Necessity of low effective dimension

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October 2002, Orig: July 2002

Abstract

Practitioners have long noticed that quasi-Monte Carlo methods work very well on functions that are nearly superpositions of low dimensional functions. The reason is that the low dimensional coordinate projections of QMC rules can have very good equidistribution properties at sample sizes for which the original rule itself cannot have good equidistribution. This paper explores a converse proposal: that low effective dimension is necessary for QMC to be much better than MC in high dimensions with practical sample sizes.

1 Introduction

In some high dimensional applications Quasi-Monte Carlo (QMC) methods of integration give very good results that are not easily explained by the Koksma-Hlawka inequality or other discrepancy bounds. By inspecting the proofs of upper bounds on error one might suspect that the asymptotes would set in at a number n of evaluations that grows at least exponentially with the dimension d. Indeed, Sloan and Wozniakowski (1998) show that in a worst case setting, that QMC (using lattices) is no better than estimating the integrand by zero until $n \geq 2^d$. Yet in numerical examples, particularly some arising in computational finance (Paskov and Traub 1995; Ninomiya and Tezuka 1996), it is sometimes observed that QMC methods in dimensions as high as 360 can provide very good accuracy at practically relevant sample sizes n.

One explanation that has been offered is that the integrands may have effective dimension smaller than d. Specifically, the integrand may be nearly a sum of lower dimensional parts as described in Caflisch, Morokoff, and Owen (1997). Then if the QMC rule used has good equidistribution in its low dimensional coordinate projections, an accurate result is not surprising.

As Tezuka (2002) notes, a second class of high dimensional integrands for which good results have been seen in QMC are certain isotropic integration problems of Capstick and Keister (1996). Such problems reduce to computing the expectation of a function of the norm of a d dimensional spherical Gaussian random vector. Papageorgiou and Traub (1997) report good results for QMC on such problems. Recently Owen (2001) has shown that polynomials in the squared norm have effective dimension no larger than their degree. Furthermore, numerical investigation of a 25 dimensional isotropic function published in Papageorgiou and Traub (1997) show that it is very nearly a superposition of functions of 3 or fewer of the input variables.

Because the isotropic integrands appeared to be also of low effective dimension, it is interesting to conjecture that low effective dimension is somehow a necessary condition for QMC to work well at values of n below those where the discrepancy bounds apply.

It is clear that $|\hat{I}_n - I|$ can be small without f necessarily having low superposition dimension. For instance any f continuous on $[0,1]^d$, of whatever effective dimension, always has at least one point x with $f(x) = I$ and so $n = 1$ is compatible with $\hat{I}_n = I$. We will frame the problem in a way that rules out such cases, because no general purpose integration algorithms are based on finding such an x.

In this paper we find that low effective dimension is necessary for scrambled $(0, m, d)$-nets to have a much smaller variance than ordinary Monte Carlo, in high dimensions and for practical sample sizes. We do however uncover a surprising free lunch phenomenon: it is possible to have a scrambled net variance of zero on certain nonzero functions of effective dimension $m+1$ or $m+2$, but this effect requires a sample size n of at least $(d-1)^{d-2}$.

Section 2 introduces some notation, including the ANOVA decomposition of $L^2[0,1]^d$. Section 3 discusses effective dimension and formula (5) there shows how low effective dimension can lead to upper bounds on quadrature error. We are interested in a converse which we base on scrambled nets as outlined in Section 4. Theorem 1 there shows that if a scrambled (t, m, d)-net (for $1 \le m < d$) has variance below $0.01/\underline{\Gamma}$ times that of ordinary Monte Carlo sampling, that the function f is necessarily of superposition dimension at most m. The quantity $\underline{\Gamma} \le 1$ is a minimum gain coefficient for the net, and Section 5 describes how far below unity $\underline{\Gamma}$ can be, for $(0, m, d)$-nets. Section 6 discusses the results and considers how generally necessity of low superposition dimension might hold. Section 7 proves some results on minimized gain coefficients.

2 Notation

We consider approximating $I = \int_{[0,1]^d} f(x)dx$ by

$$\hat{I}_n = \frac{1}{n}\sum_{i=1}^{n} f(x_i) \tag{1}$$

for points $x_1, \dots, x_n \in [0,1]^d$. Equation (1) includes Monte Carlo (MC) and quasi-Monte Carlo (QMC) methods that dominate practice when d is large.

If $f \in L^2[0,1]^d$, then simple Monte Carlo sampling with independent x_i uniformly distributed on $[0,1]^d$ yields a random $\hat{I}_n$ with mean I and variance σ^2/n. The error $|\hat{I}_n - I|$ is of order $n^{-1/2}$ in probability, written $O_p(n^{-1/2})$. The law of the iterated logarithm establishes that the slightly larger error bound $|\hat{I}_n - I| = O([n^{-1}\log\log(n)]^{1/2})$ holds with probability 1.

If $f \in \text{BVHK}[0,1]^d$, the space of functions of bounded variation in the sense of Hardy and Krause, then

$$|\hat{I}_n - I| \le D_n^*(x_1, \dots, x_n)\|f\|_{\text{HK}} \tag{2}$$

The first indications that QMC could be significantly better than MC arose from constructions of points $x_1, \dots, x_n$ for which $D_n^* = O(n^{-1+\epsilon})$.

The sample size n at which the asymptotic error rates for QMC should set in is thought to grow exponentially with dimension d. Sloan and Wozniakowski (1998) show that in a worst case sense QMC is no better than estimating the integrand by zero until $n \ge 2^d$. Owen (1997b) finds that scrambled Faure sequences become much better than Monte Carlo at roughly $n \ge d^d$ while Owen (1998b) estimates a threshold at roughly $n \ge 4^d$ for Niederreiter-Xing sequences.

For $f \in L^2[0,1]^d$ there is an analysis of variance (ANOVA) decomposition with

$$f(x) = \sum_{u \subseteq \{1,\dots,d\}} f_u(x). \tag{3}$$

The function $f_u(x)$ depends on $x = (x^1, \dots, x^d)$ only through components x^j with $j \in u$. It also satisfies $\int_0^1 f_u(x)dx^j = 0$ whenever $j \in u$ for any values of x^k, $k \ne j$. The name ANOVA arises because the variance of f is $\sigma^2 = \int (f(x) - I)^2 dx$, attributable to subsets u of inputs via

$$\sigma^2 = \sum_u \sigma_u^2 \tag{4}$$

where $\sigma_\emptyset^2 = 0$ and $\sigma_u^2 = \int f_u(x)^2 dx$ for u with cardinality $|u| > 0$. To rule out trivial cases we assume $0 < \sigma^2 < \infty$.

3 Effective dimension

Caflisch, Morokoff, and Owen (1997) define the effective dimension of a function in two senses. The function f has effective dimension s in the superposition sense if

$$\sum_{|u|\le s} \sigma_u^2 \ge 0.99\sigma^2$$

and it has effective dimension s in the truncation sense if

$$\sum_{u\subseteq\{1,\dots,s\}} \sigma_u^2 \ge 0.99\sigma^2.$$

The idea of effective dimension appears in Paskov and Traub (1995) where they remark that certain integrands from finance are not essentially determined by just a small number of leading input variables. Sloan and Wozniakowski (1998) introduce classes of functions in which the importance of each successive variable x^j decays as j increases. Such functions can have small truncation dimension relative to their nominal dimension.

The definitions above capture two notions in which f is almost s dimensional. As Caflisch, Morokoff, and Owen (1997) remark, the choice of 99'th percentile is arbitrary. This paper uses the 99'th percentile for definiteness sake. Hickernell (1998) makes the threshold percentile a parameter in the definition.

The quadrature error in a QMC rule $x_1,\dots,x_n$ satisfies the bound

$$\left|\hat{I}_n - I\right| \le \sum_{|u|>0} D_{n,|u|}(x_1^u,\dots,x_n^u)\|f_u\| \tag{5}$$

where x_i^u is the coordinate projection of x_i onto the subset u of input variables, $D_{n,|u|}$ is a discrepancy for n points in $[0,1]^{|u|}$ and $\|f_u\|$ is a compatible norm. A version of formula (5) appears in Caflisch, Morokoff, and Owen (1997) and several versions are given by Hickernell (1998).

The upper bound (5) shows how low superposition dimension can guarantee good performance in QMC. Suppose that the function f belongs to a class in which $\|f_u\|$ is small whenever $|u| > s$ for $1 \le s < d$. Then (5) provides for a small error, when we use a method with $D_{n,|u|}$ small for $|u| \le s$.

Many widely studied discrepancies allow for tight versions of (5). For those discrepancies, given $x_1,\dots,x_n$ we may find f such that $|\hat{I}_n - I| = D_{n,|u|}(x_1^u,\dots,x_n^u)\|f_u\|$ and $f = f_u$. Then, given lower bounds on $D_{n,|u|}$ for large $|u|$, low effective dimension is necessary for $\hat{I}_n - I$ to be uniformly small over functions with $\|f\| \le 1$.

4 Scrambled nets

Digital nets are defined in Niederreiter (1992). A method of scrambling of them was proposed in Owen (1995). The discrepancy of scrambled nets was studied in Hickernell and Yue (2000). The variance formulas for scrambled nets below are from Owen (1997a).

The variance of $\hat{I}_n$ when x_i are scrambled versions of $a_i \in [0,1]^d$ is

$$\frac{1}{n}\sum_{|u|>0}\sum_{\kappa}\Gamma_{u,\kappa}\sigma^2_{u,\kappa}.$$

Here $\Gamma_{u,\kappa}$ is the gain coefficient corresponding to the subset $u \subseteq \{1,\dots,d\}$ and the vector κ containing $|u|$ nonnegative integers, defined as

$$\Gamma_{u,\kappa} = \frac{1}{n(b-1)^{|u|}}\sum_{i=1}^{n}\sum_{j=1}^{n}\prod_{r\in u}\Bigl(bN_{i,j,r} - W_{i,j,r}\Bigr), \tag{6}$$

where

$$N_{i,j,r} = N_{i,j,r}(\kappa) = 1_{\lfloor b^{k_j+1}a_i^r\rfloor = \lfloor b^{k_j+1}a_j^r\rfloor}$$

and

$$W_{i,j,r} = W_{i,j,r}(\kappa) = 1_{\lfloor b^{k_j}a_i^r\rfloor = \lfloor b^{k_j}a_j^r\rfloor}$$

are indicator variables designating narrow and wide matches respectively between the components a_i^r and a_j^r. This formula holds for any $a_1,\dots,a_n \in [0,1]^d$ but it can simplify for nets, especially nets for which the quality parameter t is 0.

The notation $\Gamma_{u,\kappa}$ suppresses the dependence of the gain coefficient on b and m. When this dependence must be made explicit, the notation $\Gamma^{b,m}_{u,\kappa}$ will be used.

The variance of $\hat{I}_n$ under scrambling is a sum of contributions from every nonempty u and every vector $\kappa \in \{0,1,\dots\}^{|u|}$. Because $\sigma_u^2 = \sum_\kappa \sigma^2_{u,\kappa}$ a method with all gains $\Gamma_{u,\kappa} = 1$ has the same variance as Monte Carlo sampling.

Theorem 1 *Let $f \in L^2[0,1]^d$, let $\hat{I}_n$ be the quadrature rule* (1)*. Denote the variance of $\hat{I}_n$ by $Var_{snet}(\hat{I}_n)$ or $Var_{mc}(\hat{I}_n)$ depending on whether the x_i are a scrambled (t,m,d)-net with $1 \le m < d$ in base b or simple Monte Carlo respectively. Suppose that $Var(\hat{I}_{rqmc}) \le \epsilon\, Var(\hat{I}_{mc})$ for $0 < \epsilon < 1$. Then the function f satisfies*

$$\frac{\sum_{|u|>m}\sigma_u^2}{\sigma^2} \le \epsilon\left(\min_{|u|>m,\kappa\in\{0,1,\dots\}^{|u|}}\Gamma_{u,\kappa}\right)^{-1}.$$

Proof: Under the hypothesis of the theorem,

$$\epsilon \geq \frac{\mathrm{Var}_{\mathrm{snet}}(\hat{I}_n)}{\mathrm{Var}_{\mathrm{mc}}(\hat{I}_n)} \geq \sum_{|u|>m} \sum_{\kappa} \frac{\Gamma_{u,\kappa}\sigma^2_{u,\kappa}}{\sigma^2} \geq \left(\min_{|u|>m,\kappa} \Gamma_{u,\kappa} \right) \sum_{|u|>m} \frac{\sigma^2_u}{\sigma^2}. \quad \square$$

The following corollary is immediate:

Corollary 1 *If scrambled* (t, m, d)*-net integration of* f *has variance smaller than* $0.01/\min_{|u|>m,\kappa} \Gamma_{u,\kappa}$ *times that of ordinary Monte Carlo, then* f *has effective dimension at most* m*.*

5 Lower bounds on gain coefficients

To draw any practical conclusions from Theorem 1 and the Corollary requires lower bounds on gain coefficients $\Gamma^{b,m}_{u,\kappa}$ for $|u| > m$. From the defining property of a (t, m, d)-net it follows (Owen 1997a) that $\Gamma_{u,\kappa} = 0$ when $|u| + |\kappa| \leq m - t$. When $t > 0$ and $|u| + |\kappa| > m - t$ the net property does not uniquely define $\Gamma_{u,\kappa}$.

From here on, we restrict attention to the gain coefficients for (t, m, d)-nets with $t = 0$. For $(0, m, d)$-nets, it is known that

$$\Gamma_{u,\kappa} = 1 + (1-b)^{-u} \left[(-b)^{m-k} \binom{u-1}{m-k} - \sum_{j=0}^{m-k} \binom{u}{j} (-b)^j \right]. \tag{7}$$

Here, and in the following, the integers $|u|$ and $|\kappa|$ are replaced by u and k in expressions for Γ. This reduces clutter and leads to no loss of generality because for a $(0, m, d)$-net the gain depends on the subset u and the vector κ only through their cardinality and component sum respectively. We suppose also that b is a prime power. Most digital net constructions use prime power bases. Niederreiter (1987) shows how to construct digital nets in more general bases $b \geq 2$ from those with prime power bases, but the resulting nets have comparatively small dimension d.

It follows easily from (7) that $\Gamma_{u,k} = 1$ for $k \geq m$. Also $(0, m, d)$-nets in base b can only exist when $d \leq b + 1$. Thus for any b and m, the interesting gain coefficients can be arranged into a $b + 1$ by m table. As a consequence of Theorem 1 we are particularly interested in

$$\underline{\Gamma} = \underline{\Gamma}^{b,m} \equiv \min_{u>m,k\geq 0} \Gamma^{b,m}_{u,k},$$

	0	1	2	3	4	≥ 5
1					1	$\cdots$
2				1.06667	1	$\cdots$
3			1.13778	0.99556	1	$\cdots$
4		1.21363	0.98607	1.00030	1	$\cdots$
5	1.29454	0.97090	1.00124	0.99998	1	$\cdots$
6	0.94933	1.00327	0.99990	1.00000	1	$\cdots$
7	1.00686	0.99967	1.00001	1.00000	1	$\cdots$
8	0.99919	1.00003	1.00000	1.00000	1	$\cdots$
9	1.00009	1.00000	1.00000	1.00000	1	$\cdots$
10	1.00000	1.00000	1.00000	1.00000	1	$\cdots$
$\vdots$	$\vdots$	$\vdots$	$\vdots$	$\vdots$	$\vdots$	$\vdots$
17	1.00000	1.00000	1.00000	1.00000	1	$\cdots$

Table 1: Shown are the gain coefficients for randomized $(0, 4, d)$-nets in base 16. The value $\Gamma_{|u|,|\kappa|}$ appears in the row with $|u|$ on the left and in the column headed by $|\kappa|$. The largest relevant value of $|u|$ is 17 because $|u| \leq d \leq b + 1 = 17$. The upper left corner of exact zeros is left blank. For $|\kappa| \geq m = 4$ the gain is exactly one. The other values have been rounded. Rows 11 through 16 look the same as rows 10 and 17.

for $m < d$. If $\underline{\Gamma}$ is near one then a variance reduction of slightly over 100-fold for scrambled $(0, m, d)$-nets implies that f has effective dimension at most m.

Table 1 shows the gain coefficients for scrambled $(0, 4, d)$ nets in base 16. These nets have $n = 65536$ points in $[0, 1]^d$. The smallest gain coefficient for $|u| > 4$ is $\underline{\Gamma} = \Gamma_{6,0} = 720896/759375 \doteq 0.94933$. Theorem 1 shows that if scrambled net sampling has variance ϵ times as large as ordinary Monte Carlo sampling then the fraction of the variance of f due to ANOVA components of dimension 5 or more is at most $\epsilon/0.94933 = \epsilon 1.05338$. To conclude that f has effective dimension 5 or less we need to find that the scrambled net variance is no larger than 0.0095 times the Monte Carlo variance.

The values $\Gamma^{16,4}_{u,k}$ in Table 1 below the row for $u = 4$ are alternately above and below unity as u or k increases. When $u > m$ the gain $\Gamma_{u,k}$ is at least 1 for odd $m - u + k$ and at most 1 for even $m - u + k$. Moving from left to right in the table the gains approach one. When u is m plus an odd positive number, the gains decrease to unity as k increases through even values beginning with 0. Similarly when $u - m > 0$ is odd and k increases through odd values beginning with 1, the gains increase to unity. When u

is m plus an even positive number, the trends described above are reversed. Lemma 1 below shows that these monotone trends hold in generality. It follows that the search for $\underline{\Gamma}$ can be restricted to cases of the form $\Gamma_{m+2r,0}$ for $r \geq 1$ or $\Gamma_{m+2r+1,1}$ for $r \geq 0$.

It also holds in Table 1 that $\Gamma_{m+2r+1,1} \geq \Gamma_{m+2r+2,0}$ when $r \geq 0$ and $m + 2r + 2 \leq b + 1$. Lemma 2 below shows that this pattern holds in generality, and so the search for the minimum Γ can ordinarily be restricted to $\Gamma_{m+2r+2,0}$ for $r \geq 0$. There is an exception when $m = b$, for then $u = m+2 = b+2$ is inapplicable and so the minimizer must be $\Gamma_{b+1,1}$. Finally the terms $\Gamma_{m+2r+2,0}$ in Table 1 are nondecreasing as $r \geq 0$ increases. This too is a general phenomenon (Lemma 3 below) and so the minimizer is $\underline{\Gamma} = \Gamma_{m+2,0}$ when $m \leq b - 1$.

Theorem 2 *Let $b \geq 2$ be an integer. For a non-negative integer $m \leq b - 1$*

$$\underline{\Gamma} = \min_{m<u\leq b+1} \min_{k\geq 0} \Gamma_{u,k} = \Gamma_{m+2,0},$$

and for $m = b$

$$\underline{\Gamma} = \min_{m<u\leq b+1} \min_{k\geq 0} \Gamma_{u,k} = \Gamma_{m+1,1}.$$

Proof: See Section 7.

The minimizing gain coefficients simplify. They can be surprisingly small as the next proposition shows.

Proposition 1 *Let $b \geq 2$ and $m \geq 0$ be integers. Then*

$$\Gamma^{b,m}_{m+2,0} = \left(\frac{b}{b-1}\right)^m \frac{b-m-1}{b-1}, \quad \textit{for } m \leq b-1 \textit{ and,}$$
$$\Gamma^{b,m}_{m+1,1} = \left(\frac{b}{b-1}\right)^m \frac{b-m}{b}, \quad \textit{for } m \leq b.$$

In particular $\Gamma^{b,b-1}_{b+1,0} = \Gamma^{b,b}_{b+1,1} = 0.$

Proof: The result follows after a short manipulation of binomial coefficients. The alternating sum within the square brackets of (7) matches all but $u-m+k$ terms of $\sum_{j=0}^{u} \binom{u}{j}(-b)^j$, which equals $(1-b)^u$ by the binomial theorem. For the cases here $u - m + k = 2$.

This proposition provides an astonishing example of an apparently free lunch. For a $(0, m, d)$-net certain hypercubical subsets of $[0, 1]^d$ are guaranteed to contain a number of points equal to b^m times their volume. We say these sub-cubes are "balanced" by the net. For $m < d$ the balanced sub-cubes have at least $d - m$ sides of length 1, and in that sense are less than fully d dimensional. It is a surprise to be able to integrate exactly some fully d dimensional integrands using nets that do not balance any fully d dimensional sub-cubes.

The phenomenon in Proposition 1 does not help with high dimensional problems. First, the smallest gain coefficients are for dimensions only one or two higher than m. Second, the number of points in such nets is $n = b^m$ which is either b^{b-1} or b^b. Because $b \geq d - 1$ this phenomenon does not apply for $n < (d-1)^{d-2}$.

To further study $\underline{\Gamma}$ we suppose that $m < b + 1$ so that $\underline{\Gamma}^{b,m} = \Gamma^{b,m}_{m+2,0}$. The smallest values of this gain arise with small b and large m:

Proposition 2 *If $m \geq 1$ and $b \geq m + 1$ then $\Gamma^{b,m}_{m+2,0}$ increases with b. If $b \geq 2$ and $0 \leq m \leq b - 1$ then $\Gamma^{b,m}_{m+2,0}$ decreases with m.*

Proof: Although $\Gamma^{b,m}_{m+2,0}$ is defined for integers, we may interpolate by real values. Then

$$
\begin{aligned}
\frac{\partial}{\partial b} \log\Bigl(\Gamma^{b,m}_{m+2,0}\Bigr) &= \frac{m}{b} - \frac{m}{b-1} + \frac{1}{b-m-1} - \frac{1}{b-1} \\
&= \frac{m(m+1)}{b(b-1)(b-m-1)} \\
&\geq 0, \quad \text{and,} \\
\frac{\partial}{\partial m} \log\Bigl(\Gamma^{b,m}_{m+2,0}\Bigr) &= \log\Bigl(\frac{b}{b-1}\Bigr) - \frac{1}{b-m-1} \\
&\leq \frac{1}{b-1} - \frac{1}{b-m-1} \\
&\leq 0. \quad \Box
\end{aligned}
$$

Very small values of $\underline{\Gamma}$ are possible for $n \geq (d-1)^{d-2}$. Here we investigate numerically how small $\underline{\Gamma}$ can be for large dimensions and practical sample sizes. We restrict attention to $\Gamma^{b,m}_{b+2,0}$ as this is the minimum gain when $m \leq b - 1$. Consider $d \geq 20$ and $n \leq 10^7$. For $d \geq 20$ the smallest prime power $b \geq d-1$ is $b = 19$. For $b = 19$ and $n \leq 10^7$ the largest m we can have is $\lfloor \log_{19}(10^7) \rfloor = 5$. Therefore for $d \geq 20$ and $n \leq 10^7$, the minimum gain must be at least $\Gamma^{19,5}_{7,0} = 0.946403$, which is not much below one. Table 2 records the results of similar calculations varying both the lower bound on d and the upper bound on n.

	10^4	10^5	10^6	10^7	10^8	10^9	10^{10}
10	0.80090	0.67576	0.50682	0.28509	0.00000	0.00000	0.00000
15	0.97090	0.94933	0.94933	0.92056	0.88374	0.83791	0.78205
20	0.98008	0.98008	0.96556	0.94640	0.92214	0.89225	0.89225
30	0.99608	0.99198	0.98631	0.98631	0.97897	0.96985	0.96985
50	0.99868	0.99868	0.99732	0.99548	0.99548	0.99312	0.99312
100	0.99990	0.99970	0.99970	0.99939	0.99939	0.99898	0.99898
360	0.99999	0.99999	0.99998	0.99998	0.99995	0.99995	0.99995

Table 2: This table shows minimum possible gain coefficients for scrambled $(0, m, d)$-nets. The rows are labelled with dimensions d and the columns are labelled with sample sizes n. Let $b = b(d)$ be the smallest prime power no smaller than $d - 1$. Shown is the smallest value of $\Gamma_{u,k}^{b,m}$ subject to $b \geq b(d)$, $b^m \leq n$, $m < u \leq d$, and $k \geq 0$. Zeros for $d = 10$ correspond to $(0, 8, 10)$-nets in base 9. These have $\Gamma_{10,0}^{9,8} = 0$ and $n = 9^8 = 43,046,721$.

For large dimensions and practical sample sizes $\Gamma_{u,k}^{b,m}$ cannot be appreciably smaller than 1. In those settings, a variance reduction of just over 100 implies that f has effective dimension at most m. When the sample size can reach b^{b-2} then $\Gamma_{u,k}^{b,m}$ can become surprisingly small.

6 Discussion

The conclusion of this paper is that low effective dimension is necessary for scrambled $(0, m, d)$-nets to be much better than Monte Carlo for large d and practical n. A surprising free lunch phenomenon was found in which the scrambled net variance could be zero for some nonzero functions of effective dimension $b + 1$ when $m = b$ or $b - 1$, but the free lunch was only seen for $n \geq (d - 1)^{d-2}$.

There are three important features to Theorem 1. The first is that performance of scrambled nets is studied relative to Monte Carlo, not absolutely. The second is that it is not asymptotic. The sample sizes used are of the form b^m for $m < d$, including values below those at which QMC asymptotics are thought to take effect. The third is that it provides a conclusion about the function f itself, without reference to a containing function class.

These features are important because they capture what surprised many observers: QMC can be much better than MC for specific functions with large d at surprisingly small n. A non-asymptotic analysis is essential because $\mathrm{Var}_{\mathrm{snet}}(\hat{I}_n)/\mathrm{Var}_{\mathrm{mc}}(\hat{I}_n) \to 0$, for any $f \in L^2[0, 1]^d$, regardless of effective dimension.

Simple counterexamples with spiky integrands show that low effective dimension cannot be sufficient for good performance of QMC, either absolutely or relatively. For example, let $f(x) = \epsilon^{-1} 1_{x^1 \le \epsilon}$. Then f has truncation and superposition dimension both equal to 1 but cannot be integrated well by QMC for $n \ll 1/\epsilon$.

It is also easy to see that small truncation dimension is not necessary for QMC to be much better than MC. The linear function $f(x) = \sum_{j=1}^d x^j$ is easy for QMC methods, but has truncation dimension at least $0.99d$, for any re-ordering of the variables. Truncation dimension is an important aspect of infinite dimensional problems. Owen (1998a) shows by a martingale argument that any square integrable function on $[0,1]^\infty$ necessarily has finite effective dimension in the truncation sense, for any threshold less than 100 percent.

Recent work of Sloan (2002) on function classes with successively less important dimensions shows that a small quadrature error can be obtained for some functions having high superposition dimension. The importance of input j decays rapidly, as quantified by a series of constants γ_j for $j \ge 1$. Let f^* be a purely 1000 dimensional function in that class involving only dimensions $1,000,001$ through $1,001,000$. Then f^* can be integrated with a small error despite having superposition dimension 1000. These tractability results are not at odds with the thesis of this paper. The former study performance relative to the zero rule $\hat{I} = 0$ while this paper considers performance relative to Monte Carlo methods. The function f^* would have a small norm in order to "fit in the space" defined by the γ_j sequence. A small norm for f^* would also lead to a small Monte Carlo variance and it is not clear that QMC would beat MC for this f^*.

Low superposition dimension is necessary for scrambled $(0, m, d)$-nets to beat MC by a wide margin at modest sample sizes in high dimensions. But this does not show that low superposition dimension is universally necessary for this phenomenon. Perhaps other general purpose QMC methods can beat MC by a wide margin for modest n and integrands of high superposition dimension.

To show similar results for scrambled (t, m, d)-nets with $t > 0$ requires lower bounds on gain coefficients $\Gamma_{u,\kappa}$ for $t > 0$. The definition of a (t, m, d)-net is not sharp enough to determine gain coefficients when $t > 0$. Upper bounds on gain coefficients appear in Owen (1998b), Niederreiter and Pirsic (2001), and Yue and Hickernell (2002). A quadrature rule may be described by a great many nonnegative t-values, one for each of a class of subintervals of $[0,1]^d$. The net nomenclature specifies only the largest of these. When the largest is zero then they are all zero. But in general a net with $t > 0$ can have smaller t even $t = 0$ when projected into a set u of components. Schmid (2001) describes this phenomenon. Yue (1999) provides gain coefficients for some leading subsequences of $(0, d)$-sequences in base b that like $(\lambda, 0, m, d)$-nets are not necessarily nets.

It is interesting to speculate on whether necessity of low superposition dimension might hold outside of scrambled nets. Heinrich, Hickernell, and Yue (2001) show that scrambled nets are asymptotically optimal quadrature rules in various settings. The function classes are defined by the decay of certain Haar wavelet coefficients and three approximation senses are considered: worst case, random case, and average case, in their terminology. The random case setting is closest to the one considered here, but their results are not relative to Monte Carlo and are asymptotic.

7 Proofs

We begin by recalling that $\binom{n}{r} = 0$ if $r < 0$ or $r > n$ and that the binomial identity $\binom{n}{r} = \binom{n-1}{r} + \binom{n-1}{r-1}$ holds even when $r > n - 1$ or $r < 0$. We will also use

$$\frac{\binom{n}{r}}{\binom{n}{r-1}} = \frac{n - r + 1}{r} \tag{8}$$

but only for $0 < r \le n + 1$.

This first lemma establishes that certain monotone alternations seen in gain tables hold generally.

Lemma 1 *For non-negative integers b, m, r, and s, with $b \ge 2$, $m \le b$ and $m + 2r + 1 \le b + 1$,*

$$\Gamma_{m+2r+1,2s} \ge \Gamma_{m+2r+1,2s+2} \ge 1, \tag{9}$$

$$\Gamma_{m+2r+1,2s+1} \le \Gamma_{m+2r+1,2s+3} \le 1. \tag{10}$$

For non-negative integers b, m, r, and s, with $b \ge 2$, $m \le b$ and $m + 2r \le b + 1$,

$$\Gamma_{m+2r,2s} \le \Gamma_{m+2r,2s+2} \le 1, \tag{11}$$

$$\Gamma_{m+2r,2s+1} \ge \Gamma_{m+2r,2s+3} \ge 1. \tag{12}$$

Proof: We prove (11). The proofs of the other three propositions use the same sequence of techniques. If $2s \ge m$ then $\Gamma_{m+2r,2s} = \Gamma_{m+2r,2s+2} = 1$, so without loss of generality we suppose $2s < m$. Use $u = m + 2r$ to shorten some intermediate expressions.

$$
\begin{aligned}
&\Gamma_{m+2r,2s+2} - \Gamma_{m+2r,2s} \\
&= (1-b)^{-u}\Bigg[(-b)^{m-2s-2}\binom{u-1}{m-2s-2} - \sum_{j=0}^{m-2s-2}\binom{u}{j}(-b)^j \\
&\quad - (-b)^{m-2s}\binom{u-1}{m-2s} + \sum_{j=0}^{m-2s}\binom{u}{j}(-b)^j\Bigg] \\
&= (1-b)^{-u}\Bigg[(-b)^{m-2s-2}\binom{u-1}{m-2s-2} - (-b)^{m-2s}\binom{u-1}{m-2s} \\
&\quad + \binom{u}{m-2s-1}(-b)^{m-2s-1} + \binom{u}{m-2s}(-b)^{m-2s}\Bigg] \\
&= (1-b)^{-u}(-b)^{m-2s-2}\Bigg[\binom{u-1}{m-2s-2} - b^2\binom{u-1}{m-2s} \\
&\quad - b\binom{u}{m-2s-1} + b^2\binom{u}{m-2s}\Bigg] \\
&= (b-1)^{-u}b^{m-2s-2}(-1)^{-m-2r+m-2s-2}\Bigg[\binom{u-1}{m-2s-2} - b^2\binom{u-1}{m-2s} \\
&\quad - b\binom{u-1}{m-2s-1} - b\binom{u-1}{m-2s-2} + b^2\binom{u-1}{m-2s} + b^2\binom{u-1}{m-2s-1}\Bigg] \\
&= (b-1)^{-u}b^{m-2s-2}\Bigg[\binom{u-1}{m-2s-2}(1-b) + \binom{u-1}{m-2s-1}(b^2-b)\Bigg].
\end{aligned}
$$

If $2s = m-1$ then the first term in square brackets vanishes and so the entire factor in square brackets is nonnegative. If $2s < m-1$ then we apply (8) within the square brackets, obtaining

$$\begin{aligned}
&\binom{u-1}{m-2s-2}(1-b) + \binom{u-1}{m-2s-1}(b^2-b) \\
&= (b-1)\binom{u-1}{m-2s-2}\left(b\frac{(u-1)-(m-2s-1)+1}{m-2s-1} - 1\right) \\
&= (b-1)\binom{u-1}{m-2s-2}\left(b\frac{2r+2s+1}{m-2s-1} - 1\right) \\
&\geq (b-1)\binom{u-1}{m-2s-2}\left(\frac{b}{m-2s-1} - 1\right) \\
&\geq (b-1)\binom{u-1}{m-2s-2}\left(\frac{b}{m-1} - 1\right) \\
&\geq 0,
\end{aligned}$$

where we have used $m - 2s - 1 > 0$ and $m \leq b$. It follows that $\Gamma_{m+2r,2s+2} - \Gamma_{m+2r,2s} \geq 0$ establishing (11). $\square$

To simplify some manipulations, we introduce the term

$$S_u^m = \sum_{j=0}^{m} \binom{u}{j} (-b)^j.$$

Differences $S_u^m - S_u^{m-r}$ reduce to sums of r terms. Also the binomial identity yields $S_{u+1}^m = S_u^m - bS_u^{m-1}$ and $S_{u+2}^m = S_u^m - 2bS_u^{m-1} + b^2 S_u^{m-2}$.

The next lemma shows that for any small gain coefficient with $k = 1$ there is ordinarily one with $k = 0$ that is no larger.

Lemma 2 *For non-negative integers b, m, and r, with $b \geq 2$, $m \leq b$ and $m + 2r + 1 \leq b + 1$,*

$$\Gamma_{m+2r+1,1} \geq \Gamma_{m+2r+2,0}. \tag{13}$$

Proof:

$$
\begin{aligned}
&\Gamma_{m+2r+1,1} - \Gamma_{m+2r+2,0} \\
&= (1-b)^{-m-2r-1}\left[(-b)^{m-1}\binom{m+2r}{m-1} - S^{m-1}_{m+2r+1}\right] \\
&\quad - (1-b)^{-m-2r-2}\left[(-b)^{m}\binom{m+2r+1}{m} - S^{m}_{m+2r+2}\right] \\
&= (1-b)^{-m-2r-2}\left[(-b)^{m-1}\binom{m+2r}{m-1}(1-b) - (-b)^{m}\binom{m+2r+1}{m}\right. \\
&\quad \left. - (1-b)S^{m-1}_{m+2r+1} + S^{m}_{m+2r+1} - bS^{m-1}_{m+2r+1}\right] \\
&= (1-b)^{-m-2r-2}\left[(-b)^{m-1}\binom{m+2r}{m-1}(1-b) - (-b)^{m}\binom{m+2r+1}{m}\right. \\
&\quad \left. + (-b)^{m}\binom{m+2r+1}{m}\right] \\
&= (1-b)^{-m-2r-2}(-b)^{m-1}\binom{m+2r}{m-1}(1-b) \\
&= (b-1)^{-m-2r-1}b^{m-1}\binom{m+2r}{m-1}(-1)^{-m-2r-2+m-1-1} \\
&\geq 0. \quad \Box
\end{aligned}
$$

The final lemma shows that the elements $\Gamma_{m+2r,0}$ in the $k=0$ column of the gain table increase with r.

Lemma 3 *For nonnegative integers b, m, and r, with $b \geq 2$, $1 \leq m \leq b$ and $m+2r+2 \leq b+1$,*

$$\Gamma_{m+2r+2,0} \geq \Gamma_{m+2r,0}. \tag{14}$$

Proof:

$$
\begin{aligned}
&\Gamma_{m+2r+2,0} - \Gamma_{m+2r,0} \\
&= (1-b)^{-m-2r-2}\left[(-b)^m\binom{m+2r+1}{m} - S^m_{m+2r+2}\right] \\
&- (1-b)^{-m-2r}\left[(-b)^m\binom{m+2r-1}{m} - S^m_{m+2r}\right] \\
&= (1-b)^{-m-2r-2}\left[(-b)^m\binom{m+2r+1}{m} - (1-b)^2(-b)^m\binom{m+2r-1}{m}\right. \\
&\qquad \left. - S^m_{m+2r+2} + (1-b)^2 S^m_{m+2r}\right] \\
&= (1-b)^{-m-2r-2}\left[(-b)^m\binom{m+2r+1}{m} - (1-b)^2(-b)^m\binom{m+2r-1}{m}\right. \\
&\qquad \left. - S^m_{m+2r} + 2bS^{m-1}_{m+2r} - b^2 S^{m-2}_{m+2r} + (1-2b+b^2)S^m_{m+2r}\right] \\
&= (1-b)^{-m-2r-2}\left[(-b)^m\binom{m+2r+1}{m} - (1-b)^2(-b)^m\binom{m+2r-1}{m}\right. \\
&\qquad \left. b^2(S^m_{m+2r} - S^{m-2}_{m+2r}) - 2b(S^m_{m+2r} - S^{m-1}_{m+2r})\right] \\
&= (1-b)^{-m-2r-2}(-b)^m\left[\binom{m+2r+1}{m} - (1-b)^2\binom{m+2r-1}{m}\right. \\
&\qquad \left. - b\binom{m+2r}{m-1} + b^2\binom{m+2r}{m} - 2b\binom{m+2r}{m}\right].
\end{aligned}
$$

The product outside the square brackets is positive. The factor within square brackets simplifies to

$$
\begin{aligned}
&(b-1)^2\binom{m+2r-1}{m-1} + (1-b)\binom{m+2r}{m-1} \\
&= (b-1)^2\binom{m+2r-1}{m-1}\left[1 - \frac{m+2r}{b-1}\frac{1}{2r+1}\right] \\
&\geq 0,
\end{aligned}
$$

because $m + 2r \leq b - 1$. □

Proof of Theorem 2: Suppose $m \leq b-1$. For $u = m + 2r \leq b+1$ with $r \geq 0$ the minimum value of $\Gamma_{u,k}$ for $k \geq 0$ is $\Gamma_{u,0}$ by the alternating gain Lemma 1. Similarly for $u = m + 2r + 1 \leq b + 1$ with $r \geq 0$ the minimum value of $\Gamma_{u,k}$ for $k \geq 0$ is $\Gamma_{u,1}$. Therefore the minimizing $\Gamma_{u,k}$ has the form

$\Gamma_{m+2r,0}$ or $\Gamma_{m+2r+1,1}$. But Lemma 2 shows that $\Gamma_{m+2r+1,1} \geq \Gamma_{m+2r+2,0}$ in this case. Therefore the minimizing $\Gamma_{u,k}$ has the form $\Gamma_{m+2r,0}$. Finally Lemma 1 show that the minimizing $\Gamma_{u,k}$ is $\Gamma_{m+2,0}$.

When $m = b$ then $m + 2 > b + 1$ and the only eligible $\Gamma_{u,k}$ entries are $\Gamma_{b+1,k}$. Lemma 1 then shows that the minimizing value is $\Gamma_{b+1,1}$. □

Acknowledgments

I thank Grzegorz Wasilkowski for helpful comments, and I also thank an anonymous reviewer for comments that motivated important changes in this paper. This work was supported by the NSF under grant DMS-0072445.

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