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THE L^2 DISCREPANCY OF THE ROTH SEQUENCE IN $[0,1]^2$ FOR AN ARBITRARY NUMBER OF POINTS*

by

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ABSTRACT

An exact expression for the L^2 discrepancy D of the Roth sequence R_n in the unit square is computed for any $2^{M-1} \leqq n < 2^M$ points. Previously such a result was known only for powers of two. D is a measure of equidistributivity and has direct application in estimating the error of numerical integration formulae employing quasirandom sequences. The calculated $D(R_n)$ has approximately forty terms, typically consisting of a multiple summation over the bits of n with the inductive form

$$(e_t, e_{t-1}, \ldots, e_0)M := \sum_{r=t}^{M-1} n_{M-1-r} \left(2^{M-1-r}\right)^{e_t} (e_{t-1}, \ldots, e_0)r, \quad 0 \leqq t \leqq 4,$$

where $(e_{-1}, \ldots, e_0)r := 1$ and $(e_t, \ldots, e_0)M \equiv 0$ for $M \leqq t$. The computation, utilizing special algorithms developed for the manipulation of these summations and known formulae for n a power of two, indicates precisely the detailed structure of $D(R_n)$.

1. INTRODUCTORY REMARKS

This is an interim report giving some preliminary results of a Ph.D. dissertation investigation under Professor John H. Halton. The central theme of the planned thesis is the theoretical analysis of low-discrepancy quasirandom sequences with the goal of illuminating their detailed structure. This is expected to facilitate precise formulation and rigorous proofs of interesting qualitative behavior already observed experimentally such as global monotonicity, local anomalies and the relative performance of different sequences with respect to error bounds for quadrature formulae. It is anticipated that such a study will provide further justification for the use of certain point sets and lead to the discovery of additional low-discrepancy sequences of practical value [3,4].

This report is confined to the calculation of the L^2 discrepancy for an important well-known sequence in two dimensions. For the first time a formula (27) is obtained for an arbitrary number n of points in terms of the bits of n and involving summations up to an index of only $[\log_2 n]$ rather than $n - 1$. Because of the length and complexity of the computations it is felt that the attainment of this result would have been infeasible without the development of special symbolic manipulation routines which alleviated much of the tedium and increased the reliability of the intermediate calculations.

The further exploitation of these techniques should permit the extension of these findings to three dimensions in the forseeable future. A description of the computational aids employed and the analysis of the formulae (27 and 35) obtained here, including their asymptotic behavior, will be saved for a later report.

Being essentially theoretical in nature this effort can be viewed as a complement to some of Warnock's work which is broader in scope but has an experimental flavor. Incidentally, an expanded version of [3] just appeared as a Computer Sciences Department Ph. D. thesis.

2. DERIVATION OF THE MAIN RESULT

Let P_n represent a set of n points in the unit square S^2. For a given positive integer M, n is expressed in binary notation as

$$(1)\qquad 2^{M-1} \leqq n := (1\, n_{M-2} \cdots n_1\, n_0)_2 := \sum_{i=0}^{M-1} n_i \cdot 2^i < 2^M ,$$

where $n_i \in \{0,1\}$, $0 \leqq i \leqq M-2$, and $n_{M-1} \equiv 1$. Let the number of points of P_n in the rectangle $R(p) = \{q \mid q \leqslant p \in S^2\}$ be denoted by $\nu(P_n, p)$. Let (x_j, y_j) be the location of point $j = 0,1,\ldots,n-1$ of P_n, and take $p \equiv (x,y)$. If $H(z)$ is the Heaviside function

$$(2)\qquad H(z) := \begin{cases} 1, & z \geqq 0 \\ 0, & z < 0 \end{cases}$$

then ν can be expressed as

$$(3)\qquad \nu(P_n, p) := \sum_{j=0}^{n-1} H(x-x_j) \cdot H(y-y_j) .$$

For arbitrary $j = 0,1,\ldots,n-1$, let $\varphi_2(j)$ denote the binary fraction of j with the order of the bits reversed, i.e.

$$(4)\qquad 2^M \varphi_2(j) := (j_0\, j_1 \cdots j_{M-1})_2 = \sum_{i=0}^{M-1} j_{M-1-i} \cdot 2^i .$$

Then the Roth sequence [1, p. 43] can be defined as

$$(5)\qquad \left(\frac{j}{2^M}, \varphi_2(j)\right), \quad j = 0,1,\ldots,2^M - 1 .$$

Suppose this sequence is generalized from 2^M points to an arbitrary number in the range of 1 as follows. Scale the abscissas of 5 by the factor $2^M/n$ leaving the ordinates unchanged:

$$(6) \qquad (\tfrac{j}{n}, \varphi_2(j)), \quad j = 0,1,\ldots,n-1 .$$

The principal objective of this report is the calculation of

$$(7) \qquad J_n := \int_0^1 dx \int_0^1 dy \, (\nu(P_n, p) - n\,xy)^2$$

for the sequence of 6. Note the xy symmetry of 7 for 6 when n is a power of two. This computation extends the result of [2] for the Roth sequence of 5. J_n is related to the L^2 discrepancy T_n of P_n as $T_n := \sqrt{J_n}/n$.

For the trivial case $M = 1$, the only point of P_1 is at the origin, by 1 and 6. Hence, 7 becomes

$$J_1 = \int_0^1 dx \int_0^1 dy \, (1 - xy)^2 = \frac{11}{18} .$$

Henceforth it is assumed that $M > 1$, i.e., $n \geqq 2$.

In order to apply previously derived formulas for 2^η points, $\eta = 1,2,3,\ldots,$ it is convenient to subdivide the x interval as

$$(8) \qquad \bar{x}_m := \sum_{i=0}^{m-1} n_{M-1-i} \frac{2^{M-1-i}}{n}, \quad 1 \leqq m \leqq M \quad (\bar{x}_0 \equiv 0).$$

Then since $n_{M-1} \equiv 1$, 7 can be rewritten as

$$(9)\qquad J_n = \int_0^{\frac{2^{M-1}}{n}} dx \int_0^1 dy\, (\nu(P_n, p) - n\,xy)^2$$

$$+ \sum_{m=1}^{M-1} n_{M-1-m} \int_{\bar{x}_m}^{\bar{x}_{m+1}} \mathbf{dx} \int_0^1 dy\, (\nu(P_n, p) - n\,xy)^2 .$$

For the sequence of 6 with n defined by 1, there are 2^{M-1} points of P_n equally spaced in the interval $[0, x_1)$. Thus, with the change of variable $x \leftarrow n\,x/2^{M-1}$, the first term of 9 becomes

$$(10)\qquad I_0 := \frac{2^{M-1}}{n} \int_0^1 dx \int_0^1 dy\, (\nu(P_{2^{M-1}}, p) - 2^{M-1} xy)^2$$

$$= \frac{2^{M-1}}{n} J_{2^{M-1}}$$

by 7. The remainder of 9 can be expressed as

$$(11)\qquad \sum_{m-1}^{M-1} n_{M-1-m}\, I_m$$

where attention is now focussed on

$$(12)\qquad I_m := \int_{\bar{x}_m}^{\bar{x}_{m+1}} dx \int_0^1 dy\, (\nu(P_n, p) - nxy)^2 .$$

From 8, if $n_{M-1-m} = 0$, then $\bar{x}_{m+1} = \bar{x}_m$ and $I_m = 0$. If $n_{M-1-m} = 1$, then there are 2^{M-1-m} points of 6 equally spaced in the interval $[\bar{x}_m, \bar{x}_{m+1})$. These points are raised by an amount

$$(13) \qquad \bar{y}_m := y_{n\bar{x}_m} = \sum_{i=0}^{m-1} n_{M-1-i}\, 2^{i-M}, \; 1 \leq m < M \quad (\bar{y}_0 \equiv 0)$$

with respect to the 2^{M-1} points beginning at the origin. Therefore, 12 is separated into two parts by subdividing the y interval at $\bar{y}_m$

$$(14) \qquad I_m = \int_{\bar{x}_m}^{\bar{x}_{m+1}} dx \int_0^{\bar{y}_m} dy(\nu(P_n, p) - nxy)^2 + \int_{\bar{x}_m}^{\bar{x}_{m+1}} dx \int_{\bar{y}_m}^{1} dy(\nu(P_n, p) - nxy)^2 .$$

For $\bar{x}_m \leq x < \bar{x}_{m+1}$, ν can be decomposed as

$$(15) \qquad \nu(P_n, p) = \nu(P_{n\bar{x}_m}, (1, y)) + \nu(P_{u_m}, (\frac{n}{u_m}(x - \bar{x}_m), y - \bar{y}_m))$$

where

$$(16) \qquad u_m := 2^{M-1-m}, \quad 0 \leq m < M .$$

The second component of 15 is taken as zero for $y < \bar{y}_m$. It is valid to omit this second component in the first term of 14 since $y = \bar{y}_m$ only on a set of measure zero. The separation between $\bar{x}_m$ and $\bar{x}_{m+1}$ for 6 is

$$(17) \qquad \bar{x}_{m+1} - \bar{x}_m = \begin{cases} 0, & n_{M-1-m} = 0 \\ \dfrac{u_m}{n}, & n_{M-1-m} = 1 \end{cases}$$

from 8, so with the change of variable $x \leftarrow n(x-\bar{x}_m)/u_m$, 14 becomes

$$(18)\qquad I_m = \frac{u_m}{n}\int_0^1 dx \left(\int_0^{\bar{y}_m} dy(\nu(P_{n\bar{x}_m},(1,y)) - (u_m x + n\bar{x}_m)y)^2 \right.$$
$$\left. + \int_{\bar{y}_m}^1 dy(\nu(P_{n\bar{x}_m},(1,y)) + \nu(P_{u_m},(x,y-\bar{y}_m)) - (u_m x + n\bar{x}_m)y)^2 \right) .$$

For the purpose of calculation let

$$(19)\qquad A_m := \int_0^1 dy\ \nu^2(P_{n\bar{x}_m},(1,y))$$

$$(20)\qquad B_m := \int_0^1 dx \int_{\bar{y}_m}^1 dy\ \nu(P_{u_m},(x,y-\bar{y}_m)) \cdot \nu(P_{n\bar{x}_m},(1,y))$$

$$(21)\qquad C_m := \int_0^1 dy\ y\ \nu(P_{n\bar{x}_m},(1,y))$$

$$(22)\qquad D_m := \int_0^1 dx \int_0^{1-\bar{y}_m} dy(\nu(P_{u_m},(x,y)) - (u_m x + n\bar{x}_m)(y+\bar{y}_m))^2$$
$$+ \left(\frac{u_m^2}{3} + nu_m\bar{x}_m + n^2\bar{x}_m^2\right)\frac{\bar{y}_m^3}{3} .$$

Note the change of variable $y \leftarrow y - \bar{y}_m$ in the integral of D_m. Then collecting results 10-12 and 18, 7 can be expressed as

$$(23)\qquad J_n = \frac{1}{n}\left(u_0 J_{u_0} + \sum_{m=1}^{M-1} n_{M-1-m}\, u_m (A_m + 2B_m - (u_m + 2n\bar{x}_m)C_m + D_m)\right)$$

where 16 and 19-22 are used.

Observe that for $n = u_0$, 23 is useless since $n_{M-1-m} = 0$,

$1 \leq m \leq M-1$ by 1 and 17. However, it is already known [2] that

$$(24) \qquad J_{u_0} = \frac{M^2}{64} + \frac{23M}{192} + \frac{23}{96} - \frac{M-5}{8 \cdot 2^M} - \frac{1}{18 \cdot 2^{2M}} .$$

The component expressions 19-22 of J_n are computed in the appendices. The following shorthand notation is used to express results which involve multiple summations over the binary digits of n $\{n_{M-1-r} \mid 0 \leq r \leq M-1\}$ and powers of two. Let $\{e_k \mid k = 0, 1, \ldots, t\}$ be arbitrary integers denoting the exponents on the u_r's. Then the summation of order t is defined as

$$\text{a)} \quad (e_0)s := \sum_{r=0}^{s-1} n_{M-1-r} u_r^{e_0}$$

(25)

$$\text{b)} \quad (e_t, e_{t-1}, \ldots, e_0)s := \sum_{r=t}^{s-1} n_{M-1-r} u_r^{e_t} (e_{t-1}, \ldots, e_0)r .$$

The summations are taken as zero if $s \leq t$, where $t = 0$ in 25a) and $t > 0$ in 25b). Note that in this notation, from 8, 13, 16 and 25a)

$$\text{a)} \quad \bar{x}_m = \frac{1}{n}(1)m, \quad 0 \leq m \leq M$$

(26)

$$\text{b)} \quad \bar{y}_m = \frac{1}{2}(-1)m, \quad 0 \leq m < M .$$

A useful property for manipulating the product of a single summation $(e)s$ of the form 25a) and any summation $(e_t, e_{t-1}, \ldots, e_0)s$ of the form 25 of order $t \geq 0$ is given by Theorem 1. Note that the integer

s must be the same in both factors.

Theorem 1. For the summations of 25 the following identity holds (for all $t = 0,1,2,3,\dots$):

$$\begin{aligned}(e)s \cdot (e_t, e_{t-1}, \dots, e_0)s \equiv{} & (e+e_t, e_{t-1}, \dots, e_0)s \\ & + (e_t, e+e_{t-1}, \dots, e_0)s \quad + \cdots + (e_t, e_{t-1}, \dots, e+e_0)s \\ & + (e, e_t, e_{t-1}, \dots, e_0)s + (e_t, e, e_{t-1}, \dots, e_0)s \\ & + \cdots + (e_t, e_{t-1}, \dots, e_0, e)s\end{aligned}$$

$t+1$ summations of order t and $t+2$ summations of order $t+1$.

Proof. By 25 the left-hand side of the identity is $\sum_{r'=0}^{s-1} n_{M-1-r'} u_{r'}^{e} \cdot$ $\cdot \sum_{r=t}^{s-1} n_{M-1-r} u_r^{e_t} (e_{t-1}, \dots, e_0)r$, $t > 0$. This expression can be decomposed into the following three parts for $r' = r$, $r' > r$ and $r' < r$:

i) $$\sum_{r=t}^{s-1} n_{M-1-r}^2 u_r^{e+e_t} (e_{t-1}, \dots, e_0)r$$

ii) $$\sum_{r'=t+1}^{s-1} n_{M-1-r'} u_{r'}^{e} \sum_{r=t}^{r'-1} n_{M-1-r} u_r^{e_t} (e_{t-1}, \dots, e_0)r$$

iii) $$\sum_{r=t}^{s-1} n_{M-1-r} u_r^{e_t} \sum_{r'=0}^{r-1} n_{M-1-r'} u_{r'}^{e} (e_{t-1}, \dots, e_0)r \, .$$

Since $n_{m-1-r}^2 \equiv n_{M-1-r}$, i) is $(e+e_t, e_{t-1}, \dots, e_0)s$ by 25b). The inner summation of ii) is $(e_t, e_{t-1}, \dots, e_0)s$, so the whole summation is $(e, e_t, e_{t-1}, \dots, e_0)s$ by 25b). The inner summation of iii) is $(e)r \cdot (e_{t-1}, \dots, e_0)r$, an expression of the same form as the original left-hand side but with the summation order reduced by one. Hence, the identity follows by induction on t using 25 since for $t = 0$

$$(e)s' \cdot (e_0)s' = \sum_{r'=0}^{s'-1} n_{M-1-r'} u_{r'}^{e} \sum_{r''=0}^{s'-1} n_{M-1-r''} u_{r''}^{e_0}$$

$$= \sum_{r''=0}^{s'-1} n_{M-1-r''} u_{r''}^{e+e_0} + \sum_{r'=1}^{s'-1} n_{M-1-r'} u_{r'}^{e} \sum_{r''=0}^{r'-1} n_{M-1-r''} u_{r''}^{e_0}$$

$$+ \sum_{r''=1}^{s'-1} n_{M-1-r''} u_{r''}^{e_0} \sum_{r'=0}^{r''-1} n_{M-1-r'} u_{r'}^{e}$$

$$= (e+e_0)s' + (e,e_0)s' + (e_0,e)s'. \qquad \blacksquare$$

Combining the results A28, B17, C5 and D18 from the appendices, 23 becomes

$$(27)\quad J_n = \frac{1}{n}\Bigg(\sum_{m=0}^{M-1} n_{M-1-m} \frac{M-m}{8} \Bigg(\frac{M-m}{8} u_m - u_m(1,-1)m + u_m(0)m -$$

$$- \frac{u_m}{2}(u_m-1)(-1)m + \frac{23}{24} u_m - \frac{1}{2}\Bigg)$$

$$+ (1,1,1,-1,-1)M + \frac{1}{2}(1,1,-1,1,-1)M$$

$$+ \frac{1}{2}(2,1,-1,-1)M + \frac{1}{4}(2,-1,1,-1)M + \frac{1}{2}(1,2,-1,-1)M$$

$$+ \frac{1}{2}(1,1,1,-2)M - \frac{1}{2}(1,1,-1,0)M + \frac{1}{4}(1,1,-1,-1)M$$

$$- \frac{1}{2}(1,0,1,-1)M + \frac{1}{4}(1,-1,1,-1)M +$$

$$+\frac{1}{6}(3,-1,-1)M+\frac{1}{4}(2,1,-2)M$$

$$-\frac{1}{4}(2,-1,0)M+\frac{1}{8}(2,-1,-1)M+\frac{1}{4}(1,2,-2)M-\frac{35}{24}(1,1,-1)M$$

$$+\frac{1}{8}(1,1,-2)M+\frac{1}{2}(1,0,0)M+\frac{1}{4}(1,0,-1)M-\frac{1}{4}(1,-1,0)M$$

$$-\frac{1}{24}(1,-1,-1)M-\frac{1}{4}(0,1,-1)M+\frac{1}{12}(3,-2)M-\frac{25}{48}(2,-1)M$$

$$+\frac{1}{16}(2,-2)M+\frac{17}{24}(1,0)M-\frac{11}{16}(1,-1)M-\frac{1}{48}(1,-2)M$$

$$\left.+\frac{1}{4}(0,0)M+\frac{1}{24}(0,-1)M+\frac{23}{96}(1)M+\frac{5}{16}(0)M-\frac{1}{72}(-1)M\right)$$

where 26a) and the notation of 25 are utilized.

This rather lengthy expression 27 is the main result of this report. Although the formula still seems amenable to evaluation only with the aid of a computer, the homologous structure of the terms invites detailed analysis that promises a greater understanding of J_n for the Roth sequence than previously known formulae. The techniques for manipulating a typical term of 27 are currently being explored.

3. A SUPPLEMENTARY RESULT

Let P'_n be the same set as P_n except that the point at the origin is replaced by a point at $(1,1)$. By definition of ν it follows that $\nu(P'_n,p) \equiv \nu(P_n,p) - 1$ for all $p \in S^2$ except $p = (1,1)$ where both ν's equal n. Using 7 one can write

$$(28) \qquad J'_n = \int_0^1 dx \int_0^1 dy(\nu(P'_n,p) - nxy)^2$$

$$= J_n + 1 - 2 \int_0^1 dx \int_0^1 dy(\nu(P_n,p) - nxy).$$

With 8, 13 and 15-17 the last integral can be expressed as

$$(29) \qquad \sum_{m=0}^{M-1} n_{M-1-m} \int_{\bar{x}_m}^{\bar{x}_{m+1}} dx \int_0^1 dy(\nu(P_n,p) - nxy)$$

$$= \sum_{m=0}^{M-1} n_{M-1-m} \int_{\bar{x}_m}^{\bar{x}_{m+1}} dx(\int_0^{\bar{y}_m} dy(\nu(P_{n\bar{x}_m},(1,y)) - nxy)$$

$$+ \int_{\bar{y}_m}^1 dy(\nu(P_{n\bar{x}_m},(1,y)) + \nu(P_{u_m},(\frac{n}{u_m}(x-\bar{x}_m),y-\bar{y}_m)) - nxy)).$$

Proceeding in the same fashion as in the calculation of I_m, the first component of the summand of 29 becomes

$$(30) \qquad \frac{u_m}{n} \int_0^1 dx \int_0^{\bar{y}_m} dy(\nu(P_{n\bar{x}_m},(1,y)) - (u_m x + n\bar{x}_m)y)$$

$$= \frac{u_m}{n} \int_0^{\bar{y}_m} dy \ \nu(P_{n\bar{x}_m},(1,y)) - \frac{u_m}{2n} (\frac{u_m}{2} + n\bar{x}_m)\bar{y}_m^2 .$$

The second component of the summand becomes

$$(31)\qquad \frac{u_m}{n}\int_0^1 dx \int_{\bar{y}_m}^1 dy(\nu(P_{n\bar{x}_m},(1,y)) + \nu(P_{u_m},(x,y-\bar{y}_m)) - (u_m x + n\bar{x}_m)y)$$

$$= \frac{u_m}{n}\int_{\bar{y}_m}^1 dy\ \nu(P_{n\bar{x}_m},(1,y)) + \frac{u_m}{n}\int_0^1 dx \int_{\bar{y}_m}^1 dy\ \nu(P_{u_m},(x,y-\bar{y}_m))$$

$$- \frac{u_m}{2n}\left(\frac{u_m}{2} + n\bar{x}_m\right)(1-\bar{y}_m^2)\ .$$

Thus, with the definitions

$$(32)\qquad B'_m := \int_0^1 dx \int_{\bar{y}_m}^1 dy\ \nu(P_{u_m},(x,y-\bar{y}_m))$$

$$(33)\qquad C'_m := \int_0^1 dy\ \nu(P_{n\bar{x}_m},(1,y))$$

and combining 30 and 31, 29 can be rewritten as

$$(34)\qquad \frac{1}{n}\sum_{m=0}^{M-1} n_{M-1-m}\, u_m\left(B'_m + C'_m - \frac{1}{2}\left(\frac{u_m}{2} + n\bar{x}_m\right)\right).$$

From the results B18 and C8 of the appendices and applying 26a) in 34, 28 becomes

$$(35)\qquad J'_n = J_n + 1 - \frac{1}{n}\left(\sum_{m=0}^{M-1} n_{M-1-m}\ \frac{M-m}{4}\ u_m - (1,1,-1)M\right.$$

$$\left. - \frac{1}{2}(2,-1)M + (1,0)M - \frac{1}{2}(1,-1)M + \frac{3}{4}(1)M + \frac{1}{2}(0)M\right)$$

where the notation of 25 is used. The slight modification P'_n proposed by Warnock [3] evidently has a smaller discrepancy than the Roth sequence P_n according to experimental observations. It is simple to check that J_1' is only 1/9, which is precisely 1/2 less than J_1.

Just recently the author was successful in proving

Theorem 2. $J_n' < J_n$ for $n = 1,2,3,\ldots$.

The proof, which uses 35 and induction on the number of nonzero bits of n, will appear in a later report. A similar effort is underway to prove the more difficult hypothesis that T_n is monotone decreasing with n.

4. FORMULA EVALUATION AND VERIFICATION

An alternate formula for J_n involving summations up to an index of $n-1$ instead of $[\log_2 n]$ is readily obtained as follows. Using 2 and 3, 7 can be rewritten as

$$(36) \qquad J_n = \sum_{j=0}^{n-1} (1-x_j)(1-y_j) + 2\sum_{j=1}^{n-1}\sum_{k=0}^{j-1} (1-\max\{x_j,x_k\})(1-\max\{y_j,y_k\})$$
$$-\frac{n}{2}\sum_{j=0}^{n-1} (1-x_j^2)(1-y_j^2) + \frac{n^2}{9} .$$

From the fact that $x_j > x_k$ if $j > k$ for P_n or P_n' (see 6), for the Roth sequence 36 can be simplified to

$$(37) \qquad J_n = -2\sum_{j=1}^{n-1} (1-x_j)\sum_{k=0}^{j-1} \max\{y_j,y_k\} - \sum_{j=0}^{n-1} (1-x_j)y_j$$
$$+\frac{n}{2}\left(\sum_{j=0}^{n-1} (1-x_j^2)y_j^2 - \frac{2n}{9} + \frac{1}{2} + \frac{1}{4n}\right)$$

where A13 and A16 are also applied. From 2, 3 and 28 it is easily seen that a corresponding formula for J_n' is

$$(38) \qquad J_n' = J_n + 2\sum_{j=0}^{n-1} (1-x_j)y_j - \frac{n}{2} .$$

A straightforward FORTRAN program based on 37 and 38 was used to check the validity of 27 and 35 which are implemented with a much longer program designed to be reasonably efficient (timewise) in evaluating the discrepancies for many consecutive values of n. With

DOUBLE PRECISION on a UNIVAC 1108 computer exact agreement to eight decimal places was observed for $2 \le n \le 511$. The checking program ran for approximately six minutes while the running time of the program implementing 27 and 35 was only about thirty seconds* (see Table 1). Of course, the latter program would become even more efficient than the checking program for larger ranges of n. Graphs of these discrepancies $\sqrt{J_n}/n$ and $\sqrt{J'_n}/n$ using the symbols X and Y, respectively, are depicted in Figures 1, 2, 3 and 4.

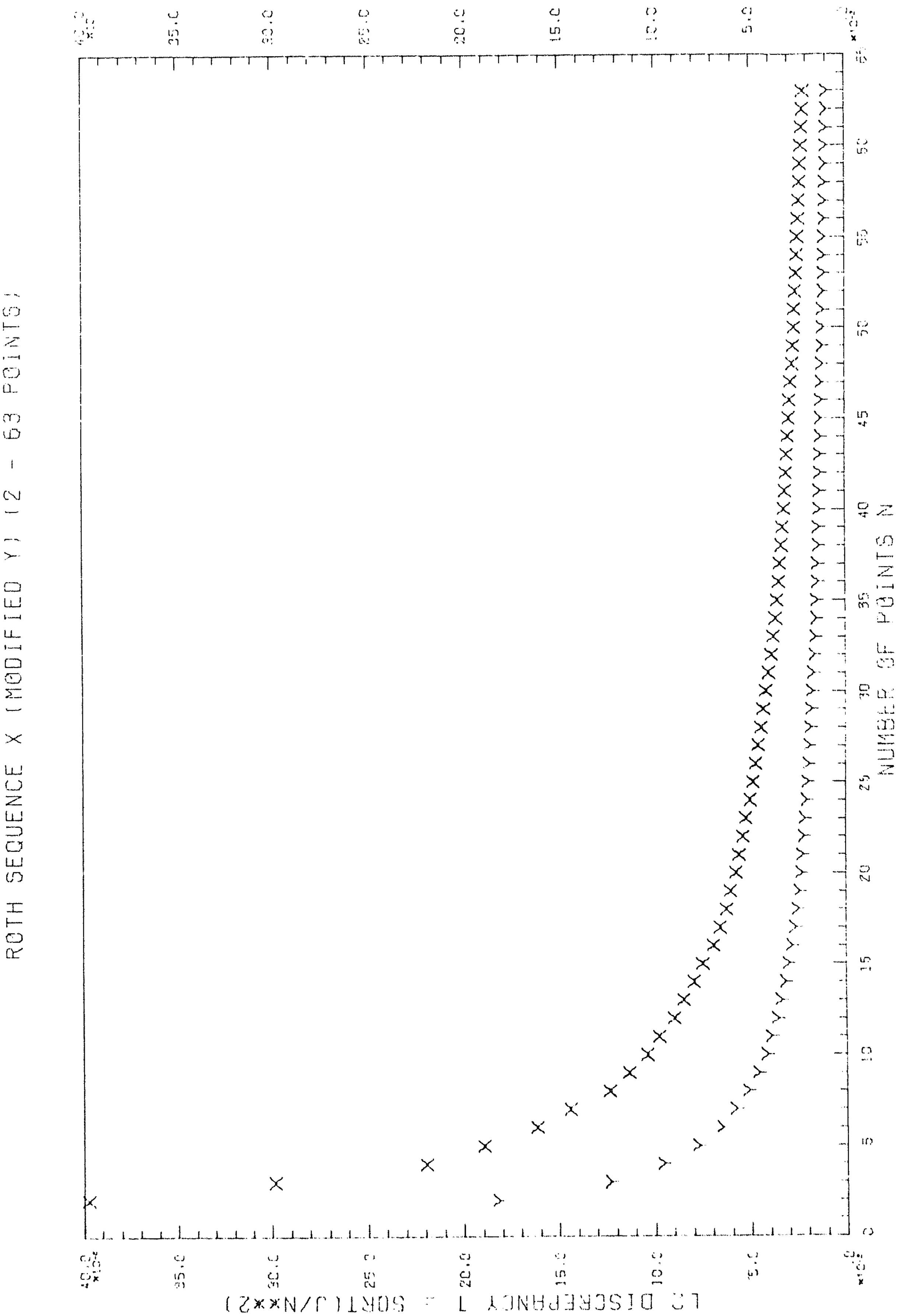
Table 1

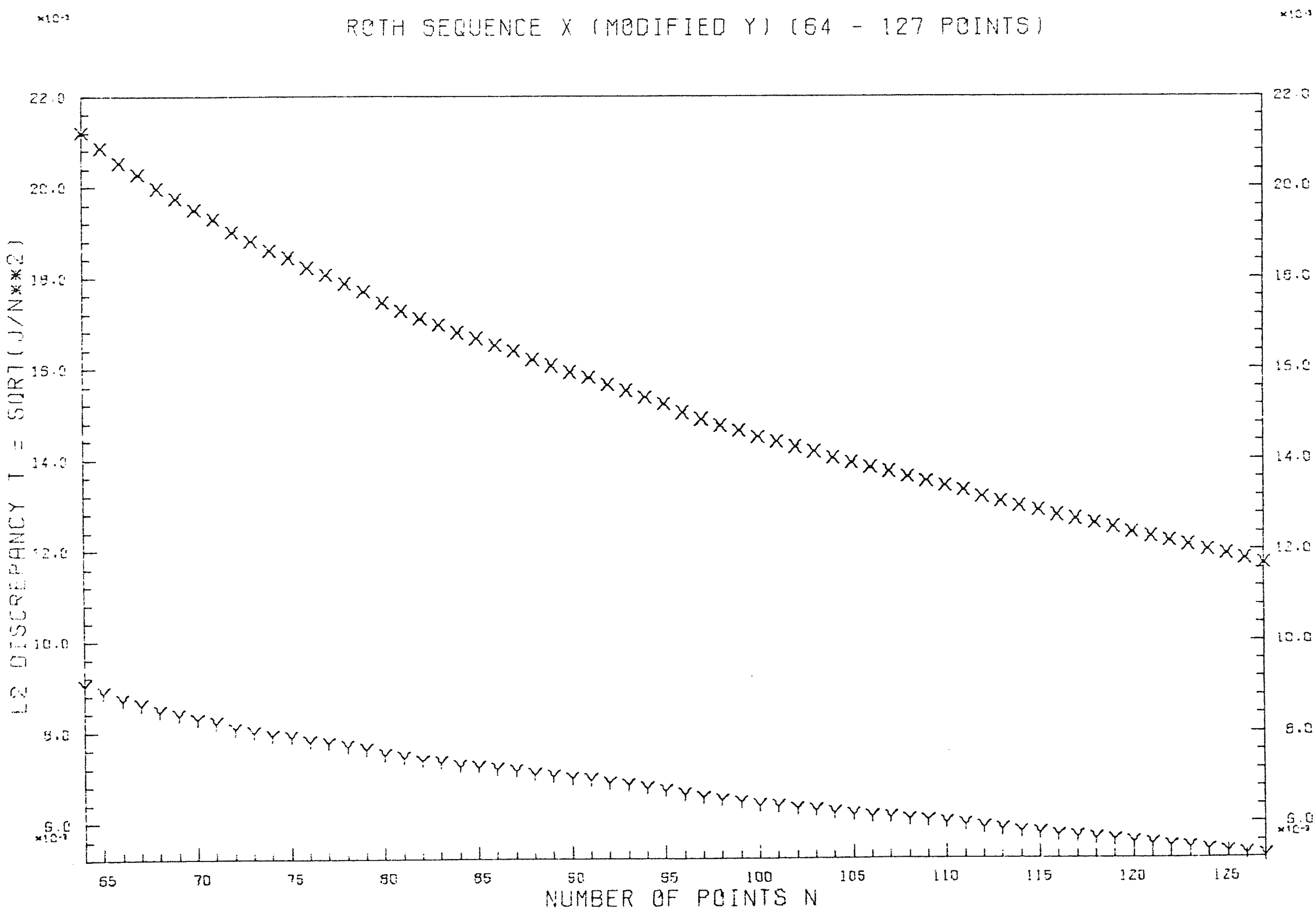
Execution and Input/Output Time for Evaluating

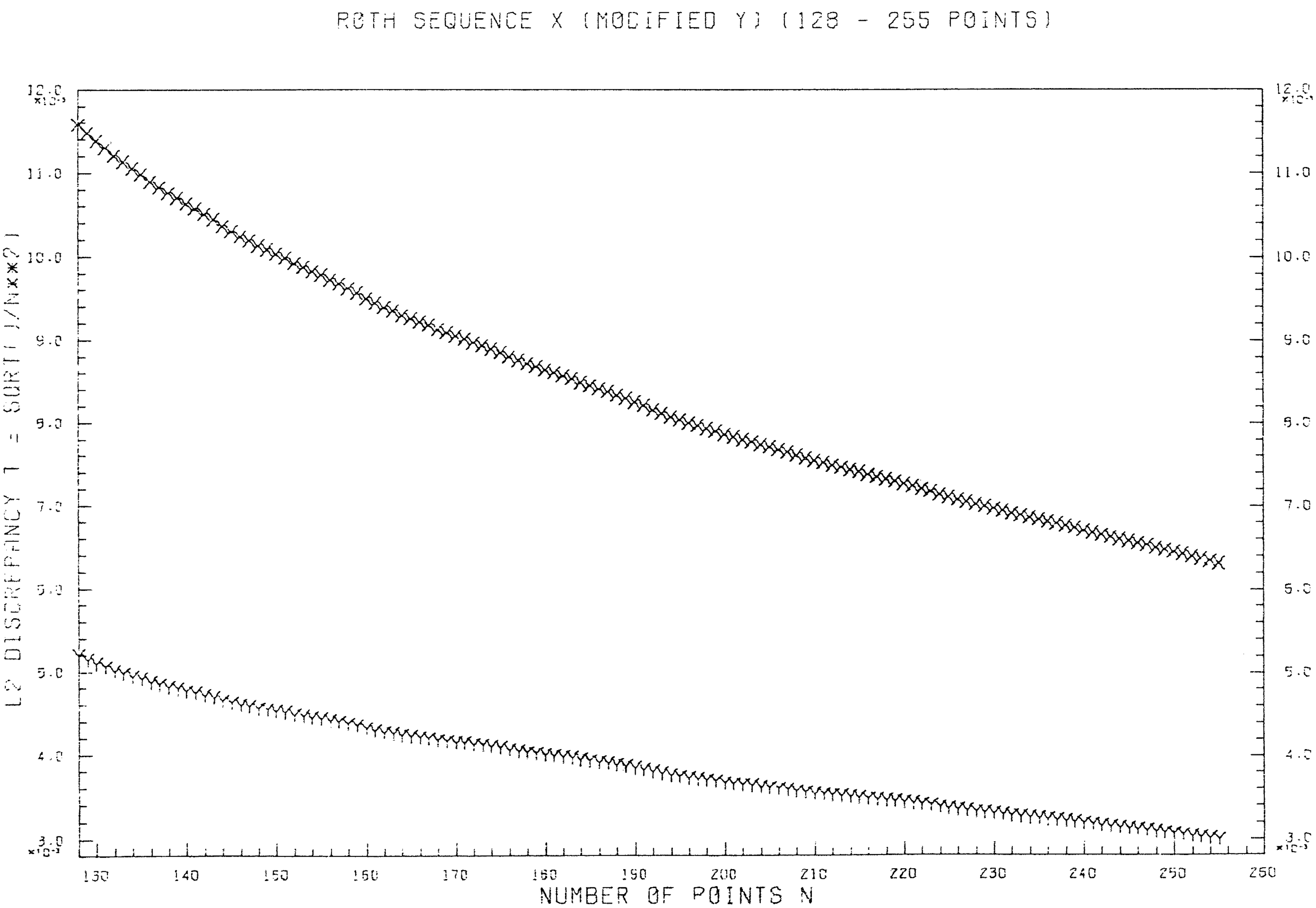
J_n, J'_n, $\sqrt{J_n}/n$ and $\sqrt{J'_n}/n$, $2 \le n \le N$.

Formulae 27 and 35		Formulae 37 and 38	
N	Time (sec.)	N	Time (sec.)
63	6.559	256	55.868
127	13.485	482	299.318
255	21.134	512	356.972
511	31.377		

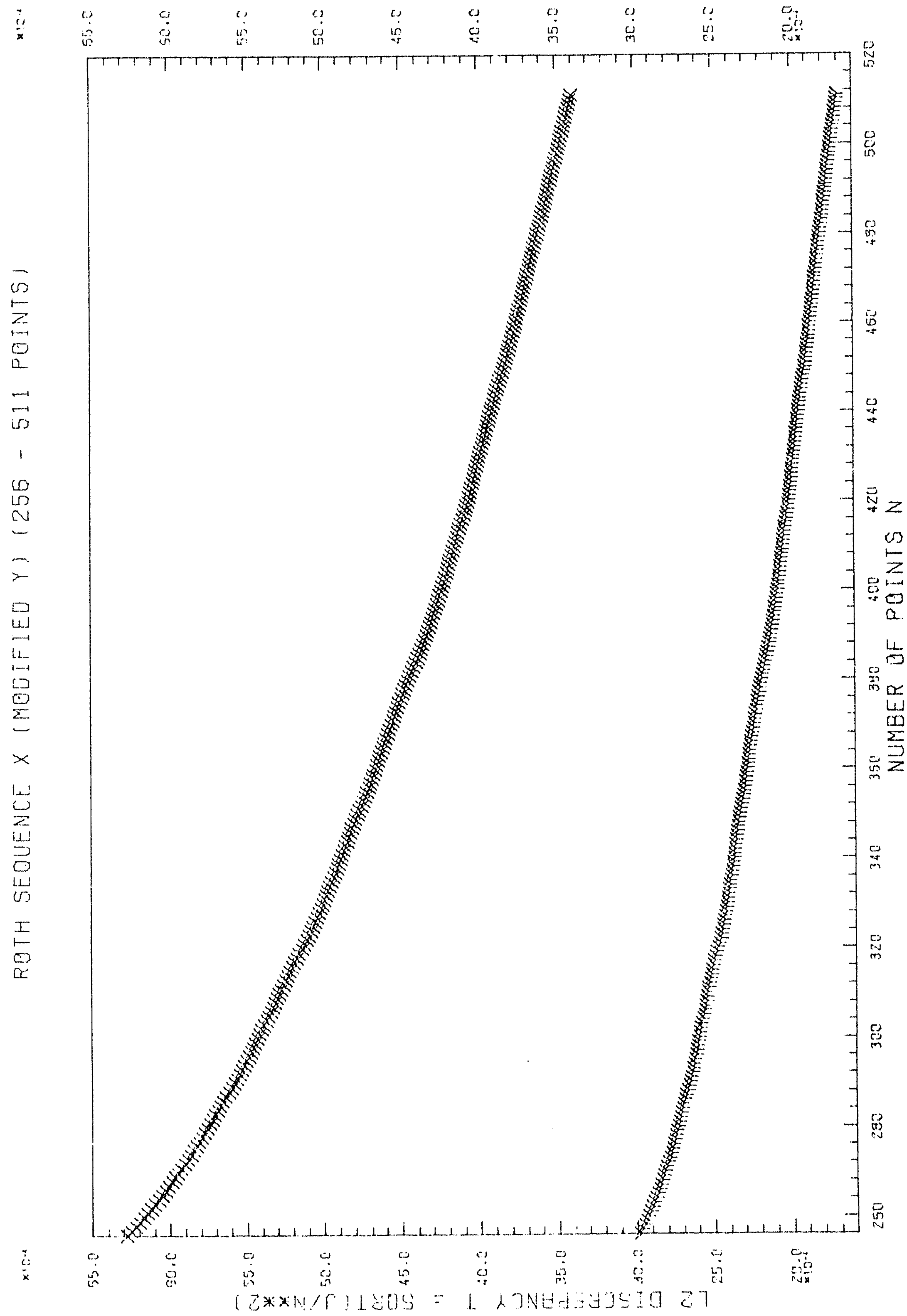
*J_n can be computed more efficiently using recursive finite difference formulae. The computation time for 37 can be reduced by roughly a factor of n. Further analysis of 27 will probably lead to a better algorithm but a less dramatic improvement.


ROTH SEQUENCE X (MODIFIED Y) (2 - 63 POINTS)
NUMBER OF POINTS N
L2 DISCREPANCY T = SQRT(J/N**2)
0
5
10
15
20
25
30
35
40
45
50
55
60
65
5.0
10.0
15.0
20.0
25.0
30.0
35.0
40.0


ROTH SEQUENCE X (MODIFIED Y) (64 - 127 POINTS)
x10^-3
L2 DISCREPANCY T = SQRT(J/N**2)
22.0
20.0
18.0
16.0
14.0
12.0
10.0
8.0
6.0
65
70
75
80
85
90
95
100
105
110
115
120
125
NUMBER OF POINTS N



ROTH SEQUENCE X (MODIFIED Y) (128 - 255 POINTS)
L2 DISCREPANCY T = SQRT(1/N**2)
NUMBER OF POINTS N
12.0 x10^-3
11.0
10.0
9.0
8.0
7.0
6.0
5.0
4.0
3.0 x10^-3
130
140
150
160
170
180
190
200
210
220
230
240
250
260


ROTH SEQUENCE X (MODIFIED Y) (256 - 511 POINTS)
NUMBER OF POINTS N
L2 DISCREPANCY T = SQRT(J/N**2)

5. CONCLUDING REMARKS

From the further study of the structural formulae 27 and 35, one should be able to prove the interesting Warnock conjecture that

a) the discrepancies of the Roth sequence and its modification are strictly monotone decreasing with the number of points.

This was suggested by earlier experimental results and seems plausible as evidenced by Figures 1-4. It has been proved (see Theorem 2) that

b) placing the original point of the Roth sequence at (1,1) uniformly yields a strict improvement in the discrepancy.

It is obvious from the definition of P_n' that $\lim_{n\to\infty} J_n' = \lim_{n\to\infty} J_n$ because altering one point cannot change the discrepancy very much for large n. A careful examination of 35 must reveal analytically just how slowly J_n' and J_n converge to each other.

More investigations of this sort are planned for other low-discrepancy sets in the unit cube as well as the unit square. An important goal is the theoretical calculation and analysis of

c) $$\int_0^1 dx \int_0^1 dy \int_0^1 dz\ (\nu(Q_n,(x,y,z)) - n\,xyz)^2$$

for the Hammersley sequence $(\frac{j}{n}, \varphi_2(j), \varphi_3(j))$, $j = 0,1,\ldots,n-1$, where $\varphi_3(j)$ is the radical-inverse function of j to the base 3. It may be instructive to first compute J_n for the Halton sequence $(\varphi_2(j), \varphi_3(j))$, $j = 0,1,\ldots,n-1$ [1].

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APPENDIX A

Using 2 and 3 with n replaced by $n\bar{x}_m$ and $x = 1$ in 3 the ν of 19 becomes

$$\text{(A1)} \qquad \nu(P_{n\bar{x}_m}, (1,y)) = \sum_{j=0}^{n\bar{x}_m - 1} H(y - y_j) \ .$$

This equals the number of points of 6 whose coordinates lie in the rectangle

$$R'((\bar{x}_m, y)) := \{(x,\eta) \mid x \in [0,\bar{x}_m),\ \eta \in [0,y],\ 0 \leq y \leq 1\}.$$

The 2^{M-1-i} points of 6 in the rectangular strip

$$\{(x,y) \mid x \in [\bar{x}_i, \bar{x}_{i+1}),\quad y \in [0,1],\quad 0 \leq i \leq m-1\}$$

are equally spaced in y with a point at $(\bar{x}_i, \bar{y}_i)$; $\bar{x}_0$ and $\bar{y}_0$ are taken as zero. Hence, the number of points in R' can also be expressed as*

$$\text{(A2)} \qquad \sum_{i=0}^{m-1} n_{M-1-i} \left(1 + [2^{M-1-i}(y - \bar{y}_i)]\right) H(y - \bar{y}_i), \quad 0 \leq y < 1 \ .$$

Thus, using 16 and A2, 19 can be rewritten as

---

*Throughout this report $[z]$ denotes the largest integer no larger than z and $\{z\} := z - [z]$.

$$\text{(A3)} \qquad A_m = \int_0^1 dy \left(\sum_{i=0}^{m-1} n_{M-1-i} H(y-\bar{y}_i)(1+[u_i(y-\bar{y}_i)]) \right)^2$$

$$= \sum_{i=0}^{m-1} n_{M-1-i} (1 - \bar{y}_i + 2A_i^4 + A_i^3)$$

$$+ \; 2 \sum_{i=1}^{m-1} n_{M-1-i} \sum_{j=0}^{i-1} n_{M-1-j} (1 - \bar{y}_i + A_i^4 + A_{ij}^2 + A_{ij}^1)$$

where

$$\text{(A4)} \qquad A_{ij}^1 := \int_{\bar{y}_i}^1 dy\, [u_i(y-\bar{y}_i)]\, [u_j(y-\bar{y}_j)]$$

$$\text{(A5)} \qquad A_{ij}^2 := \int_{\bar{y}_i}^1 dy\, [u_j(y-\bar{y}_j)]$$

$$\text{(A6)} \qquad A_i^3 := \int_{\bar{y}_i}^1 dy\, [u_i(y-\bar{y}_i)]^2$$

$$\text{(A7)} \qquad A_i^4 := \int_{\bar{y}_i}^1 dy\, [u_i(y-\bar{y}_i)] \,.$$

The fact that the summation of A3 is one too large for $y = 1$ does not affect the validity of the integral since the integrand is incorrect only on a set of measure zero. The expansion of A3 is straightforward observing that $\bar{y}_i \geqq \bar{y}_j$ for $i \geqq j$, $n_{M-1-i}^2 \equiv n_{M-1-i}$, and $H^2(y-\bar{y}_i) \equiv H(y-\bar{y}_i)$.

For convenience let

$$\text{(A8)} \qquad \alpha_{ij} := u_j(\bar{y}_i - \bar{y}_j)$$

$$1 \leqq i \leqq m, \quad 0 \leqq j \leqq i$$

$$\text{(A9)} \qquad \beta_{ij} := -u_j\bar{y}_i + \{\alpha_{ij}\}.$$

With the change of variable $y \leftarrow y - \bar{y}_i$, A4 becomes

$$\text{(A10)} \qquad A^1_{ij} = \int_0^{1-\bar{y}_i} dy\ [u_i y][u_j y + \alpha_{ij}]$$

$$= \sum_{k=0}^{u_i-2} k \int_{k/u_i}^{(k+1)u_i} dy\ [u_j y + \alpha_{ij}]$$

$$+ (u_i - 1) \int_{1-\frac{1}{u_i}}^{1-\bar{y}_i} dy\ [u_j y + \alpha_{ij}]$$

since $1/u_i$ divides $1 - \bar{y}_i$ with a quotient of $[u_i(1 - \bar{y}_i)] \equiv u_i - 1$, for $i > 0$. The latter follows from 1, 13 and 16:

$$\text{(A11)} \qquad u_i - 1 = [u_i - \tfrac{1}{2} - 2^{-1-i}] \equiv [u_i - 2^{-M}(2^i - 1)u_i] \leqq [u_i(1 - \bar{y}_i)]$$

$$\leqq [u_i(1 - 2^{-M})] \equiv [u_i - 2^{-1-i}] = u_i - 1.$$

Since $i > j$ in A3, $1/u_j$ divides $1/u_i$ exactly 2^{i-j} times. Hence, with the change of variable $y \leftarrow y - k/u_i$ the first integral of A10 becomes

$$\text{(A12)} \quad \int_0^{1/u_i} dy\,(ku_j/u_i + [u_j y + \alpha_{ij}]) = ku_j/u_i^2 + [\alpha_{ij}] \int_0^{(1-\{\alpha_{ij}\})/u_j} dy$$

$$+ \sum_{r=0}^{u_j/u_i-2} (r+1+[\alpha_{ij}]) \int_0^{1/u_j} dy + (u_j/u_i + [\alpha_{ij}]) \int_0^{\{\alpha_{ij}\}/u_j} dy$$

$$= \frac{1}{u_i} \left(\left(k+\frac{1}{2}\right)\frac{u_j}{u_i} + \alpha_{ij} - \frac{1}{2}\right)$$

using the facts that $[\alpha_{ij} + 1 - \{\alpha_{ij}\}] \equiv [\alpha_{ij}] + 1$ and that

$$\text{(A13)} \qquad \sum_{r=1}^{s} r = \frac{s(s+1)}{2} .$$

Using A9, let

$$\text{(A14)} \qquad \rho_{ij} := u_j \left(\frac{1}{u_i} - \bar{y}_i\right) - 1 + \{\alpha_{ij}\} = \frac{u_j}{u_i} - 1 + \beta_{ij} .$$

Then with the change of variable $y \leftarrow y - (1 - \frac{1}{u_i})$ the second integral of A10 becomes

$$\text{(A15)} \quad \int_0^{\frac{1}{u_i} - \bar{y}_i} dy\,(u_j(1-\frac{1}{u_i}) + [u_j y + \alpha_{ij}]) = u_j(1 - \frac{1}{u_i})(\frac{1}{u_i} - \bar{y}_i)$$

$$+ [\alpha_{ij}] \int_0^{(1-\{\alpha_{ij}\})/u_j} dy + \sum_{r=0}^{[\rho_{ij}]-1} (r+1+[\alpha_{ij}]) \int_0^{1/u_j} dy$$

$$+ ([\rho_{ij}]+1+[\alpha_{ij}]) \int_0^{\{\beta_{ij}\}/u_j} dy = \frac{1}{u_j}\left(-\frac{[\rho_{ij}]^2}{2} + [\rho_{ij}](\rho_{ij} - \frac{1}{2})\right.$$

$$\left. - 1 + \{\alpha_{ij}\} + u_j(\frac{1}{u_i} - \bar{y}_i)(u_j(1-\bar{y}_i) - \rho_{ij} + \alpha_{ij})\right) .$$

Thus, using A13 again and the fact that

$$\text{(A16)} \qquad \sum_{r=1}^{s} r^2 = \frac{1}{6}\, s(s+1)(2s+1)$$

from A10, A12 and A15, A4 becomes

$$\text{(A17)} \qquad A^1_{ij} = \frac{u_j}{u_i}\left(\frac{u_i^2}{3} - \frac{5}{4}u_i + \frac{17}{12} - \frac{1}{2u_i}\right) + \left(\alpha_{ij} - \frac{1}{2}\right)\left(\frac{u_i}{2} - \frac{3}{2} + \frac{1}{u_i}\right)$$

$$+ \frac{u_i - 1}{u_j}\left(-\frac{[\rho_{ij}]^2}{2} + [\rho_{ij}](\rho_{ij} - \frac{1}{2}) - 1 + \{\alpha_{ij}\}\right.$$

$$\left. + u_j\left(\frac{1}{u_i} - \bar{y}_i\right)(u_j(1 - \bar{y}_i) - \rho_{ij} + \alpha_{ij})\right) .$$

With the change of variable $y \leftarrow y - \bar{y}_i$ and using A8 and A11, A5 becomes

$$\text{(A18)} \qquad A^2_{ij} = \int_0^{1-\frac{1}{u_i}} dy\, [u_j y + \alpha_{ij}] + \int_{1-\frac{1}{u_i}}^{1-\bar{y}_i} dy\, [u_j y + \alpha_{ij}] .$$

Using A13 the first integral of A18 becomes

$$\text{(A19)} \qquad [\alpha_{ij}] \int_0^{(1-\{\alpha_{ij}\})/u_j} dy + \sum_{r=0}^{u_j(1-\frac{1}{u_i})-2} (r + 1 + [\alpha_{ij}]) \int_0^{1/u_j} dy$$

$$+ (u_j(1 - \frac{1}{u_i}) + [\alpha_{ij}]) \int_0^{\{\alpha_{ij}\}/u_j} dy$$

$$= (1 - \frac{1}{u_i})(\frac{u_j}{2}(1 - \frac{1}{u_i}) + \alpha_{ij} - \frac{1}{2}) .$$

The second integral of A18 is given by A15, so with A17-19, $A^1_{ij} + A^2_{ij}$ becomes

$$\text{(A20)} \qquad A^1_{ij} + A^2_{ij} = \frac{u_j}{u_i}\left(\frac{u_i^2}{3} - \frac{3}{4}u_i + \frac{5}{12}\right) + \frac{1}{2}(\alpha_{ij} - \frac{1}{2})(u_i - 1)$$
$$+ \frac{u_i}{u_j}\left(-\frac{[\rho_{ij}]^2}{2} + [\rho_{ij}](\rho_{ij} - \frac{1}{2}) - 1 + \{\alpha_{ij}\}\right.$$
$$\left. + u_j\,(\frac{1}{u_i} - \bar{y}_i)(u_j(1 - \bar{y}_i) - \rho_{ij} + \alpha_{ij})\right).$$

Similarly, using A11, A6 becomes

$$\text{(A21)} \qquad A^3_i = \int_0^{1-\bar{y}_i} dy\,[u_i y]^2 = \sum_{r=0}^{u_i-2} r^2 \int_{r/u_i}^{(r+1)/u_i} dy + (u_i - 1)^2 \int_{1-1/u_i}^{1-\bar{y}_i} dy$$
$$= \frac{u_i^2}{3} - \frac{1}{2}u_i + \frac{1}{6} - (u_i - 1)^2\bar{y}_i$$

and A7 becomes

$$\text{(A22)} \qquad A^4_i = \int_0^{1-\bar{y}_i} dy\,[u_i y] = \sum_{r=0}^{u_i-2} r \int_{r/u_i}^{(r+1)/u_i} dy + (u_i - 1)\int_{1-1/u_i}^{1-\bar{y}_i} dy$$
$$= \frac{u_i}{2} - \frac{1}{2} - (u_i - 1)\bar{y}_i$$

where A13 and A16 are applied.

Combining A20-22 using A9 and A14, A3 becomes

(A23)
$$A_m = \sum_{i=0}^{m-1} n_{M-1-i}\left(\frac{u_i^2}{3} + \frac{u_i}{2} + \frac{1}{6} - u_i^2\bar{y}_i\right)$$
$$+ 2\sum_{i=1}^{m-1} n_{M-1-i} \sum_{j=0}^{i-1} n_{M-1-j}\left(\frac{u_j}{u_i}\left(\frac{u_i^2}{3} + \frac{u_i}{4} - \frac{1}{12}\right)\right.$$
$$+ \frac{u_i}{u_j}\left(-\frac{[\beta_{ij}]^2}{2} - (u_j\bar{y}_i + \frac{1}{2} - \{\alpha_{ij}\})[\beta_{ij}] - u_j(u_j + [\alpha_{ij}])\bar{y}_i\right)$$
$$\left. + \frac{\alpha_{ij}}{2} + \frac{1}{4} - u_i\bar{y}_i + \frac{1}{2}(\alpha_{ij} + \frac{1}{2})u_i\right) .$$

From 13, 16, A8 and A9 observe that

(A24)

a) $$\{\alpha_{ij}\} = \frac{n_{M-1-j}}{2}$$

b) $$[\beta_{ij}] = \begin{cases} -[\alpha_{ij}] - 1, & j > 0 \\ -[\alpha_{i0}], & j = 0 . \end{cases}$$

Since $n_{M-1} \equiv 1$, $\{\alpha_{i0}\} = 1/2$ by A24a). It is valid to take $\{\alpha_{ij}\} \equiv 1/2$ in A23, because $\{\alpha_{ij}\} \neq 1/2$ iff $n_{M-1-j} = 0$ by 1 and A24a), but in this case the effect of the erroneous $\{\alpha_{ij}\}$ is nullified by the zero n_{M-1-j} coefficient of the double summation. From 13, taking $\bar{y}_0 = y_0 = \varphi_2(0) \equiv 0$, and 26b) and A8

(A25)
$$\alpha_{ij} = \begin{cases} \frac{u_j}{2}((-1)i - (-1)j), & j > 0 \\ \frac{u_0}{2}(-1)i, & j = 0 . \end{cases}$$

Hence, in A24b) and A23 one can use

$$\text{(A26)} \qquad [\alpha_{ij}] = \begin{cases} \frac{1}{2}(u_j((-1)i - (-1)j) - 1), & j > 0 \\ \frac{1}{2}(u_0(-1)i - 1), & j = 0 \end{cases}$$

where $\{\alpha_{ij}\}$ is taken as 1/2.

Using the notation of 25 along with 26b), A24b), A25 and A26, and after some calculation distinguishing the $j = 0$ terms from the others, A23 can be rewritten as

$$\begin{aligned} \text{(A27)} \qquad A_m = {} & \frac{1}{3}(2)m + \frac{1}{2}(1)m + \frac{1}{6}(0)m - \frac{1}{2}(2,-1)m \\ & + 2\left(\frac{1}{3}(1,1)m + \frac{1}{4}(0,1)m - \frac{1}{12}(-1,1)m\right) \\ & + \sum_{i=1}^{m-1} n_{M-1-i}\, u_i \left(-\frac{1}{4}((-1)i)^2(1)i - \frac{1}{4}\sum_{j=0}^{i=1} n_{M-1-j}\, u_j((-1)j)^2 \right. \\ & \left. + \frac{1}{2}(-1)i(1,-1)i - \frac{1}{2}(-1)i(0)i - \frac{1}{2}(-1)i(1)i\right) \\ & + \frac{1}{2}(1,0,-1)m - \frac{1}{4}(1,-1)m - \frac{1}{2}(0,1,-1)m \\ & + \frac{1}{2}\sum_{i=1}^{m-1} n_{M-1-i}(-1)i(1)i + \frac{1}{2}(1,0)m + \frac{1}{2}(0,0)m - \frac{1}{2}(1,1,-1)m. \end{aligned}$$

This intermediate result can be simplified by applying Theorem 1. After further calculation A_m takes the form

(A28)
$$A_m = -\frac{1}{2}(1,-1,-1,1)m - (1,1,-1)m - \frac{1}{2}(1,-1,1)m$$
$$- (1,-1,0)m - \frac{1}{4}(1,-2,1)m + \frac{1}{2}(0,-1,1)m$$
$$- \frac{1}{2}(2,-1)m + \frac{2}{3}(1,1)m - (1,-1)m$$
$$+ \frac{1}{2}(0,1)m + (0,0)m - \frac{1}{6}(-1,1)m + \frac{1}{3}(2)m$$
$$+ \frac{1}{2}(1)m + \frac{1}{6}(0)m .$$

APPENDIX B

The first factor in the integrand of 20 involves only 2^{M-1-m} points of 6. Because of the previous variable transformations (cf. 15) these points map one to one on the set of points with coordinates (cf. 4 and 6)

$$\text{(B1)}\quad \begin{aligned} &\text{a)} \quad x_j' := \frac{j}{u_m} \\ &\text{b)} \quad y_j' := \varphi_2'(j) \end{aligned} \qquad 0 \leqq j \leqq u_m - 1$$

where

$$\text{c)} \quad \begin{cases} u_m\, \varphi_2'(j) := (j_0 j_1 \cdots j_{M-2-m})_2, & 1 \leqq m < M-1 \\ \varphi_2'(0) := 0, & m = M-1\ . \end{cases}$$

Thus, from 3 with n replaced by u_m

$$\text{(B2)} \qquad \nu(P_{u_m}, (x, y-y_m)) = \sum_{j=0}^{u_m-1} H(x-x_j')\, H(y-\bar{y}_m-y_j')\ .$$

The second factor in the integrand of 20 is given by A2. Integrating with respect to x, and using 2, A2 and B2, 20 can be rewritten as

$$\text{(B3)} \qquad B_m = \sum_{j=0}^{u_m-1} (1-x_j') \int_{\bar{y}_m}^{1} dy\ H(y-\bar{y}_m-y_j') \sum_{i=0}^{m-1} n_{M-1-i}(1 + [u_i(y-\bar{y}_i)])$$

since $\bar{y}_m \geqq \bar{y}_i$ by 13. By B1bc), $y_j' \leqq 1 - 2^{-M+1+m}$. Hence, from this and 13

$$\text{(B4)} \qquad \bar{y}_m + y_j' \leqq 2^{-M} \sum_{i=0}^{m-1} 2^i + (1 - 2^{-M+1+m}) = 1 - 2^{-M+1+m} - 2^{-M} < 1$$

and B3 becomes

$$\text{(B5)} \qquad B_m = \sum_{j=0}^{u_m - 1} (1 - x_j') \sum_{i=0}^{m-1} n_{M-1-i} (1 - \bar{y}_m - y_j' + B_{ij}^1)$$

where

$$\text{(B6)} \qquad B_{ij}^1 := \int_{\bar{y}_m + y_j'}^{1} dy\, [u_i(y - \bar{y}_i)].$$

Using A9 define

$$\text{(B7)} \qquad \sigma_{mij} := u_i(1 - \bar{y}_m - y_j') - 1 + \{\alpha_{mi}\} = u_i(1 - y_j') - 1 + \beta_{mi}.$$

With the change of variable $y \leftarrow y - \bar{y}_m - y_j'$, B6 becomes

$$\text{(B8)} \qquad \int_0^{1-\bar{y}_m - y_j'} dy[u_i(y+y_i') + \alpha_{mi}] = \int_0^{1-\bar{y}_m - y_j'} dy(u_i y_j' + [u_i y + \alpha_{mi}])$$

$$= u_i y_j'(1 - \bar{y}_m - y_j') + \int_0^{1-\bar{y}_m - y_j'} dy\, [u_i y + \alpha_{mi}]$$

because $u_i y_j'$ is a nonnegative integral multiple of two by 16 and B1 bc). The final integral of B8 can be expressed as

$$\text{(B9)} \qquad [\alpha_{mi}] \int_0^{(1-\{\alpha_{mi}\})/u_i} dy + \sum_{r=0}^{[\sigma_{mij}]-1} (r+1+[\alpha_{mi}]) \int_0^{1/u_i} dy$$

$$+ ([\sigma_{mij}] + 1 + [\alpha_{mi}]) \int_0^{\{\beta_{mi}\}/u_i} dy \ .$$

Thus, B6 becomes

$$\text{(B10)} \qquad B^1_{ij} = \frac{1}{u_i} \left(\frac{[\sigma_{mij}]^2}{2} + [\sigma_{mij}] \left(u_i y'_j + \{\beta_{mi}\} + [\alpha_{mi}] + \frac{1}{2} \right) \right.$$

$$\left. + \{\beta_{mi}\} + (u_i y'_j + [\alpha_{mi}])(1 - \{\alpha_{mi}\} + \{\beta_{mi}\}) \right)$$

where A13 and B7 are applied. Interchanging the summations of B5, substituting B10 utilizing B7 and rearranging terms yields

$$\text{(B11)} \qquad B_m = \sum_{i=0}^{m-1} n_{m-1-i} \left(u_i \frac{1}{2} \sum_{j=0}^{u_m-1} (1 - x'_j)(1 - y'^2_j) \right.$$

$$+ (\alpha_{mi} + \frac{1}{2}) \sum_{j=0}^{u_m-1} (1 - x'_j)(1 - y'_j)$$

$$+ \frac{1}{u_i} \left(\frac{[\beta_{mi}]^2}{2} + [\beta_{mi}](u_i + \{\beta_{mi}\} + [\alpha_{mi}] - \frac{1}{2} \right) - u_i \bar{y}_m$$

$$\left. + (\{\beta_{mi}\} - \{\alpha_{mi}\})(u_i + [\alpha_{mi}]) \right) \sum_{j=0}^{u_m-1} (1 - x'_j) \Bigg) \ .$$

From [2] it is known that

$$\text{a)} \quad \frac{1}{2}\sum_{j=0}^{u_m-1} (1 - x_j')(1 - y_j'^2) = K_{u_m} + \frac{u_m}{6}$$

(B12)

$$\text{b)} \quad \sum_{j=0}^{u_m-1} (1 - x_j')(1 - y_j') = I_{u_m} + \frac{u_m}{4}$$

where

$$\text{a)} \quad K_{u_m} := \frac{M-m}{16}\left(1 - \frac{1}{u_m}\right) + \frac{1}{48}\left(11 + \frac{7}{u_m} - \frac{2}{u_m^2}\right)$$

(B13)

$$\text{b)} \quad I_{u_m} := \frac{M-m}{8} + \frac{1}{8}\left(3 + \frac{2}{u_m}\right) .$$

The last summation of B11 is

$$\text{(B14)} \qquad \sum_{j=0}^{u_m-1} (1 - x_j') = u_m - \frac{1}{u_m}\sum_{j=0}^{u_m-1} j = \frac{1}{2}(u_m + 1)$$

using B1a) and A13. Substituting B12 and B14 into B11, B_m becomes

$$\text{(B15)} \qquad B_m = \sum_{i=0}^{m-1} n_{M-1-i} \left(\left(K_{u_m} + \frac{u_m}{6}\right)u_i + \left(I_{u_m} + \frac{u_m}{4}\right)\left(\alpha_{mi} + \frac{1}{2}\right)\right.$$
$$+ \frac{u_m+1}{2u_i}\left(\frac{[\beta_{mi}]^2}{2} + [\beta_{mi}]\left(u_i + \{\beta_{mi}\} + [\alpha_{mi}] - \frac{1}{2}\right) - u_i\bar{y}_m\right.$$
$$\left.\left. + (\{\beta_{mi}\} - \{\alpha_{mi}\})(u_i + [\alpha_{mi}])\right)\right) \quad .$$

Observe that A8, A9, and A24-26 hold with ij replaced by mi, with $\{\alpha_{mi}\} \equiv 1/2$ valid for B15. Using the notation of 25 along with

26b) and A24-26, B_m can be expressed as

(B16) $$B_m = \left(K_{u_m} + \frac{u_m}{6}\right)(1)m + \frac{1}{2}\left(I_{u_m} + \frac{u_m}{4}\right)\Big((-1)m(1)m - (1,-1)m + (0)m\Big)$$

$$+ \frac{u_m+1}{2}\left(-\frac{1}{8}((-1)m)^2(1)m - \frac{1}{8}\sum_{i=0}^{m-1} n_{M-1-i}\, u_i((-1)i)^2\right.$$

$$\left. + \frac{1}{4}(0,-1)m + (-1)m\left(\frac{1}{4}(1,-1)m - \frac{1}{2}(1)m - \frac{1}{4}(0)m - \frac{1}{8}\right)\right) .$$

Application of Theorem 1, 25b) and B13 yields

(B17) $$B_m = \frac{M-m}{8}\left(\frac{1}{2}(-1,1)m + \frac{1}{2}\left(1 - \frac{1}{u_m}\right)(1)m + (0)m\right)$$

$$+ \frac{1}{16}(u_m+1)\Big(-2(-1,-1,1)m - 4(1,-1)m$$

$$- 4(-1,0)m - (-2,1)m - 4(-1)m\Big) - \frac{1}{8}\left(u_m + \frac{1}{2} - \frac{1}{u_m}\right)(-1,1)m$$

$$+ \frac{1}{48}\left(8u_m + 11 + \frac{7}{u_m} - \frac{2}{u_m^2}\right)(1)m + \frac{1}{8}\left(1 + \frac{2}{u_m}\right)(0)m .$$

With 2, B1 and B2, 32 can be rewritten as

(B18) $$B'_m = \sum_{j=0}^{u_m-1} (1 - x'_j)(1 - \bar{y}_m - y'_j)$$

$$= I_{u_m} + \frac{u_m}{4} - \frac{1}{2}(u_m+1)\bar{y}_m$$

$$= \frac{M-m}{8} + \frac{u_m}{4} + \frac{3}{8} + \frac{1}{4u_m} - \frac{1}{4}(u_m+1)(-1)m$$

using B12b), B13b) and 26b).

APPENDIX C

Using 2, 16, A1 and A2, 21 can be rewritten as

(C1) $$C_m = \sum_{i=0}^{m-1} n_{M-1-i}\left(\frac{1}{2}\left(1-\bar{y}_i^2\right) + C_i^1\right)$$

where

(C2) $$C_i^1 := \int_{\bar{y}_i}^{1} dy\ y[u_i(y-\bar{y}_i)] = \int_0^{1-\bar{y}_i} dy\,(y+\bar{y}_i)\,[u_i\,y]$$

$$= \bar{y}_i A_i^4 + \int_0^{1-\bar{y}_i} dy\ y[u_i\,y]$$

with the change of variable $y \leftarrow y - \bar{y}_i$ and by A22. From A11 the last integral of C2 becomes

(C3) $$\sum_{r=0}^{u_i-2} r \int_{r/u_i}^{(r+1)/u_i} dy\ y + (u_i-1)\int_{1-1/u_i}^{1-\bar{y}_i} dy\,y = \sum_{r=0}^{u_i-2} r\left(\int_0^{1/u_i} dy\ y + \frac{r}{u_i}\int_0^{1/u_i} dy\right)$$

$$+ \frac{u_i-1}{2}\left((1-\bar{y}_i)^2 - (1-\frac{1}{u_i})^2\right)$$

$$= \frac{u_i}{3} - \frac{1}{4} - \frac{1}{12u_i} + \frac{u_i-1}{2}(\bar{y}_i-2)\bar{y}_i$$

with the change of variable $y \leftarrow y - r/u_i$ and by A13 and A16. Substituting this result in C2 and using A22, C1 becomes

(C4) $$C_m = \sum_{i=0}^{m-1} n_{M-1-i}\left(-\frac{u_i}{2}\bar{y}_i^2 - \frac{1}{2}(u_i-1)\bar{y}_i + \frac{u_i}{3} + \frac{1}{4} - \frac{1}{12u_i}\right).$$

Using the notation of 25 and applying 26b) and Theorem 1

$$\text{(C5)} \qquad C_m = -\frac{1}{4}(1,-1,-1)m - \frac{1}{4}(1,-1)m - \frac{1}{8}(1,-2)m$$

$$+ \frac{1}{4}(0,-1)m + \frac{1}{3}(1)m + \frac{1}{4}(0)m - \frac{1}{12}(-1)m \,.$$

With 2, 16, A1 and A2, 33 can be rewritten as

$$\text{(C6)} \qquad C'_m = \sum_{i=0}^{m-1} n_{M-1-i}\left(1 - \bar{y}_i + C'^1_i\right)$$

where

$$\text{(C7)} \qquad C'^1_i := \int_{\bar{y}_i}^{1} dy\ [u_i(y-\bar{y}_i)] = \int_0^{1-\bar{y}_i} dy\ [u_i y]$$

$$= \sum_{r=0}^{u_i-2} r \int_{r/u_i}^{(r+1)/u_i} dy + (u_i - 1)\int_{1-1/u_i}^{1-\bar{y}_i} dy = (u_i - 1)\left(\frac{1}{2} - \bar{y}_i\right)$$

as in C3. Hence, C6 becomes

$$\text{(C8)} \qquad C'_m = \sum_{i=0}^{m-1} n_{M-1-i}\left(\frac{1}{2}(u_i + 1) - u_i\bar{y}_i\right)$$

$$= \frac{1}{2}\left(-(1,-1)m + (1)m + (0)m\right)$$

using the notation of 25 and 26b).

APPENDIX D

22 can be rewritten as

$$D_m = D_m^1 - 2n\bar{x}_m D_m^2 - 2\bar{y}_m u_m D_m^3 - 2n\bar{x}_m \bar{y}_m D_m^4 - \frac{\bar{y}_m^3}{3}\left(\frac{2}{3}u_m + \frac{n\bar{x}_m}{2}\right)u_m + \frac{\bar{y}_m^2}{3}u_m^2 + \frac{n\bar{x}_m\bar{y}_m}{2}u_m + \frac{n^2\bar{x}_m^2}{3} \tag{D1}$$

where

$$D_m^1 := \int_0^1 dx \int_0^{1-\bar{y}_m} dy\, G_{u_m}^2(x,y) \tag{D2}$$

$$D_m^2 := \int_0^1 dx \int_0^{1-\bar{y}_m} dy\, y\, G_{u_m}(x,y) \tag{D3}$$

$$D_m^3 := \int_0^1 dx\, x \int_0^{1-\bar{y}_m} dy\, G_{u_m}(x,y) \tag{D4}$$

$$D_m^4 := \int_0^1 dx \int_0^{1-\bar{y}_m} dy\, G_{u_m}(x,y) \tag{D5}$$

and

$$G_{u_m}(x,y) := \nu(P_{u_m},(x,y)) - u_m xy. \tag{D6}$$

From the results of [2]

$$D_m^1 = J_{u_m} - \int_0^1 dx \int_{1-\bar{y}_m}^1 dy\, G_{u_m}^2(x,y) \tag{D7}$$

(D8) $$D_m^2 = K_{u_m} - \int_0^1 dx \int_{1-\bar{y}_m}^1 dy\ y\ G_{u_m}(x,y)$$

(D9) $$D_m^3 = K_{u_m} - \int_0^1 dx\ x \int_{1-\bar{y}_m}^1 dy\ G_{u_m}(x,y)$$

(D10) $$D_m^4 = I_{u_m} - \int_0^1 dx \int_{1-\bar{y}_m}^1 dy\ G_{u_m}(x,y)$$

where J_{u_m} is given by 24 with M replaced by $M-m$, i.e.,

(D11) $$J_{u_m} = \frac{(M-m)^2}{64} + \frac{23(M-m)}{192} + \frac{23}{96} - \frac{M-m-5}{16u_m} - \frac{1}{72u_m^2}$$

and K_{u_m} and I_{u_m} are given by B13.

Using 2, 3, B1, B4 and D6 the integral of D7 becomes

(D12) $$\int_0^1 dx \int_{1-\bar{y}_m}^1 dy\left(\sum_{j=0}^{u_m-1} H(x-x_j') - u_m xy\right)^2 = \bar{y}_m \sum_{j=0}^{u_m-1} (1-x_j')$$
$$+ 2\bar{y}_m \sum_{j=1}^{u_m-1} j(1-x_j') - \frac{u_m}{2}\left(1-(1-\bar{y}_m)^2\right)\sum_{j=0}^{u_m-1}(1-x_j'^2)$$
$$+ \frac{u_m^2}{9}\left(1-(1-\bar{y}_m)^3\right)$$
$$= \frac{\bar{y}_m^3}{9} u_m^2 + \frac{\bar{y}_m^2}{4}\left(u_m - \frac{1}{3}\right) + \frac{\bar{y}_m}{3}$$

where A13, A16 and B14 are applied.

Similarly, the integrals of D8, D9 and D10 become

(D13) $$-\frac{\bar{y}_m^3}{6}u_m + \frac{\bar{y}_m^2}{4}(u_m - 1) + \frac{\bar{y}_m}{2}$$

(D14) $$\frac{\bar{y}_m^2}{6}u_m + \frac{\bar{y}_m}{4}\left(1 - \frac{1}{3u_m}\right)$$

(D15) $$\frac{\bar{y}_m^2}{4}u_m + \frac{\bar{y}_m}{2}$$

respectively. Combining D7-10 with D12-15, substituting into D1 and collecting terms, D_m becomes

(D16) $$\begin{aligned} D_m = J_{u_m} &- 2(n\bar{x}_m + \bar{y}_m u_m)K_{u_m} - 2n\bar{x}_m\bar{y}_m I_{u_m} \\ &+ \bar{y}_m^2\left(\frac{u_m^2}{3} + \frac{1}{2}\left(n\bar{x}_m + \frac{1}{2}\right)u_m + \frac{1}{2}\left(n\bar{x}_m - \frac{1}{6}\right)\right) \\ &+ \bar{y}_m\left(\frac{n\bar{x}_m}{2}u_m + n\bar{x}_m - \frac{1}{3}\right) + \frac{n^2\bar{x}_m^2}{3} \quad . \end{aligned}$$

Using the notation of 25 along with 26, D_m can be expressed as

(D17) $$\begin{aligned} D_m = J_{u_m} &- (2(1)m + (-1)m\,u_m)K_{u_m} - (1)m\,(-1)m\,I_{u_m} \\ &+ \frac{1}{4}(-1)_m^2\left(\frac{1}{3}u_m^2 + \frac{1}{2}\left((1)m + \frac{1}{2}\right)u_m + \frac{1}{2}\left((1)m - \frac{1}{6}\right)\right) \\ &+ \frac{1}{2}(-1)m\left(\frac{1}{2}(1)m\,u_m + (1)m - \frac{1}{3}\right) + \frac{1}{3}(1)_m^2 \;. \end{aligned}$$

Application of Theorem 1, 25b), B13 and D11 yields

$$\text{(D18)} \qquad D_m = \frac{M-m}{8}\left(\frac{M-m}{8} - (1,-1)m - (-1,1)m - \frac{1}{2}(u_m - 1)(-1)m\right.$$

$$\left. + \left(-1 + \frac{1}{u_m}\right)(1)m - (0)m - \frac{1}{2u_m} + \frac{23}{24}\right)$$

$$+ \frac{1}{4}(u_m + 1)((1,-1,-1)m + (-1,1,-1)m + (-1,-1,1)m)$$

$$+ \frac{2}{3}(1,1)m - \frac{1}{4u_m}((1,-1)m + (-1,1)m)$$

$$+ \frac{1}{8}(u_m + 1)((1,-2)m + 2(0,-1)m + 2(-1,0)m + (-2,1)m)$$

$$+ \frac{1}{8}(2u_m + 1)((1,-1)m + (-1,1)m) + \frac{1}{24}\left(4u_m^2 + 3u_m - 1\right)(-1,-1)m$$

$$+ \frac{1}{3}(2)m + \frac{1}{24}\left(-11 - \frac{7}{u_m} + \frac{2}{u_m^2}\right)(1)m + \frac{1}{8}\left(2u_m + 1 - \frac{2}{u_m}\right)(0)m$$

$$+ \frac{1}{48}\left(-5u_m - 9 + \frac{2}{u_m}\right)(-1)m + \frac{1}{48}\left(4u_m^2 + 3u_m - 1\right)(-2)m$$

$$+ \frac{23}{96} + \frac{5}{16u_m} - \frac{1}{72u_m^2} \quad .$$

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