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ABSTRACT

Useful theoretical formulae are presented for measuring, in a quadratic-mean sense, the extent to which a class of important sequences is imperfectly distributed in the unit square. Previous results of Halton and Zaremba are generalized for sequences based on an arbitrary radix. The new discrepancy formulae are exact and much easier to analyze and evaluate than previously known versions. The formulae have direct application in providing significantly improved error-bounds in the Quasi-Monte Carlo numerical integration of difficult functions.

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1. INTRODUCTION AND SUMMARY

In [1], Halton and Zaremba obtained exact mean-square discrepancy formulae for binary equidistributed sequences. In this work their results are extended to sequences of arbitrary radix.

Halton and Zaremba analyzed the Roth sequence:

$$\{\frac{n}{2^M}, \frac{n_0}{2} + \cdots + \frac{n_i}{2^{i+1}} + \cdots + \frac{n_{M-1}}{2^M}\}_{n=0}^{2^M-1}$$

where M is a positive integer, and where, in radix-two notation, $n = (n_{M-1} \cdots n_i \cdots n_0)_2$, and what is now termed the Zaremba sequence:

$$\{\frac{n}{2^M}, \frac{n'_0}{2} + \cdots + \frac{n'_i}{2^{i+1}} + \cdots + \frac{n'_{M-1}}{2^M}\}_{n=0}^{2^M-1}$$

where $n'_i = \begin{cases} 1 - n_i, & i \text{ even} \\ n_i, & i \text{ odd} \end{cases}, \quad i = 0,1,\cdots,M-1$.

These sequences are equidistributed because the fraction of sequence points in the box

$$\{(\xi,\eta) \mid 0 \leqq \xi \leqq x \leqq 1, \quad 0 \leqq \eta \leqq y \leqq 1\}$$

determined by (x,y) approaches the area xy of the box as M approaches infinity, for any (x,y) in the unit square. If S_N is a sequence of N points, and if $\nu(S_N,(x,y))$ is the number of points of S_N in the box, then the mean-square discrepancy of S_N is given by

$$\left(\int_0^1 dx \int_0^1 dy \left(\frac{\nu(S_N,(x,y))}{N} - xy\right)^2\right)^{1/2} .$$

Halton and Zaremba computed useful theoretical formulae for this discrepancy and the Roth and Zaremba sequences. Asymptotically, their results are $M/8.2^M$ and $\sqrt{5M}/8\sqrt{3}.2^M$, respectively. Since one is most interested in a small discrepancy, the Zaremba sequence is better than the Roth sequence.

The author has obtained analogous results for the generalized sequences (1) and (2) of arbitrary radix R. The principal discrepancy formulae achieved are those of (24) and (30) which are expressed in terms of R, $N = R^M$ and $u = \mu_{M-1} \equiv M-1 \pmod R$. The corresponding asymptotic discrepancies are $(R^2-1)M/12R^{M+1}$ and $\sqrt{(R^2-1)(3R^2+13)M}/12\sqrt{5}\cdot R^{M+1}$, respectively. The Zaremba-type sequence (2) dominates the Hammersley sequence (1) in discrepancy performance in the order of $\sqrt{M}$, as was the situation between the original Roth and Zaremba sequences.

An important paper [2] of Halton deals with the theoretical performance of sequences in the unit hypercube $U^k = [0,1]^k$. Halton estimates the discrepancy of the k-dimensional Hammersley sequence (and its variations)

$$\{\frac{n}{N}, \phi_{R_1}(n), \cdots, \phi_{R_{k-1}}(n)\}_{n=0}^{N-1} \qquad \text{(cf. (3))}$$

where $R_1, \cdots, R_{k-1}$ are the first $k-1$ primes. He obtained for this construction and the quantity

$$\mathcal{J}(S_N) = \int_{U^k} dp(\nu(S_N, p) - N \prod_{i=1}^{k} x_i)^2$$

where $p = (x_1, \ldots, x_k)$, the upper-bound on $\mathcal{J}$ of

$$4^{1-k} \prod_{i=1}^{k-1} \frac{R_i^2}{(\ln R_i)^2} (\ln N + \frac{13}{6} R_i)^2$$

$$\leqq \prod_{i=1}^{k-1} \frac{R_i^2}{(\ln R_i)^2} (\ln N)^{2k-2}, \text{ if } N \geqq \max_i \{R_i^{\frac{13}{6}}\} .$$

The coefficient depending on k in this estimate is the result of corrections made by Halton and the present author, in collaboration. They also observed that the same bound prevailed if the i-th coordinate of the Hammersley sequence was perturbed by adding to ϕ_{R_i}, modulo R_i, component-by-component, the fixed fraction,* cf. (4)

$$\mu_i = (0.\overline{012 \cdots (R_i-1)})_{R_i}, \quad i = 1,2,\cdots,k-1.$$

Note that $\mathscr{D}(S_N) = N^2\mathscr{T}^2(S_N)$, if $\mathscr{T}(S_N)$ is the discrepancy of S_N in k dimensions. From this and the constructed upper bound, it follows that sequences can be found in two dimensions with a discrepancy of $O(\log N/N)$. The Roth, Zaremba, (1), and (2) sequences do at least this well because they are essentially of the same construction as the Hammersley sequence. Unfortunately, the bounding techniques do not predict the significantly better behavior (by $\sqrt{\log N}$) for the Zaremba sequences.

The question arises as to the best one can do. Roth showed [3] that there exists a constant $c_k > 0$, such that for any sequence S_N in U^k,

$$c_k \frac{(\log N)^{\frac{k-1}{2}}}{N} \leqq \mathscr{T}(S_N) .$$

For $k = 2$, this implies that the Zaremba sequences achieve the best possible asymptotic order. There is a considerable gap in the asymptotic constants, however, e.g., $c_2 = 2^{-8}$ for $\log_2 N$. Considering the effort invested in depressing the upper bound on attainable discrepancies by constructing good

*This perturbation is due to Halton and Warnock.

sequences [4,5], perhaps it would be worthwhile to attack the problem of improving Roth's lower bound with the same vigor.

These theoretical bounds are too gross to be very useful in practical applications such as numerical integration. Exact formulae, provided they can be evaluated with reasonable efficiency, are preferred. Another point in favor of cultivating various discrepancy formulae is that such work leads to less costly algorithms (usually faster programs) for evaluation.

The sequences under discussion are appealing because they have low discrepancy [5], a nice structure that is not difficult to generate [6], and a prototype quality that naturally leads to other interesting sequences. Even so, the formulae encountered in working with the sequences are sufficiently complex to require the support of an automated symbolic manipulation facility. Halton and the author have jointly developed such a system, called the SYMPØL*CALCULUS [8].

The foremost application for sequences of low discrepancy is in the numerical integration of difficult functions that are either multidimensional with large k, or expensive to evaluate, or both. For domains of integration that can be suitably related to the unit hypercube, e.g., domains that are finite unions of k-dimensional intervals, and for classes of functions whose mixed partial derivatives exist, the error of numerical integration using such sequences can be guaranteed within a certain bound. For the k-cube this bound consists of a finite sum of terms each composed of a discrepancy factor depending only on the projection of the sequence on a k'-subcube, $k' \leqq k$, and the quadratic mean for the corresponding mixed partial derivative, a factor that depends only on the function.

The mathematical substantiation of the above statements has been presented many times and is readily available [4,8,10]. Accordingly, the mathematics is merely sketched for the unit square.

Let $\mathrm{rms}(\cdot) = (\int_{U^2} dxdy(\cdot)^2)^{1/2}$ denote the (root) mean square of $(\cdot)$, and let $f(x,y)$ belong to the class of functions whose partial derivatives f_{xy}, f_x and f_y are finite in quadratic mean, i.e., $\mathrm{rms}(f_{xy})$, $\mathrm{rms}(f_x)$ and $\mathrm{rms}(f_y)$ are all finite. Furthermore, let $\langle S_N \rangle_x$ and $\langle S_N \rangle_y$ denote the projection of a sequence $S_N = \{x_n, y_n\}_{n=0}^{N-1}$ in U^2 onto the coordinate $y = 1$ and $x = 1$, respectively. Then the numerical integration error

$$\varepsilon(f, S_N) = \int_{U^2} dx\, dy\, f(x,y) - \frac{1}{N} \sum_{n=0}^{N-1} f(x_n, y_n)$$

can be estimated by

$$|\varepsilon(f, S_N)| \leqq \mathrm{rms}(f_{xy}(x,y)) \cdot \mathcal{T}(S_N) + \mathrm{rms}(f_x(x,1)) \cdot \mathcal{T}(\langle S_N \rangle_x)$$

$$+ \mathrm{rms}(f_y(1,y)) \cdot \mathcal{T}(\langle S_N \rangle_y)$$

where each $\mathcal{T}$ denotes an rms discrepancy.

The advantage of utilizing cleverly constructed sequences of low discrepancy, viz., quasirandom sequences, rather than pseudorandom sequences, which are generally expected to pass a number of statistical tests--unnecessarily, for this application--or random sequences, is that many fewer sequence points are required to achieve a given error bound. Hence, the evaluation of f in the simple quadrature formula above is much less costly. This advantage is especially pronounced in two dimensions [5], for a random sequence yields the expected value for $\mathcal{T}$ of

$$\frac{(2^{-k} - 3^{-k})^{1/2}}{N^{1/2}}$$

a quantity that decreases with increasing k, while quasirandom sequences e.g., the binary Zaremba sequence, exist with a discrepancy of $(\log_2 N)^{1/2}/8N$, a much smaller quantity for $k = 2$ and large values of N.

2. PROBLEM FORMULATION

For any positive integer M and any radix $R = 2,3,4,\ldots,$ let $\mathscr{R} = \{0,1,2,\ldots,R-1\}$, and let $N = R^M$ be the number of points in a restricted quasirandom sequence. $\mathscr{P}_N$ is used generically for either of the two-dimensional sequences

1) $$\mathscr{X}_N := \{(\frac{n}{N}, \phi_R(n))\}_{n=0}^{N-1}$$

2) $$\mathscr{Z}_N := \{(\frac{n}{N}, \phi_R(n) \oplus \mu)\}_{n=0}^{N-1}$$

where

3) $$\phi_R(n) := (0.n_0n_1\ldots n_i\ldots)_R := \frac{1}{R}\sum_{i=0}^{\infty} n_iR^{-i}$$

with $n_i \in \mathscr{R}$, $i = 0,1,2,\ldots,$ and $(\ldots n_i\ldots n_1n_0)_R := \sum_{i=0}^{\infty} n_iR^i$, the R-adic expansion of the nonnegative integer n, and where μ is the <u>non-terminating</u> fixed R-adic fraction

4) $$\mu := (0.012\ldots(R-1)0\ 1\ 2\ldots(R-1)0\ 1\ 2\ \ldots)_R$$

$$:= (0.\overline{012\ldots(R-1)})_R := \frac{1}{R}\sum_{i=0}^{R-1} iR^{-i}\sum_{j=0}^{\infty} R^{-jR}$$

$$= \frac{1}{R-1}\left(\frac{1}{R-1} - \frac{R}{R^R-1}\right).$$

The $\oplus$ of (2) denotes <u>mod R addition component-by-component</u>, i.e.,

$$\phi_R(n) \oplus \mu = (0.(n_0 \oplus 0)(n_1 \oplus 1)\cdots(n_i \oplus (i \bmod R))\cdots)_R$$

$$n_i \oplus (i \bmod R) = \begin{cases} n_i + (i \bmod R), & n_i + (i \bmod R) < R \\ R-n_i-(i \bmod R), & n_i + (i \bmod R) \geqq R. \end{cases}$$

Since $N = R^M$, and because the points of $\mathscr{P}_N$ are equally spaced in the first coordinate, by (1) and (2), it is convenient to partition U^2 into R vertical strips, each containing R^{M-1} points of $\mathscr{P}_N$, by defining the <u>boundaries</u>

5) $$\hat{x}_i := \frac{i}{R}, \; i \in \mathscr{R} .$$

Clearly, the R^{M-1} points of the <u>i^{th} strip</u>

$$\mathscr{S}_i = \{p \in U^2 \,|\, x \in [\hat{x}_i, \hat{x}_{i+1}), \; y \in [0,1]\}$$

have the labels $iR^{M-1}, iR^{M-1}+1, \ldots, (i+1)R^{M-1}-1$. In the R-adic expansion for any of these labels, n say, $n_{M-1} = i$ and $n_j \equiv 0$, for all $j \geqq M$. The set $\{n_0, n_1, \ldots, n_{M-2}\}$ assumes all R^{M-1} possible combinations of values over the labels of $\mathscr{S}_i$. Hence, the R^{M-1} points of $\mathscr{P}_N$ in $\mathscr{S}_i$ are equally spaced in the second coordinate as well, with a spacing of R^{1-M}. Furthermore, the y coordinate of the lowest point of the group is given by

6) $$\hat{y}_i := \begin{cases} iR^{-M} \equiv \dfrac{i}{N}, \text{ for } \mathfrak{X}_N \\[2ex] (i \oplus \mu_{M-1})R^{-M} + \dfrac{1}{R} \displaystyle\sum_{j=M}^{\infty} \mu_j R^{-j} \\[2ex] \equiv \dfrac{(i \oplus (M-1)) + \{N\mu\}}{N}, \text{ for } \mathfrak{Z}_N . \end{cases}$$

With the definition

7) $$\mathscr{G}(\mathscr{P}_N, p) := \nu(\mathscr{P}_N, (x,y)) - Nxy \equiv \sum_{n=0}^{N-1} H(x-x_n)H(y-y_n) - Nxy$$

where $H(z) := \begin{cases} 1, & z \geqq 0 \\ 0, & z < 0 , \end{cases}$

the objective function $\mathcal{J}(\mathcal{P}_N)$ becomes

8) $$\mathcal{J}(\mathcal{P}_N) := \int_0^1 dx \int_0^1 dy\ \mathcal{G}^2(\mathcal{P}_N, (x,y)).$$

The primary concern here is the derivation of useful formulae for (8) and the sequences of (1) and (2). In computing (8) it is helpful to be cognizant of the following auxiliary integrals and summations:

9) $$\mathcal{G}(\mathcal{P}_N) := \int_0^1 dx \int_0^1 dy\ \mathcal{G}(\mathcal{P}_N, (x,y))$$

$$\equiv \sum_{n=0}^{N-1} (1-x_n)(1-y_n) - \frac{N}{4}$$

10) $$\mathcal{X}(\mathcal{P}_N) := \int_0^1 dx\ x \int_0^1 dy\ \mathcal{G}(\mathcal{P}_N, (x,y))$$

$$\equiv \frac{1}{2} \sum_{n=0}^{N-1} (1-x_n^2)\ (1-y_n) - \frac{N}{6}$$

11) $$\mathcal{Y}(\mathcal{P}_N) := \int_0^1 dx \int_0^1 dy\ y\ \mathcal{G}(\mathcal{P}_N, (x,y))$$

$$\equiv \frac{1}{2} \sum_{n=0}^{N-1} (1-x_n)(1-y_n^2) - \frac{N}{6} .$$

Useful formulae for $\mathcal{G}(\mathcal{P}_N)$ and $\mathcal{X}(\mathcal{P}_N)$ are derived in Appendices $\mathcal{G}$ and $\mathcal{X}$, respectively.

In the case of the Zaremba sequence, formulae like (9) - (11), except that each y_n is smaller by a constant, are easier to calculate. The constant equals $\{N\mu\}/N$, the positive difference between μ and a μ that is truncated after the first M components.

With derivation techniques closely paralleling those of [11, Chapter 2], (8) can be rewritten as

12) $$\mathcal{J}(\mathcal{P}_N) = \sum_{i=0}^{R-1} \mathcal{J}_i(\mathcal{P}_N)$$

where for the i^{th} strip

13) $$\mathcal{J}_i(\mathcal{P}_N) := \int_{\hat{x}_i}^{\hat{x}_{i+1}} dx \left(\int_0^{\hat{y}_i} dy + \int_{\hat{y}_i}^{1} dy\right) \varphi^2(\mathcal{P}_N(x,y)).$$

With the change of variable $x \leftarrow R(x-\hat{x}_i)$, and by decomposing ν, (13) becomes

14) $$\mathcal{J}_i(\mathcal{P}_N) = \frac{1}{R}\int_0^1 dx \left(\int_0^{\hat{y}_i} dy(\nu(\mathcal{P}_{iw},(1,y)) - w(x+i)y)^2\right.$$

$$\left. + \int_{\hat{y}_i}^{1} dy(\nu(\mathcal{P}_{iw},(1,y)) + \nu(\mathcal{P}_w,(x,y-\hat{y}_i)) - w(x+i)y)^2\right)$$

where use is made of (5), (7), and the shorthand notation

15) $$w := R^{M-1} \equiv \frac{N}{R}.$$

One can write the following:

16) $$\mathcal{A}_i(\mathcal{P}_N) := \int_0^1 dy\ \nu^2(\mathcal{P}_{iw},(1,y))$$

17) $$\mathscr{B}_i(\mathscr{P}_N) := \int_0^1 dx \int_{\hat{y}_i}^1 dy \quad \nu(\mathscr{P}_w, (x, y-\hat{y}_i))\,\nu(\mathscr{P}_{iw}, (1, y))$$

18) $$\mathscr{C}_i(\mathscr{P}_N) := \int_0^1 dy\ y\ \nu(\mathscr{P}_{iw}, (1, y))$$

19) $$\mathscr{D}_i(\mathscr{P}_N) := \int_0^1 dx \int_0^{1-\hat{y}_i} dy(\nu(\mathscr{P}_w, (x, y)) - w(x+i)(y+\hat{y}_i))^2$$

$$+ (\frac{1}{3} + i + i^2)\frac{w^2\hat{y}_i^3}{3}$$

20) $$\mathscr{J}(\mathscr{P}_N) = \frac{1}{R}\sum_{i=0}^{R-1} (\mathscr{A}_i(\mathscr{P}_N) + 2\mathscr{B}_i(\mathscr{P}_N) - w(1+2i)\mathscr{C}_i(\mathscr{P}_N) + \mathscr{D}_i(\mathscr{P}_N)).$$

The component formulae $\mathscr{A}_i, \mathscr{B}_i, \mathscr{C}_i$ and $\mathscr{D}_i$ are derived in [11], but are omitted here.

3. RECURRENCE RELATIONS

Specializing now for $\mathscr{P}_N = \mathcal{X}_N$, (with ($\mathscr{G}$7), ($\mathscr{H}$7), $w = N/R$, and $\hat{y}_i = i/N$), (20) becomes

21)
$$\mathscr{J}(\mathcal{X}_N) = \mathscr{J}(\mathcal{X}_w) + (R-1)\left(-\frac{1}{R}\mathscr{H}(\mathcal{X}_w) + \frac{R+4}{6R}\mathscr{G}(\mathcal{X}_w) + \frac{(R+1)(R^2+1)}{90R^2} + \frac{1}{24R} - \frac{R^2+9R+1}{24RN} - \frac{2R-1}{72N^2}\right)$$

$$= \mathscr{J}(\mathcal{X}_w) + \frac{R-1}{12}\left(\frac{(R+1)(R^2-1)}{6R^2}M - \frac{(R+1)(R^2-9)}{30R^2} + \frac{R+1}{R} + \left(\frac{R^2-1}{2R}M - \frac{R+7}{2}\right)\frac{1}{N} + \frac{R+1}{6N^2}\right).$$

From this recursive relation it is a straightforward matter to postulate a $\mathscr{J}$ of the form

22)
$$\mathscr{J}(\mathcal{X}_N) = aM^2 + bM + c + \frac{dM+e}{N} + \frac{f}{N^2}$$

and solve for the unknown coefficients a, b, d, e and f, which may depend on R only, by equating like terms in the equation induced by (21) with

$$\mathscr{J}(\mathcal{X}_w) = a(M-1)^2 + b(M-1) + c + \frac{d(M-1)+e}{N/R} + \frac{R^2 f}{N^2}$$

appearing on the right-hand side. This procedure results in the partial solution

$$a = \frac{(R^2-1)^2}{144R^2} \qquad b = \frac{(R^2-1)(3R^2+60R+13)}{720R^2}$$

$$d = -\frac{R^2-1}{24R} \qquad e = \frac{1}{4} \qquad f = -\frac{1}{72} .$$

The remaining unknown c is determined using the initial condition, by (1), (3), (7) and (8),

$$\mathcal{J}(\chi_1) = \int_0^1 dx \int_0^1 dy\ (1-xy)^2 = \frac{11}{18} \tag{23}$$

corresponding to χ_w with $M = 1$ in the induction on M. Substituting (22) and (23) into (21), taking $N = R$, and solving for c using the known coefficients yields $c = 3/8$.

Thus, the complete solution for the Hammersley sequence is

$$\mathcal{J}(\chi_N) = \frac{(R^2-1)^2}{144R^2} M^2 + \frac{(R^2-1)(3R^2+60R+13)}{720R^2} M + \frac{3}{8} - \frac{R^2-1}{24RN} M + \frac{1}{4N} - \frac{1}{72N^2} \tag{24}$$

a major result. For the special binary ($R = 2$) case, (24) reduces to

$$\mathcal{J}(\chi_{2^M}) = \frac{M^2}{64} + \frac{29M}{192} + \frac{3}{8} - \frac{M}{16 \cdot 2^M} + \frac{1}{4 \cdot 2^M} - \frac{1}{72 \cdot 2^{2M}} \tag{25}$$

an expression that is well known, having been derived previously by Halton and Zaremba.

Turning now to the more complex case of $\mathscr{S}_N = \mathfrak{Z}_N$, (with ($\mathscr{S}$16), ($\mathscr{K}$13), $w = N/R$, and $\hat{y}_i = ((i \oplus u) + \{N\mu\})/N)$, with <u>$u := (M-1) \bmod R$</u>, (20) becomes

26)
$$\mathscr{H}(\mathfrak{Z}_N) = \mathscr{H}(\mathfrak{Z}_w) - \frac{(R-1)}{R}\mathscr{K}(\mathfrak{Z}_w)$$

$$+ \frac{6u^2-6Ru+R^2+3R-4}{6R}\,\mathscr{S}(\mathfrak{Z}_w)$$

$$+ \frac{u^4}{4R^2} - \frac{3R+1}{6R^2}u^3 + \frac{4R^2+3R-1}{12R^2}u^2 - \frac{R^2+R-1}{12R}u$$

$$+ \frac{8R^4+30R^2-30R-8}{720R^2} - \frac{2R^2-3R+1}{72N^2}$$

$$+ \frac{1}{N}\left(\frac{u^3}{6R} - \frac{2R+1}{4R}u^2 + \frac{4R+3}{12}u - \frac{R^3+8R^2-8R-1}{24R}\right) + F_1(\{N\mu\},N,u,R)$$

$\boxed{u\neq 0}$

$$= \mathscr{H}(\mathfrak{Z}_w) + \frac{u^5}{6R^2} - \frac{5u^4}{12R} + \frac{13R^2-1}{36R^2}u^3$$

$$- \frac{3R^4-4R^3-12R^2+26R-1}{24R^2(R-1)}u^2$$

$$+ \frac{R^5-5R^4-30R^3+110R^2-43R+39}{72R(R-1)^2}u$$

$$+ \frac{2R^7+9R^6-54R^5+13R^4-17R^3-114R^2-21R+2}{180R^2(R-1)^3}$$

$$+\frac{1}{N}\left(\frac{R+1}{12R}u^3-\frac{(R+1)^2}{8R}u^2+\frac{(R+1)(R+3)}{24}u\right.$$

$$\left.-\frac{5R^5-29R^4+32R^3-32R^2-R+1}{24R(R-1)^3}\right)+\frac{R^2-1}{72N^2}$$

$$+\frac{(R+1)R^R}{2(R-1)^2(R^R-1)}\left(R^{-1-(u-1)(\mathrm{mod}\ R)}-\frac{R}{N}\right)$$

$$+\ F_2(\{N\mu\},N,u,R)$$

$\boxed{u=0}$

$$=\mathcal{I}(\mathcal{Z}_W)+\frac{4R^8+14R^7-126R^6+314R^5-240R^4-374R^3+366R^2+46R-4}{360R^2(R-1)^4}$$

$$-\frac{5R^5-29R^4+32R^3-32R^2-R+1}{24R(R-1)^3N}+\frac{R^2-1}{72N^2}+\frac{R+1}{2(R-1)^2(R^R-1)}\left(1-\frac{R^{R+1}}{N}\right)$$

$$+\ F_3(\{N\mu\},N,0,R)$$

where F_1, F_2 and F_3 are complicated functions with the property that $F_i(0,N,u,R)\equiv 0$, $i=1,2,3$. The explicit expressions for the F's are omitted since it is easier to solve the above recursion relations for $\mathcal{I}(\check{\mathcal{Z}}_N)$ with the truncated μ and subsequently derive the expression for $\mathcal{I}(\mathcal{Z}_N)$ using (32).

In proceeding to solve the recursive relations of (26), a $\mathcal{I}$ of the form

27) $$\mathcal{I}(\check{\mathcal{Z}}_N)=au^6+bu^5+cu^4+du^3+eu^2+fu+g$$

$$+\frac{hu^3+iu^2+ju+k+k_1R^u}{N}+\frac{\ell}{N^2}+mR^{-u}$$

is postulated for the truncated μ, where the fourteen coefficients, a, b, ..., k, k_1, ℓ, m are assumed to depend only on R. For the case $u \neq 0$, i.e., $M \not\equiv 1 \pmod{R}$, with u replaced by u − 1 and N replaced by N/R in (27) for $\mathcal{J}(\check{\mathfrak{z}}_w)$, and by equating like terms in the equation induced by (26) and (27), one obtains the partial solution

$$a = \frac{1}{36R^2} \qquad b = -\frac{R-1}{12R^2} \qquad c = \frac{13R^2-30R+9}{144R^2}$$

$$d = -\frac{3R^4-17R^3+11R^2+17R-2}{72R^2\ (R-1)}$$

$$e = \frac{R^6-14R^5+4R^4+108R^3-147R^2+126R-6}{144R^2\ (R-1)^2}$$

$$f = \frac{13R^7-9R^6-291R^5+767R^4-1093R^3+309R^2-429R+13}{720R^2\ (R-1)^3}$$

$$h = -\frac{R+1}{12R\ (R-1)} \qquad i = \frac{R^3-R^2-3R-1}{8R(R-1)^2} \qquad j = -\frac{R^4-4R^3-4R^2+16R+15}{24\ (R-1)^3}$$

$$k = -\frac{R^6-6R^5+21R^4-24R^3+51R^2+6R-1}{24R\ (R-1)^4} + \frac{(R+1)R^{R+1}}{2\ (R-1)^3\ (R^R-1)}$$

$$\ell = -\frac{1}{72} \qquad m = -\frac{(R+1)R^R}{2\ (R-1)^3\ (R^R-1)} .$$

The unknown k_1 is determined in a similar manner from the equation induced by (26) with $u = 0$:

$$\frac{k+k_1}{N} = \frac{h(R-1)^3+i(R-1)^2+j(R-1)+k+k_1R^{R-1}}{N/R}$$

$$- \frac{5R^5-29R^4+32R^3-32R^2-R+1}{24R(R-1)^3N} - \frac{(R+1)R^{R+1}}{2(R-1)^2(R^R-1)N}$$

with the solution

$$k_1 = \frac{R(R+1)}{2(R-1)^3(R^R-1)} \quad .$$

The remaining unknown g is determined by the initial condition for $M = 1$, when $\mathcal{J}$ is given by (24) with $N = R$, since $\check{\mathfrak{Z}}_R \equiv \mathcal{X}_R$, i.e.,

$$\text{28)} \qquad \mathcal{J}(\check{\mathfrak{Z}}_R) \equiv \mathcal{J}(\mathcal{X}_R) = \frac{2R^4+15R^3+60R^2+30R+3}{180R^2} \quad .$$

This, along with the solutions for k, k_1, ℓ and m and the equation induced by (27) with $u = 0$, implies that

$$g = \frac{4R^8+14R^7+39R^6-346R^5+690R^4-494R^3+711R^2+106R-4}{360R^2(R-1)^4}$$

$$- \frac{R+1}{2(R-1)^3(R^R-1)} \quad .$$

Now suppose that $u = 0$, i.e., that $M \equiv 1 \pmod R$. Then the $u = 0$ recursion relation of (26) and the $M \not\equiv 1$ solution with w replacing N and $R-1$ replacing u yield

$$\text{29)} \qquad \mathcal{J}(\check{\mathfrak{Z}}_N) = g + \frac{(R^2-1)(3R^2+13)}{720R} + \frac{k+k_1}{N} + \frac{\ell}{N^2} + m$$

which actually is <u>valid only for $M \equiv R + 1$</u>. Hence, it is apparent that g depends on M, contrary to the hypothesis for (27). This anomaly is accommodated by adding

$$\left\lfloor \frac{M-1}{R} \right\rfloor \cdot \frac{(R^2-1)(3R^2+13)}{720R}$$

to the current g to reflect the increases of (27) in steps at values of n where $M \equiv 1 \pmod R$.

Therefore, the original form of (27) is amended to

$$
\begin{aligned}
30) \qquad \mu(\check{\mathfrak{z}}_N) = {} & \frac{u^6}{36R^2} - \frac{R-1}{12R^2}u^5 + \frac{13R^2-30R+9}{144R^2}u^4 \\
& - \frac{3R^4-17R^3+11R^2+17R-2}{72R^2(R-1)}u^3 \\
& + \frac{R^6-14R^5+4R^4+108R^3-147R^2+126R-6}{144R^2(R-1)^2}u^2 \\
& + \frac{13R^7-9R^6-291R^5+767R^4-1093R^3+309R^2-429R+13}{720R^2(R-1)^3}u \\
& + \frac{4R^8+14R^7+39R^6-346R^5+690R^4-494R^3+711R^2+106R-4}{360R^2(R-1)^4} \\
& - \frac{R+1}{2(R-1)^3(R^R-1)}\left(1 + R^{R-u} - \frac{R^{R+1+u}}{N}\right) \\
& + \frac{(R^2-1)(3R^2+13)}{720R}\left\lfloor\frac{M-1}{R}\right\rfloor - \frac{1}{72N^2} \\
& - \frac{1}{N}\left(\frac{R+1}{12R(R-1)}u^3 - \frac{R^3-R^2-3R-1}{8R(R-1)^2}u^2\right. \\
& + \frac{R^4-4R^3-4R^2+16R+15}{24(R-1)^3}u \\
& \left. + \frac{R^6-6R^5+21R^4-24R^3+51R^2+6R-1}{24R(R-1)^4}\right) .
\end{aligned}
$$

This expression, which is now valid for all positive integers M and R (except $R = 1$, of course), is the principal result; (30) is the complete solution for the Zaremba sequence with the truncated μ .

For the special case $R = 2$, $u^k \equiv u = 1 - \varepsilon_M$, $k = 2,3,\ldots,6$, where $\varepsilon_M = 1$ (0) if M is odd (even), and (30) reduces to

$$\text{31)} \qquad \mathcal{J}(\check{\mathcal{Z}}_{2M}) = \frac{5M}{192} + \frac{24+9\varepsilon_M}{64} + \frac{36-49\varepsilon_M}{16\cdot 2^M} - \frac{1}{72\cdot 2^{2M}}$$

using the facts that

$$\left\lfloor \frac{M-1}{2} \right\rfloor \equiv \frac{M}{2} - 1 + \frac{\varepsilon_M}{2}$$

and $\varepsilon_M^k \equiv \varepsilon_M$, $k = 1,2,\ldots$. This is a new binary result which is to be compared with the corresponding expression

$$\frac{5M}{192} + \frac{24-7\varepsilon_M}{64} + \frac{4+\varepsilon_M}{16\cdot 2^M} - \frac{1}{72\cdot 2^{2M}}$$

derived by Halton and Zaremba for the truncated ordinate perturbation $(0.10101\cdots)_2$.

The R-adic formula for $\mathcal{J}$ with the non-terminating μ is obtained via the following auxiliary expression for $\mathcal{P}_N = \mathcal{X}_N$ or $\mathcal{Z}_N$ which is developed using (1), (2), (7) and (8):

$$\text{32)} \qquad \mathcal{J}(\mathcal{P}_N) = \int_0^1 dx \int_0^1 dy \left(\sum_{n=0}^{N-1} H(x-x_n)H(y-y_n) - Nxy \right)^2$$

$$= \sum_{n=0}^{N-1} (1-x_n)(1-y_n) + 2 \sum_{n=1}^{N} n(1-x_n) - \frac{N}{2} \sum_{n=0}^{N-1} (1-x_n^2)(1-y_n^2)$$

$$- 2 \sum_{n=1}^{N-1} (1-x_n) \sum_{m=0}^{n-1} \max\{y_n, y_m\} + \frac{N^2}{9}$$

$$= -2 \sum_{n=1}^{N-1} (1-x_n) \sum_{m=0}^{n-1} \max\,\{y_n, y_m\} - \frac{N}{2} \sum_{n=0}^{N-1} x_n^2 y_n^2$$

$$+ \sum_{n=0}^{N-1} x_n y_n + \frac{5N^2}{18} - \frac{N}{2} + \frac{5}{6}$$

where the fact that $x_n > x_m$, for $n > m$, is also utilized.

Although (32) is easily derived, this formula is much less efficient than (24) and (30) for calculating the discrepancies for $\mathcal{X}_N$ and $\mathfrak{Z}_N$, at least for sufficiently large N. The relative computational efficiencies of such formulae are not pursued here. Using the summation form of (10), along with (32), and the fact that $x_n = n/N$, the $\mathcal{J}(\mathfrak{Z}_N)$ formula for the <u>non-terminating</u> μ is

33) $$\mathcal{J}(\mathfrak{Z}_N) = \mathcal{J}(\check{\mathfrak{Z}}_N) - c_N \sum_{n=0}^{N-1} (1-x_n) - \frac{N}{2} \sum_{n=0}^{N-1} (1-x_n^2)(-2c_N \check{y}_n - c_N^2)$$

$$- 2c_N \sum_{n=1}^{N-1} n(1-x_n)$$

$$= \mathcal{J}(\check{\mathfrak{Z}}_N) - 2Nc_N \mathscr{X}(\check{\mathfrak{Z}}_N)$$

$$+ \frac{c_N^2}{2}\left(\frac{2N^2}{3} + \frac{N}{2} - \frac{1}{6}\right) - \frac{c_N}{3}$$

where $\mathcal{J}(\check{\mathfrak{Z}}_N)$ and $\mathscr{X}(\check{\mathfrak{Z}}_N)$ are given by (30) and ($\mathscr{X}$13) and $c_N = \{N\mu\}/N$.

Appendix $\mathcal{G}$

For the truncated μ the integral form of (9) can be expressed as

$$\mathcal{G}1) \qquad \mathcal{G}(\check{\mathcal{P}}_N) = \frac{1}{R}\sum_{i=0}^{R-1} (\mathcal{V}_i(\check{\mathcal{P}}_N) + \mathcal{W}_i(\check{\mathcal{P}}_N)) - \frac{N}{4} .$$

where

$$\mathcal{G}2) \qquad \mathcal{V}_i(\check{\mathcal{P}}_N) := \int_0^1 dy \;\; \nu(\check{\mathcal{P}}_{iw}, (1, y))$$

$$\mathcal{G}3) \qquad \mathcal{W}_i(\check{\mathcal{P}}_N) := \int_0^1 dx \int_{\check{y}_i}^1 dy \;\; \nu(\check{\mathcal{P}}_w, (x, y-\check{y}_i))$$

and $\check{y}_i = \hat{y}_i - c_N = (i \oplus (M-1))/N = (i \oplus u)/N$. ($\mathcal{G}$ 2) becomes

$$\mathcal{G}4) \qquad \mathcal{V}_i(\check{\mathcal{P}}_N) = \sum_{j=0}^{i-1} \int_{\check{y}_j}^1 dy(1+[w(y-\check{y}_j)])$$

$$= \frac{w+1}{2} i - w \sum_{j=0}^{i-1} \check{y}_j .$$

Using (9), ($\mathcal{G}$ 3) can be rewritten as

$$\mathcal{G}5) \qquad \mathcal{W}_i(\check{\mathcal{P}}_N) = \sum_{n=0}^{w-1} \int_{x_n}^1 dx \int_{\check{y}_i+\check{y}_n}^1 dy$$

$$= \mathcal{G}(\check{\mathcal{P}}_w) + \frac{w}{4} - \frac{w+1}{2}\check{y}_i .$$

Specializing now for $\mathcal{X}_N$, by (6), ($\mathcal{G}$4) and ($\mathcal{G}$5), ($\mathcal{G}$1) results in the recursive relation

$$\mathcal{G}\,6)\qquad \mathcal{G}(\mathcal{X}_N) = \frac{1}{R}\sum_{i=0}^{R-1}\left(\frac{w+1}{2}\,i - w\sum_{j=0}^{i-1}\frac{j}{N} - \frac{w+1}{2}\,\frac{i}{N}\right)$$

$$+\ \mathcal{G}(\mathcal{X}_w) + \frac{w}{4} - \frac{N}{4}$$

$$= \mathcal{G}(\mathcal{X}_w) + \frac{1}{12}\left(R - \frac{1}{R}\right) - \frac{R-1}{4N}\ .$$

It is easily verified with (15) that the explicit formula

$$\mathcal{G}\,7)\qquad \mathcal{G}(\mathcal{X}_N) = \frac{M}{12}\left(R - \frac{1}{R}\right) + \frac{1}{2} + \frac{1}{4N}$$

satisfies ($\mathcal{G}$ 6) and the constraint or <u>initial condition</u> that $\mathcal{G}(\mathcal{X}_1) = 3/4$ which corresponds to $\mathcal{G}(\mathcal{X}_w)$ with $M = 1$.

Turning now to the more complex case for $\mathcal{Z}_N$, by (6), ($\mathcal{G}$4) and ($\mathcal{G}$5), ($\mathcal{G}$1) becomes

$$\mathcal{G}\,8)\qquad \mathcal{G}(\mathcal{Z}_N) = \frac{1}{R}\sum_{i=0}^{R-1}\left(\frac{w+1}{2}\,i - w\sum_{j=0}^{i-1}\frac{j \oplus u}{N} - \frac{w+1}{2}\,\frac{i \oplus u}{N}\right)$$

$$+\ \mathcal{G}(\check{\mathcal{Z}}_w) + \frac{w}{4} - \frac{N}{4}$$

$$= \mathcal{G}(\check{\mathcal{Z}}_w) + \frac{R-1}{4} - \frac{N+R}{2RN}\left(\frac{R-1}{2} + u - (R-\bar{u})H(u-1)\right)$$

$$-\ \frac{1}{R^2}\sum_{i=0}^{R-1}\left(\frac{(i-1)i}{2} + ui - R(i-\bar{u})H(i-\bar{u})H(u-1)\right)$$

where (15) and the fact that $H(R-\bar{u}) \equiv 1$, since $\underline{\bar{u} = R - u \pmod R}\ \varepsilon\ \mathcal{R}$, are also applied. Observe now that

$$u - (R-\bar{u})H(u-1) = 0\ ,\ \underline{\text{identically}},\ \text{even if } R = 2.$$

Further simplification of ($\mathcal{G}$8) yields

$$\mathcal{G}9)\qquad \mathcal{G}(\check{\mathfrak{z}}_N) = \mathcal{G}(\check{\mathfrak{z}}_w) + \frac{1}{12}(R - \frac{1}{R}) - \frac{R-1}{4N}$$

$$+ \frac{1}{R}(\frac{R-1}{2}((R-u) - \bar{u}) + \frac{\bar{u}}{2}(\bar{u}-R))H(u-1).$$

Since $u = 0$ implies $\bar{u} = 0$, and because of the equivalence

$$\bar{u}^2 \equiv \bar{u} \equiv 1-\varepsilon_M, \quad \text{for } R = 2, \text{ using (4)},$$

one can write ($\mathcal{G}$9) as

$$\mathcal{G}10)\qquad \mathcal{G}(\check{\mathfrak{z}}_N) = \mathcal{G}(\check{\mathfrak{z}}_w) + \frac{1}{12}(R - \frac{1}{R}) - \frac{R-1}{4N} - \frac{u}{2R}(R-u).$$

For $R = 2$, ($\mathcal{G}$10) reduces to

$$\mathcal{G}11)\qquad \mathcal{G}(\check{\mathfrak{z}}_{2^M}) = \mathcal{G}(\check{\mathfrak{z}}_{2^{M-1}}) - \frac{1}{8} + \frac{\varepsilon_M}{4} - 2^{-M-2}$$

where $\varepsilon_M = 0(1)$ for M even (odd).

The recursive relations ($\mathcal{G}$ 10) and ($\mathcal{G}$ 11) will be considered separately using <u>induction on M</u>. Relation ($\mathcal{G}$10) with $R > 2$ will be further separated into two cases determined by whether $u = 0$. One deduces that <u>$u = 0$ if and only if $M \equiv 1 \pmod{R}$</u>.

Taking the most interesting case first, suppose that $R > 2$ and that $u \neq 0$. Assume that $\mathcal{G}$ has the form

$$\mathcal{G}12)\qquad \mathcal{G}(\check{\mathfrak{z}}_N) = \frac{1}{4N} + au^3 + bu^2 + cu + d$$

where the constants a, b, c and d, which may depend on R but are independent of M, are to be determined. It is clear that the $1/4N$ term satisfies the recursion since $1/4N = 1/4w - (R-1)/4N$. The coefficients a, b and c are found by solving the equation induced by ($\mathcal{G}$ 10)

$$au^3 + bu^2 + cu = a(u-1)^3 + b(u-1)^2 + c(u-1)$$

$$+ \frac{1}{12}\left(R - \frac{1}{R}\right) - \frac{u}{2R}(R-u).$$

Equating coefficients of like powers of u results in the solution

$$a = \frac{1}{6R} \qquad b = -\frac{R-1}{4R} \qquad c = \frac{R-3}{12} \quad .$$

The constant d is determined from the initial condition for $M = 2$, the smallest value for which $u \neq 0$. Using the summation of (9), by direct calculation

$$(\mathscr{G}13) \qquad \mathscr{G}(\check{\mathfrak{Z}}_{R^2}) = 1 - \frac{R^2}{4} + \frac{1}{R^2} \sum_{n=0}^{R^2-1} n\,\check{y}_n \ .$$

The summation of $(\mathscr{G}13)$ can be written as

$$(\mathscr{G}14) \qquad \sum_{n=0}^{R^2-1} n\,\check{y}_n = \frac{1}{R} \sum_{(n_0,n_1)\,\varepsilon\,\mathfrak{R}\times\mathfrak{R}} (n_1R + n_0)\,(n_0 + (n_1 \oplus 1)R^{-1})$$

$$= \frac{1}{R}\left(2R \sum_{k=1}^{R-1} k^2 + (R + R^{-1})\left(\sum_{k=1}^{R-1} k\right)^2 - R \sum_{k=1}^{R-1} k\right)$$

$$= \frac{R^4}{4} + \frac{R^3}{6} - R^2 + \frac{R}{3} + \frac{1}{4}\ .$$

Thus, $(\mathscr{G}13)$ becomes

$$(\mathscr{G}15) \qquad \mathscr{G}(\check{\mathfrak{Z}}_{R^2}) = \frac{2R^3 + 4R + 3}{12R^2}$$

which, along with $(\mathscr{G}12)$ and the solution for a, b and c, implies that

$$d = \frac{R^2 + 6R - 1}{12R}$$

whence one obtains

$$\mathscr{g}16) \qquad \mathscr{g}(\check{\mathfrak{Z}}_N) = \frac{1}{4N} + \frac{u^3}{6R} - \frac{(R-1)}{4R}u^2 + \frac{R-3}{12}u + \frac{R^2+6R-1}{12R}$$

valid for $R > 2$ and $M \not\equiv 1 \pmod{R}$.

Now suppose that $R > 2$ but that $u = 0$. Then the recursion ($\mathscr{g}10$) and the $M \not\equiv 1$ solution ($\mathscr{g}16$) with w replacing N and $R-1$ replacing u yields the solution

$$\mathscr{g}17) \qquad \mathscr{g}(\check{\mathfrak{Z}}_N) = \frac{1}{4w} - \frac{(R-1)^3}{12R} + \frac{(R-3)(R-1)}{12} + \frac{R^2+6R-1}{12R}$$

$$+ \frac{1}{12}(R - \frac{1}{R}) - \frac{R-1}{4N}$$

$$= \frac{1}{4N} + \frac{R^2+6R-1}{12R}$$

valid for $R > 2$ and $M \equiv 1 \pmod{R}$. Note that ($\mathscr{g}7$) and ($\mathscr{g}17$) agree for $M = 1$, as they must. Since ($\mathscr{g}16$) reduces to ($\mathscr{g}17$) when $u = 0$, i.e., when $M \equiv 1 \pmod{R}$, <u>($\mathscr{g}16$) is valid for all M</u>.

For the $R = 2$ case, ($\mathscr{g}11$) is satisfied by

$$\mathscr{g}18) \qquad \mathscr{g}(\check{\mathfrak{Z}}_{2^M}) = 2^{-M-2} + \frac{\varepsilon_M}{8} + \frac{1}{2}$$

where the constant $1/2$ is forced by the initial condition $\mathscr{g}(\check{\mathfrak{Z}}_1) = 3/4$ corresponding to $\mathscr{g}(\check{\mathfrak{Z}}_w)$ with $M = 1$. It is noted that ($\mathscr{g}16$) and ($\mathscr{g}17$) each reduce to ($\mathscr{g}18$) when $R = 2$. Hence, <u>($\mathscr{g}16$) is valid</u> for $R = 2$, as well. This completes the derivation of explicit formulae for $\mathscr{g}(\check{\mathscr{P}}_N)$, namely, ($\mathscr{g}16$).

Using (9), it is now a simple matter to obtain a similar formula for $\mathscr{g}(\mathfrak{Z}_w)$

$$\mathscr{I}19) \qquad \mathscr{I}(\mathfrak{Z}_w) = \sum_{n=0}^{w-1} (1-x_n)(1-y_n) - \frac{w}{4}$$

$$= \mathscr{I}(\check{\mathfrak{Z}}_w) - c_N \sum_{n=0}^{w-1} (1-x_n)$$

$$= \mathscr{I}(\check{\mathfrak{Z}}_w) - \frac{(w+1)\{N\mu\}}{2N} \quad .$$

Appendix $\mathscr{K}$

For the truncated μ the integral form of (10) can be expressed as

$$\mathscr{K}1) \qquad \mathscr{K}(\check{\mathscr{I}}_N) = \frac{1}{R}\sum_{i=0}^{R-1}\left(\left(\frac{1}{2R}+\hat{x}_i\right)\mathcal{V}_i(\check{\mathscr{I}}_N)+\hat{x}_i\,\mathcal{W}_i(\check{\mathscr{I}}_N)\right.$$

$$\left.+\frac{1}{R}\mathscr{M}_i(\check{\mathscr{I}}_N)\right)-\frac{N}{6}$$

where $\mathcal{V}_i(\check{\mathscr{I}}_N)$ and $\mathcal{W}_i(\check{\mathscr{I}}_N)$ are given by ($\mathscr{G}$2) and ($\mathscr{G}$3), respectively, and where

$$\mathscr{K}2) \qquad \mathscr{M}_i(\check{\mathscr{P}}_N) := \int_0^1 dx\, x\int_{\check{y}_i}^1 dy\ \ \nu(\check{\mathscr{P}}_w,(x,y-\check{y}_i)).$$

Using (10), ($\mathscr{K}$2) can be rewritten as

$$\mathscr{K}3) \qquad \mathscr{M}_i(\check{\mathscr{P}}_N) = \sum_{n=0}^{w-1}\int_{x_n}^1 dx\, x\int_{\check{y}_i+\check{y}_n}^1 dy$$

$$= \mathscr{K}(\check{\mathscr{P}}_w)+\frac{w}{6}-\frac{4w^2+3w-1}{12w}\,\check{y}_i \quad .$$

Specializing now for χ_N, by (5), (6), ($\mathscr{G}$4) and ($\mathscr{G}$5), ($\mathscr{K}$1) results in the <u>recursive relation</u>

$$\mathscr{K}4) \qquad \mathscr{K}(\chi_N) = \frac{R-1}{2R}\left(\mathscr{G}(\chi_w)+\frac{w}{4}\right)-\frac{N}{6}+\frac{1}{R}\left(\mathscr{K}(\chi_w)+\frac{w}{6}\right)$$

$$+\frac{w+1}{8R}(R-1)+\frac{w+1}{12R}(R-1)(2R-1)$$

$$-\frac{w}{R}\sum_{i=0}^{R-1}\left(\frac{1}{2R}+\frac{i}{R}\right)\sum_{j=0}^{i-1}\frac{j}{N}$$

$$-\frac{1}{N}\sum_{i=0}^{R-1}\left(\frac{w+1}{2R}\,i+\frac{4w^2+3w-1}{12Rw}\right)\frac{i}{N}$$

$$= \frac{1}{R}\mathcal{X}(\chi_w) + \frac{R-1}{2R}\ \mathcal{G}(\chi_w) + \frac{R^2+R-2}{24R}$$

$$- \frac{4R^2-3R-1}{24RN} + \frac{R-1}{24N^2}$$

after some manipulation. Substitution for $\mathcal{G}(\chi_w)$ from ($\mathcal{G}$ 7) yields the following recursion in $\mathcal{X}$ alone:

($\mathcal{X}$ 5) $$\mathcal{X}(\chi_N) = \frac{1}{R}\,\mathcal{X}(\chi_w) + \frac{M(R^3-R^2-R+1)}{24R^2} + \frac{8R^2-7R-1}{24R^2}$$

$$- \frac{R^2-1}{24RN} + \frac{R-1}{24N^2} \ .$$

In solving for $\mathcal{X}(\chi_N)$, let the longer polynomials be denoted by

$$r := R^3-R^2-R+1 \qquad\qquad s := 8R^2-7R+1$$

and assume the following form:

($\mathcal{X}$ 6) $$\mathcal{X}(\chi_N) = aM+b + \frac{cM+d}{N} + \frac{e}{N^2} \ .$$

Then four of the five unknowns can be obtained by <u>equating coefficients of like terms</u> in the equation induced by ($\mathcal{X}$ 5):

$$aM + b + \frac{cM}{N} + \frac{e}{N^2} = \frac{1}{R}\left(a(M-1) + b + \frac{c(M-1)R}{N} + \frac{eR^2}{N^2}\right)$$

$$+ \frac{Mr+s}{24R^2} - \frac{R^2-1}{24RN} + \frac{R-1}{24N^2} \ .$$

The solution to the above equation is:

$$a = \frac{r}{24R(R-1)} = \frac{R^2-1}{24R} \qquad\qquad c = -\frac{R^2-1}{24R}$$

$$b = \frac{(R-1)s-r}{24R(R-1)^2} = \frac{7}{24} \qquad\qquad e = -\frac{1}{24} \ .$$

The remaining unknown is determined by the <u>initial condition</u> $\mathscr{X}(\chi_1) = 1/3$ corresponding to χ_w with $M = 1$. That is, from ($\mathscr{X}$6) with $M = 0$ and $N = 1$:

$$1/3 = b + d + e \quad \text{or} \quad d = 1/12.$$

Hence, one obtains

($\mathscr{X}$7)

$$\mathscr{X}(\chi_N) = \frac{M(R^2-1)}{24R} + \frac{7}{24} - \frac{M(R^2-1)}{24RN} + \frac{1}{12N} - \frac{1}{24N^2}$$

$$= \frac{1}{24}\left(\frac{M(R^2-1)}{R}\left(1 - \frac{1}{N}\right) + 7 + \frac{2}{N} - \frac{1}{N^2}\right).$$

Turning now to the more complex case for $\check{\mathfrak{z}}_N$, by (5), (6), ($\mathscr{G}$4), ($\mathscr{G}$5), and ($\mathscr{X}$3), ($\mathscr{X}$1) becomes

($\mathscr{X}$8)

$$\mathscr{X}(\check{\mathfrak{z}}_N) = \frac{1}{R}\left(\mathscr{X}(\check{\mathfrak{z}}_w) + \frac{w}{6}\right) + \frac{1}{R}\left(\mathscr{G}(\check{\mathfrak{z}}_w) + \frac{w}{4}\right)\sum_{i=0}^{R-1}\frac{i}{R} - \frac{N}{6}$$

$$+ \frac{1}{R^2}\sum_{i=0}^{R-1}\left(\frac{1}{2} + i\right)\left(\frac{w+1}{2}\, i - w \sum_{j=0}^{i-1}\frac{j \oplus u}{N}\right.$$

$$\left. - \frac{w+1}{2R}\sum_{i=0}^{R-1}\frac{i(i \oplus u)}{RN} - \frac{4w^2+3w-1}{12R^2 w}\sum_{i=0}^{R-1}\frac{i \oplus u}{N}\right.$$

$$= \frac{1}{R}\mathscr{X}(\check{\mathfrak{z}}_w) + \frac{R-1}{2R}\mathscr{G}(\check{\mathfrak{z}}_w) + \frac{R+1}{24} - \frac{1}{12R}$$

$$- \frac{4R^2-3R-1}{24RN} + \frac{R-1}{24N^2}$$

$$- u\left(\frac{1}{3} - \frac{1}{4N}\right) + \frac{u^2}{2R}\left(1 - \frac{1}{2N}\right) - \frac{u^3}{6R^2}$$

after considerable manipulation. For $R = 2$, ($\mathscr{X}$8) reduces to

$$(\mathscr{K}9)\qquad \mathscr{K}(\check{\mathfrak{Z}}_{2M}) = \frac{1}{2}\mathscr{K}(\check{\mathfrak{Z}}_{2M-1}) + \frac{1}{4}\,\mathscr{G}(\check{\mathfrak{Z}}_{2M-1}) - \frac{1}{24} - \frac{1}{16N} + \frac{\varepsilon_M}{8}(1-\frac{1}{N}) + \frac{1}{24N^2}$$

where $\varepsilon_M = 0(1)$ for M even (odd).

Substitution into ($\mathscr{K}$8) for $\mathscr{G}(\check{\mathfrak{Z}}_w)$, replacing N by N/R and u by $(u-1)(\mathrm{mod}\ R)$ in ($\mathscr{G}$16), yields the following recursion in $\mathscr{K}$ alone:

$$(\mathscr{K}10)\qquad \mathscr{K}(\check{\mathfrak{Z}}_N) = \frac{1}{R}\mathscr{K}(\check{\mathfrak{Z}}_w) - \frac{R^2-1}{24RN} + \frac{R-1}{24N^2} + \frac{(R-1)(R+8)}{24R} + \frac{R-3}{12R^2}u^3 - (\frac{R^2-4R-1}{8R^2} + \frac{1}{4RN})u^2 + (\frac{R^2-6R-3}{24R} + \frac{1}{4N})\,u\,.$$

In solving for $\mathscr{K}(\check{\mathfrak{Z}}_N)$, let the longer polynomials be denoted by:

$$q := R^2-1 \qquad\qquad r := R^2+7R-8$$

$$s := R^2-4R-1 \qquad\qquad t := R^2-6R-3$$

and assume the following form:

$$(\mathscr{K}11)\qquad \mathscr{K}(\check{\mathfrak{Z}}_N) = au^3 + bu^2 + cu + d + d_1R^{-u} + \frac{eu^3+fu^2+gu+h}{N} + \frac{\ell}{N^2}\ .$$

Then eight of the nine unknowns can be obtained by equating coefficients of like terms in the equation induced by ($\mathscr{K}$10) with $u \neq 0$:

$$au^3 + bu^2 + cu + d + \frac{eu^3+fu^2+gu}{N} + \frac{\ell}{N^2}$$

$$= \frac{1}{R}(a(u-1)^3 + b(u-1)^2 + c(u-1) + d + \frac{e(u-1)^3+f(u-1)^2+g(u-1)}{N/R}$$

$$+ \frac{\ell R^2}{N^2}) - \frac{q}{24RN} + \frac{R-1}{24N^2} + \frac{r}{24R}$$

$$+ \frac{R-3}{12R^2} u^3 - (\frac{s}{8R^2} + \frac{1}{4RN}) u^2 + (\frac{t}{24R} + \frac{1}{4N}) u .$$

The solution to the above equation is:

$$a = \frac{R-3}{12R(R-1)} \qquad b = - \frac{R^3 - 5R^2 + 5R - 5}{8R(R-1)^2}$$

$$c = \frac{R^5 - 8R^4 + 16R^3 - 24R^2 + 3R - 12}{24R(R-1)^3}$$

$$d = \frac{R^6 + 3R^5 - 21R^4 + 44R^3 - 27R^2 + 21R + 3}{24R(R-1)^4}$$

$$e = - \frac{1}{12R} \qquad f = \frac{R-1}{8R} \qquad g = - \frac{R-3}{24} \qquad \ell = - \frac{1}{24} .$$

The unknown d_1 is determined in a similar manner from the equation induced by $(\varkappa 10)$ with $u = 0$:

$$d + d_1 = \frac{1}{R}(a(R-1)^3 + b(R-1)^2 + c(R-1) + d + d_1 R^{1-u}) + \frac{r}{24R}$$

with the solution

$$d_1 = - \frac{(R+1)R^R}{2(R-1)^3 (R^R - 1)} .$$

It can be verified that the two equations in $1/N$ and $1/N^2$ that are induced by $(\varkappa 10)$ with $u = 0$ are already satisfied with the previously determined solution for e, f, g and ℓ. The remaining unknown h is determined by the initial condition for $M = 1$, when $\varkappa$ is given by $(\varkappa 7)$ with $N = R$, since $\mathfrak{z}_R \equiv \mathcal{X}_R$, i.e.,

$$(\mathcal{K}12) \qquad \mathcal{K}(\check{\mathcal{Z}}_R) \equiv \mathcal{K}(\mathcal{X}_R) = \frac{R^2+6R+1}{24R} .$$

This, along with the solutions for d, d_1 and ℓ and the equation induced by ($\mathcal{K}$11) with $u = 0$, implies that

$$h = -\frac{R^6-4R^5+15R^4-6R^3+13R^2+6R-1}{24R(R-1)^4} + \frac{(R+1)R^{R+1}}{2(R-1)^3(R^R-1)} .$$

Hence, ($\mathcal{K}$11) is

$$(\mathcal{K}13) \qquad \mathcal{K}(\check{\mathcal{Z}}_N) = \frac{R-3}{12R(R-1)}u^3 - \frac{R^3-5R^2+5R-5}{8R(R-1)^2}u^2$$

$$+ \frac{R^5-8R^4+16R^3-24R^2+3R-12}{24R(R-1)^3}u - \frac{1}{24N^2}$$

$$+ \frac{R^6+3R^5-21R^4+44R^3-27R^2+21R+3}{24R(R-1)^4}$$

$$- \frac{(R+1)}{2(R-1)^3} \; \frac{1-\dfrac{R^{u+1}}{N}}{R^R-1} \; R^{R-u}$$

$$- \frac{1}{N}\left(\frac{u^3}{12R} - \frac{R-1}{8R}u^2 + \frac{R-3}{24}u + \frac{R^6-4R^5+15R^4-6R^3+13R^2+6R-1}{24R(R-1)^4}\right) .$$

($\mathcal{K}$13) is valid for all values of M and R. For $R = 2$, $u^3 = u^2 = u = 1 - \varepsilon_M$, and ($\mathcal{K}$13) reduces to

$$(\mathcal{K}14) \qquad \mathcal{K}(\check{\mathcal{Z}}_{2^M}) = \frac{7}{24} + \frac{\varepsilon_M}{16} + \frac{1}{2^{M+2}}\left(\frac{1}{3} - \frac{\varepsilon_M}{4}\right) - \frac{1}{3\cdot 2^{2M+3}}$$

where $\varepsilon_M = 0(1)$ if M is even (odd), using the fact that

$$\left\lfloor\frac{M-1}{2}\right\rfloor \equiv \frac{M-1}{2} - \frac{1-\varepsilon_M}{2}$$

so that

$$2^{-2\left\lfloor\frac{M-1}{2}\right\rfloor-1} \equiv \frac{2-\varepsilon_M}{2^M}$$

and that

$$2^{-2\{\frac{M-1}{2}\}} \equiv \frac{1+\varepsilon_M}{2} \quad .$$

($\mathscr{K}$14) can also be obtained directly from ($\mathscr{K}$10) using the initial condition $\mathscr{K}(\check{\mathfrak{Z}}_1) \equiv \mathscr{K}(\mathcal{X}_1) = 1/3$ corresponding to w and M = 1.

Using (10), and the fact that $x_n = n/w$, the formula for $\mathscr{K}(\mathfrak{Z}_w)$ and the non-terminating μ is

$$\text{(}\mathscr{K}\text{15)} \qquad \mathscr{K}(\mathfrak{Z}_w) = \frac{1}{2}\sum_{n=0}^{w-1}(1-x_n^2)(1-(\check{y}_n+c_N)) - \frac{w}{6}$$

$$= \mathscr{K}(\check{\mathfrak{Z}}_w) - \frac{c_N}{2}\left(\frac{2w}{3}+\frac{1}{2}-\frac{1}{6w}\right)$$

$$= \mathscr{K}(\check{\mathfrak{Z}}_w) - \frac{\{N\mu\}}{2N}\left(\frac{2w}{3}+\frac{1}{2}-\frac{1}{6w}\right)$$

where $\mathscr{K}(\check{\mathfrak{Z}}_w)$ is given by ($\mathscr{K}$13).

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16. Abstracts

Useful theoretical formulae are presented for measuring, in a quadratic-mean sense, the extent to which a class of important sequences is imperfectly distributed in the unit square. Previous results of Halton and Zaremba are generalized for sequences based on an arbitrary radix. The new discrepancy formulae are exact and much easier to analyze and evaluate than previously known versions. The formulae have direct application in providing significantly improved error-bounds in the Quasi-Monte Carlo numerical integration of difficult functions.

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