambda} \equiv c_2(\alpha_*), \tag{28}$$

where λ may be chosen arbitrarily small. Then the Lyapounov condition (16) and CLT (15) hold. Moreover, for each $\alpha_* \geq 1$, as in (9), $c_2(\alpha_*)$ satisfies $0 < c_2(\alpha_*) \leq 1$, and (25) and (26) have $v_k(\alpha_*) = v_2(\alpha_*)$ with

$$v_2(\alpha_*) \equiv \frac{2\alpha_* - 1 - \lambda\alpha_*}{2\alpha_* - 1 - \lambda}, \quad \text{where} \quad \frac{1}{2} < v_2(\alpha_*) \leq 1. \tag{29}$$

Corollary 2 allows taking $\lambda \in (0,1)$ as arbitrarily small in (28) and (29), so $c_2(\alpha_*) \approx 1/(2\alpha_* - 1)$ and $v_2(\alpha_*) \approx 1$. The next corollary of Theorem 1 exploits (14) to yield a CLT when the integrand h is bounded.

Corollary 3 Suppose that Assumptions 1.B, 3.B (h is bounded), and 5 hold. If

$$c < \frac{1}{2\alpha_* + 1} \equiv c_3(\alpha_*),$$

then the Lindeberg condition (14) and CLT (15) hold. Moreover, for each $\alpha_* > 1/2$, as in (10), $c_3(\alpha_*)$ satisfies $0 < c_3(\alpha_*) < 1/2$, and (25) and (26) have $v_k(\alpha_*) = v_3(\alpha_*)$ with

$$v_3(\alpha_*) \equiv \frac{2\alpha_*}{2\alpha_* + 1}, \quad \text{where} \quad \frac{1}{2} < v_3(\alpha_*) < 1.$$

The following corollary of Theorem 1 imposes a moment condition on $h(U)$ (Assumption 3.C) to apply Lemma 2 to (16) to obtain a CLT, in contrast to requiring $V_{\mathrm{HK}}(h) < \infty$, as in Corollary 2.

Corollary 4 Suppose that Assumptions 1.B, 3.C (finite absolute central moment of order $2+b$ for some $b > 0$), and 5 hold. If

$$c < \frac{1}{2\alpha_*(1 + \frac{2}{b}) + 1} \equiv c_4(\alpha_*, b),$$

then the Lyapounov condition (16) and CLT (15) hold. Moreover, for each $b > 0$ and $\alpha_* > 1/2$, as in (10), $c_4(\alpha_*, b)$ satisfies $0 < c_4(\alpha_*, b) < 1/2$, and (25) and (26) have $v_k(\alpha_*) = v_4(\alpha_*, b)$ with

$$v_4(\alpha_*, b) \equiv \frac{2\alpha_*(1 + \frac{1}{b})}{2\alpha_*(1 + \frac{2}{b}) + 1}, \quad \text{where} \quad \frac{1}{2} < v_4(\alpha_*, b) < 1.$$

For $I_{m_n, r_n, \gamma}^{\mathrm{RQ}}$ in (17) to be AVCI (20), Theorem 2 assumes that (18) holds, which yields the CLTs in (15) and (19). We next consider conditions that enable verifying AVCI.

Corollary 5 Suppose that Assumptions 1.B, 2, 3.A ($V_{\mathrm{HK}}(h) < \infty$), and 5 hold. If

$$c < \frac{1}{4\alpha_* - 3} \equiv c_5(\alpha_*),$$

then the CLT (19) and AVCI (20) hold. Moreover, for each $\alpha_* \geq 1$, as in (9), $c_5(\alpha_*)$ satisfies $0 < c_5(\alpha_*) \leq 1$, and (25) and (26) have $v_k(\alpha_*) = v_5(\alpha_*)$ with

$$v_5(\alpha_*) \equiv \frac{3\alpha_* - 2}{4\alpha_* - 3}, \quad \text{where} \quad \frac{3}{4} < v_5(\alpha_*) \leq 1.$$

While Corollary 5 requires $V_{\mathrm{HK}}(h) < \infty$, we next ensure AVCI instead through a moment condition.

Corollary 6 Suppose that Assumptions 1.B and 5 hold, as well as Assumption 3.C (finite absolute central moment of order $2+b$) for $b = 2$. If

$$c < \frac{1}{4\alpha_* + 1} \equiv c_6(\alpha_*),$$

then the CLT (19) and AVCI (20) hold. Moreover, for each $\alpha_* > 1/2$, as in (10), $c_6(\alpha_*)$ satisfies $0 < c_6(\alpha_*) < 1/2$, and (25) and (26) have $v_k(\alpha_*) = v_6(\alpha_*)$ with

$$v_6(\alpha_*) \equiv c_6(\alpha_*)\left(\alpha_* - \frac{1}{2}\right) + \frac{1}{2} = \frac{3\alpha_*}{4\alpha_* + 1}, \quad \text{where} \quad \frac{1}{2} < v_6(\alpha_*) < \frac{3}{4}.$$
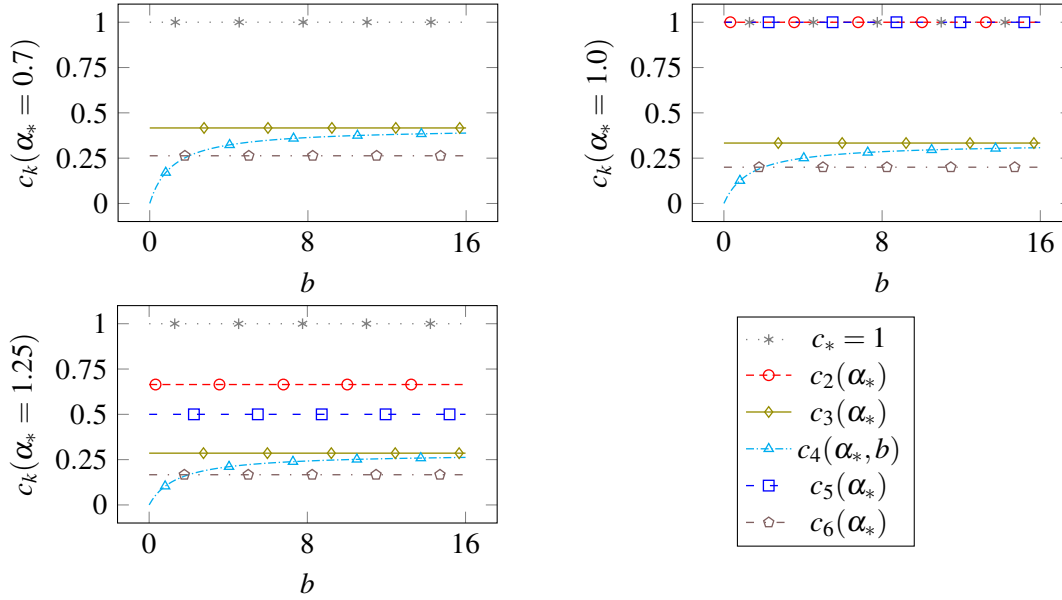
Figure 1: Plots of the upper bounds $c_k(\alpha_*)$ in (24) of c in Assumption 1.B for different Corollaries k from Section 5.1. The plots display the $c_k(\alpha_*)$ as functions of b for different fixed values of α_*. The upper left panel does not include $c_2(\alpha_*)$ and $c_5(\alpha_*)$ as these require $V_{\mathrm{HK}}(h) < \infty$, which then implies $\alpha_* \geq 1$ by (9). The plots show that stronger conditions on h correspond to loosening constraints on c.

5.2 Graphical Comparisons of the $c_k(\alpha_*)$ and the $v_k(\alpha_*)$

For the Corollaries $k = 2, 3, \ldots, 6$ in Section 5.1, we next plot their upper bounds $c_k(\alpha_*)$ for c as functions of b (from Assumption 3.C) in Figure 1 for various fixed values of $\alpha_* > 1/2$, as assumed in (10). (Our discussions omit $k = 1$ as its Assumption 4 may be difficult to verify in practice; note nevertheless that $c_1(\alpha_*) \geq c_k(\alpha_*)$ and $v_1(\alpha_*) = \alpha_* \geq v_k(\alpha_*) \forall k \geq 2$.) Figure 2's left panel graphs the $c_k(\alpha_*)$ as functions of α_* instead, where larger α_* corresponds to better RQMC performance on a single randomization by (8), and the right panel does the same for the optimal approximate RMSE rate exponents $v_k(\alpha_*)$ of (25). The plots for Corollary $k = 2$ set $\lambda = 0.01$. The figures also show $c_* = 1$ as Assumption 1.B requires $c \in (0, 1)$. The right panel of Figure 2 further includes $v_* = 1$ for reference.

Recall that Corollaries $k = 2$ and 5 require Assumption 3.A ($V_{\mathrm{HK}}(h) < \infty$), $k = 3$ imposes Assumption 3.B (bounded h), and $k = 4$ and 6 employ Assumption 3.C (order-$(2 + b)$ absolute central moment of $h(U)$ is finite). Proposition 1 gives a strict ordering of those assumptions' strengths. Figures 1 and 2 show the following properties, which Nakayama and Tuffin (2021) also establish analytically:

- $c_2(\alpha_*) > c_3(\alpha_*) > c_4(\alpha_*, b)$ for each $b > 0$ and $\alpha_* > 1/2$ ($c_2(\alpha_*)$ being valid only when $\alpha_* \geq 1$), showing that stricter conditions on integrand h permit larger values of c ensuring CLT (15).
- $c_5(\alpha_*) > c_6(\alpha_*)$ for each $b > 0$ and $\alpha_* > 1/2$, so a stronger condition on h corresponds to a larger range of values of c that yield AVCI (20).
- $c_4(\alpha_*, b)$ converges to $c_3(\alpha_*)$ as b increases, which agrees with the principle that having a finite absolute central moment of order $2 + b$ as $b \to \infty$ is "close" to meaning a bounded integrand.
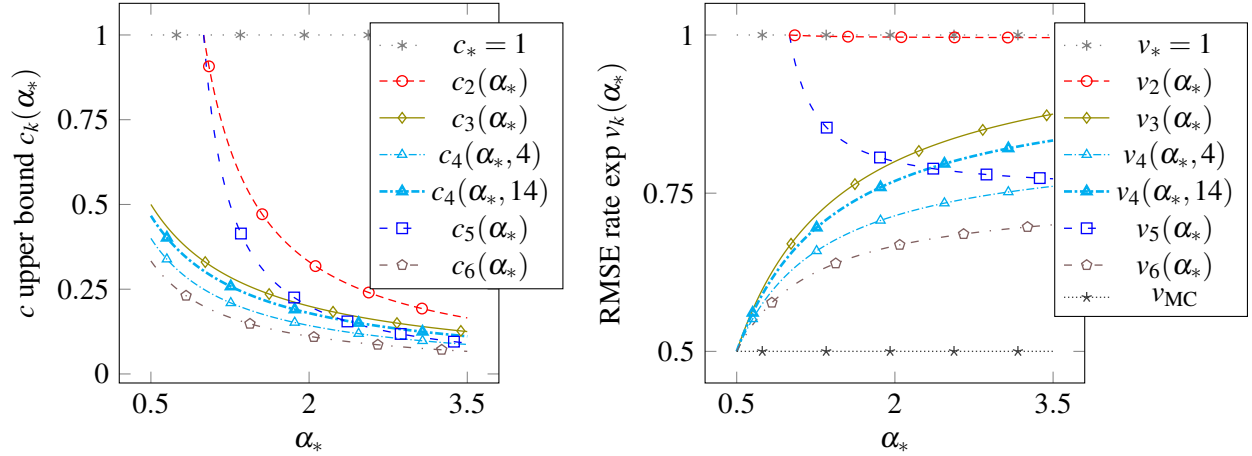
Figure 2: Plots of the upper bounds $c_k(\alpha_*)$ of c (left panel) and the negative exponent $v_k(\alpha_*)$ of the optimal rate at which the estimator RMSE decreases (right panel) as functions of α_*. Functions for $k = 2$ and 5 require $V_{\mathrm{HK}}(h) < \infty$, so they are shown for only $\alpha_* \geq 1$ because of (9). Each $c_k(\alpha_*)$ decreases in α_*, and most $v_k(\alpha_*)$ increase in α_*, so better QMC behavior usually yields better RQMC performance.

- $c_4(\alpha_*, b)$ grows as b increases (i.e., more absolute central moments are finite), so additional effort can be put on the QMC part (i.e., $m_n = n^c$ can be larger) when using the moment conditions of Corollary 4 to establish a CLT.
- $c_5(\alpha_*) \leq c_2(\alpha_*)$ and $c_6(\alpha_*) < c_3(\alpha_*)$, so securing AVCI (20) often (but not always) restricts c more than what guarantees a CLT.

The $v_k(\alpha_*)$ share the same properties and orderings as the $c_k(\alpha_*)$ by (27).

In the left panel of Figure 2, the upper bounds $c_k(\alpha_*)$ on c decrease as α_* grows, so ensuring CLT (15) or AVCI (20) for larger α_* requires putting more effort on the MC part (i.e., $r_n = n^{1-c}$ grows as c decreases) and correspondingly less on the QMC (i.e., $m_n = n^c$ shrinks as c gets smaller). By (26), the tradeoff could potentially harm the rate exponent $v_k(\alpha_*)$ governing how quickly the RQMC estimator's optimal RMSE decreases, but this does not occur for most k. The one exception is $v_5(\alpha_*)$ for the AVCI Corollary 5 when $V_{\mathrm{HK}}(h) < \infty$, which we explain by examining the corresponding $c_5(\alpha_*)$ in the left panel of Figure 2. While $c_5(\alpha_*)$ starts off at $\alpha_* = 1$ very high, it quickly drops off, so m_n must decrease rapidly as α_* grows to secure AVCI when $V_{\mathrm{HK}}(h) < \infty$, leading to less benefit from the QMC. Even so, we have that $v_5(\alpha_*) > v_6(\alpha_*)$ for all α_*, so the optimal rate exponent when establishing AVCI is better for $V_{\mathrm{HK}}(h) < \infty$ than through the moment condition of Corollary 6.

6 CONCLUDING REMARKS

We presented conditions that ensure the RQMC estimator of a mean μ obeys a Gaussian CLT or guarantee AVCI. We also examined the tradeoffs in the restrictions. While our paper gave sufficient conditions, we are currently looking into relaxing the requirements. Other current work includes devising procedures to estimate the upper bounds $c_k(\alpha_*)$ in (24) and Section 5.1, which will allow practitioners to apply our theoretical results. We are further investigating analogous theory for biased estimators, as for quantiles.

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