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On the efficiency of certain quasi-random sequences of points in evaluating multi-dimensional integrals

By

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1. Introduction

In a recent paper on Monte Carlo Methods [1], J. M. Hammersley considers the estimation of the multi-dimensional integral

$$\int_0^1 \mathrm{d}x_1 \ldots \int_0^1 \mathrm{d}x_k \, f(x_1, \ldots, x_k) \tag{1}$$

by formulae of the form $\Sigma_i w_i f(x_{i1}, \ldots, x_{ik})$. He points out that the efficiency of such an integration formula may be gauged by considering how it fares when $f(x_1, \ldots, x_k)$ is the indicator-function of the hyperbrick defined by an arbitrary point $\boldsymbol{A} \equiv (A_1, \ldots, A_k)$ in the unit hypercube $\mathfrak{U}$*. The value of the integral (1) would then be the volume $V = A_1 A_2 \ldots A_k$ of the corresponding hyper-brick.

He uses the efficiency criterion

$$J = \int_0^1 \mathrm{d}A_1 \ldots \int_0^1 \mathrm{d}A_k \, |S(\boldsymbol{A}) - NV|^2, \tag{2}$$

where N is the number of points used in the estimating formula and $S(\boldsymbol{A})$ is the number of these points falling within the hyper-brick defined by $\boldsymbol{A}$, and discusses the relative efficiencies of different distributions of points.

K. F. Roth [2] shows that a positive constant c_k exists, such that

$$J > c_k (\ln N)^{k-1} \tag{3}$$

for all distributions of the N points in $\mathfrak{U}$.

J. C. van der Corput [3] has shown that a sequence of N points can be constructed, for which

$$\sup |S(A_1, A_2) - N A_1 A_2| < C \ln N, \tag{4}$$

where C is a constant and the supremum is taken over all points (A_1, A_2) in the unit square.

Hammersley has proposed a generalisation of van der Corput's sequence to k dimensions, and asks whether $\sup |S(\boldsymbol{A}) - NV|$ can be shown not to exceed some multiple of a power of $\ln N$.

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* The unit hypercube is defined by $0 \leqq x_i \leqq 1$ $(i = 1, 2, \ldots, k)$. The hyper-brick is defined by $0 \leqq x_i \leqq A_i$ $(i = 1, 2, \ldots, k)$.

In the present paper, it is shown that, for HAMMERSLEY'S sequence, both

$$\sup |S(A) - NV| < C_k (\ln N)^{k-1} \tag{5}$$

and

$$J < B_k (\ln N)^{2k-2}, \tag{6}$$

where B_k and C_k are known positive constants. The sequence may be made rather more convenient for continuous computation at the expense of replacing $k-1$ by k in (5) and (6).

2. The quasi-random sequences in k dimensions

Let R be any integer; then any other integer n can be written in radix-R notation as

$$n \equiv n_M n_{M-1} \dots n_2 n_1 n_0 = n_0 + n_1 R + n_2 R^2 + \cdots + n_M R^M, \tag{7}$$

where

$$M = [\log_R n] = [\ln n / \ln R], \tag{8}$$

square brackets denoting the integral part, as is usual. By reversing the order of the digits in n, we can uniquely construct a fraction lying between 0 and 1,

$$\varphi = \varphi_R(n) = 0 \cdot n_0 n_1 n_2 \dots n_M = n_0 R^{-1} + n_1 R^{-2} + \cdots + n_M R^{-M-1}. \tag{9}$$

VAN DER CORPUT'S sequence of points in the unit square is $(n/N, \varphi_2(n))$ for $n = 1, 2, \dots, N$. For this, he shows that the result (4) holds. HAMMERSLEY'S suggestion is to use the k-dimensional sequence,

$$(n/N, \varphi_{R_1}(n), \varphi_{R_2}(n), \dots, \varphi_{R_{k-1}}(n)) \quad \text{for} \quad n = 1, 2, \dots, N, \tag{10}$$

in which he takes $R_1, R_2, \dots, R_{k-1}$ to be the first $k-1$ primes. Although this is clearly the most useful suggestion, we shall only require in what follows that these integers be prime to each other.

In using a sequence such as (10) for the computation of integrals of the form (1), it is necessary to compute the function $f(x_1, \dots, x_k)$ at each point of the sequence. Unfortunately, the first co-ordinate in (10) depends on N, so that we should have to decide in advance on the value of N in order to perform the calculation. It is therefore suggested that a sequence of the form

$$(\varphi_{R_1}(n), \varphi_{R_2}(n), \dots, \varphi_{R_k}(n)) \quad \text{for} \quad n = 1, 2, \dots, N, \tag{11}$$

might be more convenient in practice, at least in establishing the magnitude required for N in using (10).

3. Some preliminary results

Choose an arbitrary fraction $A \equiv 0 \cdot a_0 a_1 a_2 \dots a_M \dots$ lying between 0 and 1. By (9), if $A > \varphi$, one of the following conditions must be satisfied:

$$\left.\begin{array}{l} a_0 > n_0; \quad a_0 = n_0, \quad a_1 > n_1; \quad a_0 = n_0, \quad a_1 = n_1, \quad a_2 > n_2; \quad \dots; \\ a_0 = n_0, \quad a_1 = n_1, \dots, a_M = n_M; \end{array}\right\} \tag{12}$$

where we assume that A is given in non-terminating form.

Returning to the original integer n, we see that (12) is equivalent to requiring that, for some $m < M+3$,

$$\left.\begin{aligned} n &\equiv a_0 + a_1 R + \cdots + a_{m-2} R^{m-2} + n_{m-1} R^{m-1} \pmod{R^m}, \\ \text{where} \quad & a_{m-1} > n_{m-1} \quad \text{and} \quad n_{M+1} = 0. \end{aligned}\right\} \tag{13}$$

It is clear that only one of the conditions (13) can hold for any given n and A. Further, for a given value of m, (13) means that n must be congruent to one of a_{m-1} distinct numbers (only one in the sole case of $m = M+2$). Let p represent any one of these numbers. Then the number of integers in the sequence $1, 2, \ldots, N$ which are congruent to p, modulo R^m, is $[N/R^m] + h$, where h is a variable whose only possible values are 0 and 1.

We may now extend these considerations to several variables. R is replaced by a set of mutually-prime integers R_i. Each integer n gives rise to a set of fractions $\varphi_i = \varphi_{R_i}(n)$, and we wish to count the number of such sets satisfying the simultaneous conditions $A_i > \varphi_i$, where $\boldsymbol{A}$ is an arbitrary point in the corresponding unit hypercube. We are thus concerned with the problem of satisfying sets of simultaneous congruences,

$$n \equiv p_i \pmod{R_i^{m_i}}. \tag{14}$$

By the Chinese Remainder Theorem [4], since the moduli $R_i^{m_i}$ are prime to each other, the solutions of (14) form a complete congruence-class, modulo $\Pi_i R_i^{m_i}$. Thus the numbers of integers in the sequence $1, 2, \ldots, N$ which satisfy (14), and so which generate points $\boldsymbol{\varphi} \equiv (\varphi_i)$ lying in the hyper-brick defined by $\boldsymbol{A}$ (the meaning of all $A_i > \varphi_i$), will be $[N/\Pi_i R_i^{m_i}] + h$. To get all such points, we must sum over the possible choices of the m_i and the p_i.

4. The efficiency of the sequences

We may now proceed to calculate J for the sequences. The case of (11) is the more straightforward. Remembering that there are a_{m-1} integers p for each dimension (except when $m = M+2$, where now $M = [\log_R N]$) we see that

$$S(\boldsymbol{A}) = \sum_{\text{Each } m_i = 1}^{M_i+1} \left(\prod_{i=1}^{k} b_{i, m_i - 1} \right) \left([N/\Pi_i R_i^{m_i}] + \vartheta \right), \tag{15}$$

where $0 \leqq \vartheta \leqq 1$ * and $b_{i,m} = a_{i,m}$ except for $b_{i, M_i+1} = 1$, $a_{i,m}$ being the radix-R_i digits of A_i. Now, noting that, for each i,

$$A_i = \sum_{m=1}^{\infty} a_{i,m-1} R_i^m. \tag{16}$$

we observe that

$$N V = \sum_{\text{Each } m_i = 1}^{\infty} \left(\prod_{i=1}^{k} a_{i, m_i - 1} \right) (N/\Pi_i R_i^{m_i}). \tag{17}$$

Thus the error is

$$|S(\boldsymbol{A}) - N V| = \left| \sum_{\text{Each } m_i = 1}^{M_i+2} \left(\prod_{i=1}^{k} b_{i, m_i - 1} \right) \vartheta - \sum_{\text{Each } m_i = 1}^{\infty} \left(\prod_{i=1}^{k} a_{i, m_i - 1} \right) \{N/\Pi_i R_i^{m_i}\} \right|, \tag{18}$$

* There will be a distinct value of ϑ for each set $m_1, m_2, \ldots, m_k$.

where curly brackets denote the fractional part, and since $[N/R_i^{M_i+1}L]=0$ for any integer L. Since each of the sums above is positive, we increase the expression on the right of (18) by increasing the greater sum or decreasing the smaller. Thus ★

$$\left.\begin{aligned} |S(\boldsymbol{A})-NV| \leqq \max\Bigg(&\Bigg|\sum_{\text{Each } m_i=1}^{M_i+2}\Big(\prod_{i=1}^{k} b_{i,m_i-1}\Big)\big(\vartheta-\{N/\Pi_i R_i^{m_i}\}'\big)\Bigg|,\\ &\Bigg|\sum_{\text{Each } m_i=1}^{M_i+2}\Big(\prod_{i=1}^{k} c_{i,m_i-1}\Big)\big(\vartheta'-\{N/\Pi_i R_i^{m_i}\}\big)\Bigg|\Bigg),\end{aligned}\right\} \tag{19}$$

where the ϑ' and $\{N/\Pi_i R_i^{m_i}\}'$ vanish when any $m_i=M_i+2$ and $c_{i,m}=a_{i,m}$ except for $c_{i,M_i+1}=a_{i,M_i+1}+1$. Therefore, since $|\vartheta-\{N/\Pi_i R_i^{m_i}\}|<1$ and the same result holds for the primed quantities, and since $c_{i,m}\geqq a_{i,m}\geqq 0$,

$$|S(\boldsymbol{A})-NV| < \sum_{\text{Each } m_i=1}^{M_i+2}\Big(\prod_{i=1}^{k} c_{i,m_i-1}\Big)=\prod_{i=1}^{k}\Big(\sum_{m_i=1}^{M_i+2} c_{i,m_i-1}\Big), \tag{20}$$

whence

$$\left.\begin{aligned}\sup|S(\boldsymbol{A})-NV| &< \prod_{i=1}^{k}[M_i(R_i-1)+(2R_i-1)] <\\ &<(\ln N)^k\prod_{i=1}^{k}\Big(\frac{3R_i-2}{\ln R_i}\Big)\quad \text{if}\quad N>\text{every } R_i.\end{aligned}\right\} \tag{21}$$

Again, by (2) and (20)★★,

$$J<\prod_{i=1}^{k}\int_0^1 dA_i\Big(\sum_{m_i=1}^{M_i+2} c_{i,m_i-1}\Big)^2=\prod_{i=1}^{k}\sum_{\substack{\text{Possible}\\ \text{Digits}}} R_i^{-M_i-2}\Big(\sum_{m_i=1}^{M_i+2} c_{i,m_i-1}\Big)^2. \tag{22}$$

The squared quantity is one plus the sum of M_i+2 integers, each taking one of the values $0, 1, 2, \ldots, (R_i-1)$. Any particular sum q will occur T_q times, where T_q is the coefficient of z^q in $(1+z+z^2+\cdots+z^{R_i-1})^{M_i+2}$. We thus see that

$$\left.\begin{aligned} J &< \prod_{i=1}^{k} R_i^{-M_i-2}\,\Sigma_q T_q(q+1)^2=\prod_{i=1}^{k}R_i^{-M_i-2}\Big[\frac{d}{dz}\Big(z\frac{d}{dz}\{z\,\Sigma_q T_q z^q\}\Big)\Big]_{z=1}\\ &=\prod_{i=1}^{k}R_i^{-M_i-2}\Big[\frac{d}{dz}\Big(z\frac{d}{dz}\{z(1+z+\cdots+z^{R_i-1})^{M_i+2}\}\Big)\Big]_{z=1}\\ &=\prod_{i=1}^{k}\Big\{1+\frac{3}{2}(M_i+2)(R_i-1)+\frac{1}{4}(M_i+2)(M_i+1)(R_i-1)^2+\\ &\quad+\frac{1}{3}(M_i+2)(R_i-1)(R_i-2)\Big\},\\ \text{or}\\ J &< 4^{-k}\prod_{i=1}^{k}(M_i+3)^2(R_i-1)^2<4^{-k}\prod_{i=1}^{k}\frac{(R_i-1)^2}{\ln R_i}(\ln N+3\ln R_i)^2.\end{aligned}\right\} \tag{23}$$

★ If the first sum is the greater, $|S(\boldsymbol{A})-NV|$ will be less than the result of taking the second sum in the expression on the right of (18) up to M_i+1 only. If the second sum is the greater, we correspondingly take the first sum up to M_i+1 only, and put c for a in the second sum and terminate it at M_i+2 (This is simply the process of "rounding-up" the fractions A_i). It follows that $|S(\boldsymbol{A})-NV|$ will in either case be less than the greater of the two resulting expressions. The inequality (19) will follow if we make all sums up to M_i+2 by using the primed quantities as shown.

★★ Here $\sum\limits_{\substack{\text{Possible}\\ \text{Digits}}} = \sum\limits_{\text{Each } a_{i,m_i-1}=0}^{R_i-1}$ and $c_{i,m}$ and $a_{i,m}$ are related as previously stated.

Thus, when $N > \max_i (R_i^3)$, for instance,

$$J < \left(2^{-k} \prod_{i=1}^{k} \frac{(R_i - 1)^2}{\ln R_i}\right) (\ln N)^{2k}. \tag{24}$$

We may now turn to the case of the Hammersley sequence (10). The process described for k dimensions above now holds for $(k-1)$ dimensions only. Of the N fractions n/N $(n = 1, 2, \ldots, N)$, only the first NA fall below A, and so only the first $[NA]$ integers can be considered as candidates for a $(k-1)$-dimensional sequence of type (11). Noting that $[[NA]/L] = [NA/L]$ for any integer L, we observe, therefore, that if k is replaced by $k-1$ and N by NA, while leaving NV unchanged*, the results (15) to (20) will still hold for the present case. Thus we obtain

$$\left.\begin{aligned} \sup |S(\boldsymbol{A}) - NV| &< \prod_{i=1}^{k-1} [M_i(R_i - 1) + (2R_i - 1)] < \\ &< (\ln N)^{k-1} \prod_{i=1}^{k-1} \left(\frac{3R_i - 2}{\ln R_i}\right) \quad \text{if} \quad N > \text{every } R_i, \end{aligned}\right\} \tag{25}$$

and, similarly,

$$J < 4^{-(k-1)} \prod_{i=1}^{k-1} (M_i + 3)^2 (R_i - 1)^2 < 4^{-(k-1)} \prod_{i=1}^{k-1} \frac{(R_i - 1)^2}{\ln R_i} (\ln N + 3 \ln R_i)^2, \tag{26}$$

whence, if $N > \max_i (R_i^3)$, for example,

$$J < \left(2^{-(k-1)} \prod_{i=1}^{k-1} \frac{(R_i - 1)^2}{\ln R_i}\right) (\ln N)^{2(k-1)}. \tag{27}$$

We see that these results are the same as (5) and (6), with

$$\left.\begin{aligned} B_k &= 2^{-(k-1)} \prod_{i=1}^{k-1} \frac{(R_i - 1)^2}{\ln R_i}, \\ C_k &= \prod_{i=1}^{k-1} \left(\frac{3R_i - 2}{\ln R_i}\right). \end{aligned}\right\} \tag{28}$$

5. Some further remarks

The result (5) matches VAN DER CORPUT'S inequality (4) when $k = 2$. It confirms HAMMERSLEY'S conjecture. The result (6) is supplementary to this, and of comparable strength. There is still, unfortunately, a considerable gap between (6) and ROTH'S lower bound (3). There are evidently three possible causes for this. (i) My results may not be as strong as possible. (ii) There may be a different sequence from that of VAN DER CORPUT and HAMMERSLEY, for which a stronger result than mine may be deduced (just as the sequence (10) gives a stronger result, namely (6), than the result (24) for the sequence I propose in (11)). (iii) ROTH'S result may be too weak. Of these, I have considered only the first two possibilities.

* The V in (17) to (20) must be interpreted as $A_1 A_2 \ldots A_{k-1}$ and multiplied by NA; but we now wish to consider $V = A A_1 A_2 \ldots A_{k-1}$; thus NV must be left unchanged.

Consider (i). The result (18) is exact. The step to (19) involves an increase in value by a factor of the order of $\Pi_i(1+M_i^{-1})$, which would not appreciably close the gap between (3) and (6). From (20) to (24), an approximation of the same order is again all that occurs. It would seem, therefore, that *the step from* (19) *to* (20), *in which the sign and magnitude of* $\psi = (\vartheta - \{N/\Pi_i R_i^{m_i}\})$ *is concerned,* is the only one where an improvement might be hoped for, to lead to a strengthening of the result (6).

In the absence of any detailed information about the behavior of ψ, we may observe that, if ψ is distributed symmetrically about zero (that is, if $\pm\psi$ are equally frequent), then the sums on the right of (19) will average out to a constant multiple of $[\Pi_i(M_i+2)]^{-\frac{1}{2}}$ times the product on the right of (20). Thus sup $|S(\boldsymbol{A}) - NV|$ and $\sqrt{J}$ will each be of the order of $(\ln N)^{k/2}$ for the sequence (11), and so of the order of $(\ln N)^{(k-1)/2}$ for the Hammersley sequence. We may thus *tentatively conjecture that positive constants* B'_k, C'_k *exist, such that*

$$\sup |S(\boldsymbol{A}) - NV| < C'_k(\ln N^{(k-1)/2}) \tag{29}$$

and

$$J < B'_k(\ln N)^{k-1}, \tag{30}$$

for the Hammersley sequence, with similar results for the sequence (11).

Consider now (ii). I have considered the effect, for given N and a one-dimensional sequence, $\varphi_R(1), \varphi_R(2), \ldots, \varphi_R(N)$, of type (11), of weighting points according to the number of digits in the corresponding integer. The $(R^m - R^{m-1})$ points generated by m-digit integers are given a weight W_m. Then, if we put $W_0 = 1$, $W_{M+1} = 0$, and $S_m = W_0 - W_{m+1}$ $(m = 0, 1, 2, \ldots, M)$, we get the relations

$$\left.\begin{aligned} \sum_{m=0}^{M} S_m = W_0 - W_{M+1} = 1, \qquad \sum_{m=0}^{M} S_m R^m = N, \\ |S(\boldsymbol{A}) - NV| = \left|\sum_{m=0}^{M} S_m\{A R^m\} - 1\right|. \end{aligned}\right\} \tag{31}$$

These lead to

$$J = \tfrac{1}{3}\sum_{m=0}^{M} S_m^2 + \tfrac{1}{2}\sum_{m=0}^{M}\sum_{n=0}^{m-1} S_m S_n(1 + \tfrac{1}{3}R^{n-m}). \tag{32}$$

The unweighted case gives $S_m = 0$ $(m = 0, 1, 2, \ldots, M-1)$, $S_M = 1$, whence

$$N = R^M, \quad J = \tfrac{1}{3}. \tag{33}$$

Note that, owing to the selection of N as a power of R, the $\ln N$ factor has been eliminated. Thus we see that (33) *is an improvement on* VAN DER CORPUT'S *result, for* $N = R^M$ *only.* It can be shown that the corresponding k-dimensional result simply multiplies the $(\ln N)^{2k}$ factor by $(k-1)^k/k^k$. (Only in the case of $k=1$ does this essentially alter the nature of J.) If we minimise (32), subject to the first equation in (31), we obtain the result that $J \sim \frac{1}{12}$, so that unequal weighting does not seem to be worth-while.

6. Computation of sequences

The following scheme is suitable for computing the successive members of the sequence,

$$\varphi_R(1), \varphi_R(2), \varphi_R(3), \ldots, \varphi_R(N), \ldots, \tag{34}$$

using only the operations available in digital computers. The operations listed below are carried out consecutively, unless a "jump" instruction intervenes.

Put $\varphi=0$

(I) Put $x=1-\varphi$ ← Enter

Put $y=1/R$

(II) Jump to (III) if $x>y$

Put new y = old y/R

Jump to (II)

$\boxed{\text{If } x>y}$

(III) Put new φ = old $\varphi+(R+1)\,y-1$ → Leave

The three-step loop starting at (II) finds the most significant (*i.e.* leftmost) digit, in the radix-R expression for the current fraction φ, which is less than $(R-1)$. The next value of φ is then computed by (III). For each successive value of φ, the routine is entered at (I) and left at (III).

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