OPTIMAL SAMPLING FOR COORDINATE MEASUREMENT: ITS DEFINITION AND ALGORITHM

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Abstract

Accuracy in discrete sampling with coordinate measuring machines is first defined as the discrepancy of a finite point set, the lower bound for which was established by a Fields medalist. Then, from number theory, a particular sequence of numbers is used to compute the sampling locations -- resulting in a nearly quadratic reduction in the sample size, over the uniform or random distributions, at the same level of accuracy. Finally, experimental errors in the measurement of machined surfaces modeled as random processes are compiled, validating the number-theoretic predictions.

1. INTRODUCTION

Quality has many connotations and implications, such as customer satisfaction, management style, etc. In the engineering context, quality can be associated with precision in manufacturing. In the life cycle of a product, precision is expressed as tolerances in dimensioned drawings during the design stage. Viewing the ideal shape (with nominal dimensions) as the input to a manufacturing channel [1], its output (the realized shape) is corrupted by noise in the channel. As there are encoding and decoding schemes in signal communications, tolerance specification serves as a decoding scheme: inspection detects errors (but does not correct them). The difficulty in error correction is deeper than that which meets the eye. The signal in the manufacturing channel is not only complex in its dimensionality (as products are usually three-dimensional rather than one-dimensional bit streams), there are semantics embedded in the signal as the functionality of the product.

Inspection, as an error detection scheme, should be in itself error free. Confidence in the inspection process is however questionable. In 1988, R. Walker of Westinghouse issued an alert, through a medium called GIDEP (Government Industry Data Exchange Program) [2]: that the vendors of coordinate measuring machines (CMMs) used different algorithms in their machines -- resulting in a disagreement of as high as 60%! (An immediate conclusion one can draw is that good parts may have been rejected and bad parts may have been in service.) This phenomenon was subsequently termed as the *divergence of methods* [3].

There are actually two places where methods are invoked during inspection: for data gathering (or *sampling*) and for data interpretation (or *fitting*). Section 2 of this paper reviews the methods for both and bring out an important finding --the choice of a metric is subjective and is dependent on the implicit function of the design; but within the same metric there exists an absolute (hence objective) bound in accuracy leading to an optimal sampling strategy. Section 3 clarifies optimality as accuracy and time in coordinate measurement. Based on the work by K.F. Roth, the Fields medalist, accuracy in approximation is expressed by a mathematical notion called the *discrepancy* of a finite set of points, for which a lower bound exists [4]. For a finite set of N sample points, the time for sampling and for fitting can also be quantified in terms of N. Then, a sampling strategy based on the Hammersley sequence [5] is compared to uniform sampling. It shows a remarkable improvement of nearly-quadratic reduction in the number of samples, hence time, yet maintaining the same level of accuracy. (Loosely speaking, a quadratic reduction of 250,000 points yields 500.) Finally, implementation of the algorithm and simulation of inspection on machined surfaces [6] are conducted. The results confirm the theoretical prediction. This paper thus contributes to the convergence of sampling methods.

2. SOURCE OF DIVERGENCE

Because the notions of distance and metric are central to the source of divergence, it is useful to review them first. Then, divergence in fitting algorithms is given a context.

2.1 Distance and Metric

The basic idea in fitting is that of an *elevation in dimensionality*. Sample points are not only numerous, they are also zero-dimensional, topologically. By fitting a curve through points, or a surface through curves, hence elevating the dimensionality, two objectives are achieved. One, the size of data storage is reduced -- for later algorithmic processing. Two, a group behavior emerges -- for interpretation and decision-making.

While there is abundant literature on approximation such as [7], distance is the basic element in computation. Consider the familiar Euclidean *distance* between two points (x_1, y_1, z_1) and (x_2, y_2, z_2). For each of the three components of a vector, the difference, e.g. (x_1-x_2), is first captured. Then, the differences are squared, summed, and a square root taken over the sum, hence the root-mean-square or RMS difference:

$$d_2 = [(x_1-x_2)^2 + (y_1-y_2)^2 + (z_1-z_2)^2]^{1/2} \qquad (1)$$

The *metric* applied to (1) is the so-called L_2 metric and it has the general form under the L_p metric [8] as:

$$d_p = [\,|x_1-x_2|^p + |y_1-y_2|^p + |z_1-z_2|^p]^{1/p} \qquad (2)$$

Absolute value is taken so as to accommodate the odd and even nature of the exponent p. When $p \geq 2$, one finds a variety of distances, each having its own merit. In particular, when $p = \infty$, (2) becomes a mechanism for selecting the largest of the three components -- as supremum, or the maximal element in the set:

$$d_\infty = sup\,[\,|x_1-x_2|,\ |y_1-y_2|,\ |z_1-z_2|\,] \qquad (3)$$

Transition from (2) to (3) can be understood by assuming that one of the terms, say $|y_1-y_2|$, is the largest of the three. Dividing the entire right hand side of (2) by this term yields

$$d_p = \left\{ \left[\left(\frac{|x_1-x_2|}{|y_1-y_2|}\right)^p + \left(\frac{|y_1-y_2|}{|y_1-y_2|}\right)^p + \left(\frac{|z_1-z_2|}{|y_1-y_2|}\right)^p \right] |y_1-y_2|^p \right\}^{1/p} \qquad (4)$$

2

The first and the third terms in (4) vanish when p becomes very large, hence effectively rendering the supremum as in (3). Figure 1 illustrates the various d_p.

Figure 1

2.2 Fitting Algorithms

Having seen that distance can adopt infinitely many measures, it should not be surprising that there are a variety of algorithms for elevating the dimensionality of point data -- by fitting them into curves and surfaces [9]. The word "fitting" implies a pre-conceived notion of some ideal geometry. Indeed, there must be some polynomial of a fixed degree into which the data fits; for, otherwise, fitting becomes arbitrary.

The kinds of ideal geometries in computer aided design (CAD) are: linear, quadratic, cubic, and higher order. Examples of linear geometry are lines and planes; and examples of quadratic geometry are cylinders, cones and spheres. When the geometry is cubic or higher, there are few familiar shapes with the possible exception of a torus (which can be used to blend surfaces as fillets). In CAD, these high order surfaces are called free-form surfaces, implying the degrees of freedom that a designer has in expressing the desired shape through a set of control points. By virtue of the degree of local control the designer has on the shape, there are various interpolators [10, 11], such as Hermite, Bernstein and other polynomials, giving rise to Coons, Bezier, B-spline, non-uniform B-spline (NURB) curves and surfaces that are familiar to the CAD community.

Conceptually, there are three basic criteria to fit data to these ideal geometries: INNER, OUTER, and THROUGH. (By the distinction of INNER and OUTER, there is an implied direction that indicates the material side of the workpiece under inspection.) Data can be fitted so that they all lie on the inside (the material side) of the ideal geometry, or conversely, on the outside. While one can take the two extremes by taking both the INNER and OUTER, giving rise to a "tolerance zone," fitting an ideal geometry THROUGH the data, such that some lie on the inside and others on the outside, is a third alternative -- giving a sense of an "average." (It may be conjectured that the criterion for fitting data and the choice of a metric depend on the functionality of the component as implied by the intent of the design [12].) To ensure that the ideal geometry satisfies any of the three criteria, a distance function must be invoked, which can be linear, as in (3), or non-linear as in (1) or (2). Thus, fitting algorithms are seen as linear or non-linear optimization problems in general [13] whereby some form of a (linear or non-linear) distance is minimized [14] as constrained by an ideal (linear or non-linear) geometry. When the ideal geometry is

simple, as in the case of lines, circles, planes, and cylinders, analytic solutions are possible [15].

After the data has been fitted, it is compared to the ideal geometry. Here, again, the notion of distance must be invoked. For speed, one may choose the largest component, as in (3), for an approximation to distance. For accuracy, the RMS distance as in (1) is adopted. Recall that the objective of fitting point data is to elevate the dimensionality. Now that the zero-dimensional points have been raised to one-dimensional curves or two-dimensional surfaces, the distance between the fitted and the ideal curves and surfaces once again invokes that of the points: to find the distance between two curves, for example, one computes the distance between a pair of closest points on the two curves, and treats it as the distance between the curves. Adopting the paradigm of the Lp metric, one can take the square of the closest points, the cube, . . . as so on -- as distances. Without compounding the divergence in methods for assessing the distance between the elevated entities, the *irony of elevation* may be noted: the dimensionality of point data is elevated from zero to one (or two); yet the distance used is for zero-dimensional entities.

3. SAMPLING ALGORITHM

Discrete sampling is inherently an approximation process. If the number of samples is infinite, one may imagine that the error in approximation approaches zero. And when the sample size is finite, the error must be non-zero. This observation induces two practice questions: For any sampling sequence of size N, how small can the error be? (Section 3.1 answers this question.) And, in what way should the N samples be located in space? (This is answered in Section 3.2.) Together, these two sections address the accuracy and the time for coordinate measurement.

3.1 Sampling Error

It has been noted that once a metric is adopted, the variety of methods is less divergent than otherwise. But this still leaves open the question: Suppose one adopts the L_2 (or L_∞) metric, what is the best method for sampling? In the last section, the measure of "goodness" has been heuristic (or subjective): taking the least of the squares or minimizing the maximum. This section reports an objective criterion for assessing sampling errors.

Not that such a criterion contradicts the works of Gauss, Newton and Tschebychev [7,9,14], it was discovered at least a century later by K.F. Roth of the Imperial College, who received the equivalent of a Nobel in mathematics -- the Fields medal -- in 1958. Roth's contribution is in establishing a lower

bound in the *discrepancy* D between a finite set of N points and any function, in d dimensions [4].

$$D \cong O(N^{-1}(\log N)^{\frac{d-1}{2}}) \tag{5}$$

The significance of (5) is that the lower bound is expressed only in terms of N and d; it is devoid of any constraint on the function which the samples approximate. Most important to coordinate measurement is that one can determine if a finite set of samples of size N, giving rise to a discrepancy D, meets Roth's bound: hence giving the least amount of error possible. For calibration of the sampling sequences in the next section, Roth's bound in low dimensions are:

$$d = 2, \quad D \cong O(\sqrt{\log N} / N) \tag{6}$$

$$d = 1, \quad D \cong O(1/N) \tag{7}$$

As important as discrepancy is to coordinate measurement, the concept may be unfamiliar. The remainder of this section gives an outline of the basic idea along with definitions.

It is convenient to begin in two dimensions with a unit square [0,1] x [0,1] in which a region of interest bounded by some function resides. The area of the region can be approximated with points $p_1, p_2, \ldots p_N$ by the fraction:

$$area \cong \frac{1}{N} \sum_{i=1}^{N} \chi(p_i) \tag{8}$$

where $\chi(p_i)$ is the characteristic function indicating whether a point $p_i \in [0,1]^2$ is in or not in the region:

$$\chi(p_i) = 1 \quad \text{if } p_i \text{ is in the region}$$
$$0 \quad \text{otherwise}$$

Generalizing (8) to d dimensions whereby the unit square becomes a unit hypercube $I^d = [0,1]^d$ bounding a function f(t), $t \in I^d$, one has:

$$\int_{I^d} f(t) \, dt \cong \frac{1}{N} \sum_{i=1}^{N} \chi(p_i) \tag{9}$$

Calling the difference between the two sides of (9) as the residual:

$$R(t, N, p_i) = \int_{I^d} f(t) \, dt - \frac{1}{N} \sum_{i=1}^{N} \chi(p_i) \tag{10}$$

the discrepancy in the L_2 norm, or L_2 *discrepancy*, is defined as [16]:

$$D_2 = \left\{ \int_{I^d} [R(t,N,p_i)]^2 dt \right\}^{1/2} \tag{11}$$

Note the square root, the mean (by taking the integral in the sense of (9)), and the squaring of R. Likewise, in the L_∞ norm, the L_∞ *discrepancy* is defined by:

$$D_\infty = \sup_{I^d} |R(t,N,p_i)| \tag{12}$$

While there is a similarity between d_2 in (1) and D_2 in (11), and likewise between d_∞ in (3) and D_∞ in (12), it is noted that f(t) in (10) is a real-valued function that must be Riemann integrable. A variation of the residual (10) is to take the difference between the volume of a hypercube and its approximation [16]:

$$R^*(t,N,p_i) = \prod_{j=1}^{d} t_j - \frac{1}{N} \sum_{i=1}^{N} \chi \, (p_i) \tag{13}$$

giving rise to D_2^* and D_∞^*, respectively:

$$D_2^* = \left\{ \int_{I^d} [R^*(t,N,p_i)]^2 dt \right\}^{1/2} \tag{14}$$

$$D_\infty^* = \sup_{I^d} |R^*(t,N,p_i)| \tag{15}$$

And Roth [4] established the lower bound:

$$D_\infty^* \geq D_2 > k \, N^{-1}(\log N)^{\frac{d-1}{2}} \tag{16}$$

where the constant k is in terms of the dimension d only. The existence of such a bound triggered a flurry of activities in the construction of sequences of numbers, one of which is the subject in the next section.

3.2 Sample Size and Locations

It may be intuitive that, the larger the sample size, the more accurate the measurement is. Such an intuition is confirmed by (7) in that the minimal error of approximation is inversely proportional to the sample size of N, in one dimension. But as the dimensionality of the sample points increases, the error

is also directly proportional to some power of the logarithm of N, as in (6). The outstanding question is: are there sequences of numbers that approach or even reach Roth's bound, as in (5)? The answer turns out to be in the affirmative, from the works of researchers in number theory.

Before going into sequences, a word on the dimensionality d of the samples is in order. For a surface under inspection to be visible to an inspection machine, the surface can only be assumed to be single-valued. When the machine is a point sampling machine, it may be assumed that a command coordinate pair (x_i, y_i) is issued and a value z_i is read. When the machine is a line sampling machine, it may be assumed that a command coordinate (x_i) is issued and a pair (y_i, z_i) is read. The dimensionality of a sample, though always 3 after the data is read in, differs by the type of machinery used. In this work, sampling with the CMM is discussed; hence d = 2. To choose freely among the pairs (x_i, y_i), (x_i, z_i), and (y_i, z_i), the command coordinate (s_i, t_i) is identified with the term sample.

The sequence of numbers that Roth used to exhibit the tightness of his bound [17] is the *Hammersley sequence* [5]. Its coordinates (s_i, t_i) in two dimensions are defined by:

$$s_i = i/N \tag{17}$$
$$t_i = \sum_{j=0}^{k} b_j 2^{-j-1}$$

where

$i \in [0, N-1]$
N = total number of points
k = $\lceil \log i \rceil$ = ceiling of (log i)
b_j = binary digits for representing i

As the binary representation of integers is used, logarithm will be taken to the base 2.

Suppose N = 10 Hammersley points are used for inspection. The procedure for computing the Hammersley coordinates are as follows:

1. Determine k: Since $i \in [0,9]$, $\lceil \log i \rceil = 4$.

2. Determine b_j: The four-bit representation $(b_3 b_2 b_1 b_0)$ for i are: (0 0 0 0), (0 0 0 1), $\cdots$ (1 0 0 1).

3. Compute s_i: According to (17), the s_i coordinates for the N = 10 points are: 0/10, 1/10, 2/10, ... 9/10.

4. Compute t_i: The binary representation for the t_i coordinate is obtained by taking the "mirror image" of the binary representation for i, about the decimal point. For instance, for i = 1 = (0 0 0 1) or s_1 = 1/10, the mirror image is (1 0 0 0) or t_1 = 8/16. For i = 7 = (0 1 1 1) or s_1 = 7/10, the mirror image is (1 1 1 0) or t_7 = 14/16.

The N = 10 Hammersley points are illustrated in Figure 2. The 10x10 grid is to be interpreted as the locations for the 100 uniform samples.

Figure 2

In the construction of his sequence, Hammersley shows [5] that the discrepancy in d dimensions is of the order:

$$D_H \cong O(N^{-1}(\log N)^{d-1}) \tag{18}$$

which is off by a factor of one-half power as compared to the absolute lower bound established by Roth in (5). While slightly suboptimal, the Hammersley sequence shows a nearly quadratic reduction in the number of points needed by uniform sampling -- for the same level of accuracy as measured by discrepancy.

More precisely, it is known from Monte Carlo methods that, as the number of samples N approach infinity, the error becomes indistinguishable from that of a uniform sequence [16]. In particular, the error for a uniform sequence is $O(N^{-1/d})$. To compare the number of uniform points N_U against the Hammersley points N_H, suppose that they yield the same discrepancy in two dimensions:

$$\frac{1}{\sqrt{N_U}} = \frac{1}{N_H} \log N_H \tag{10}$$

where N_U denote the number of uniform points and N_H the number of Hammersley points. It becomes immediately obvious that there are almost quadratically many N_U as there are N_H:

$$N_U = \left(\frac{N_H}{\log N_H}\right)^2 \tag{19}$$

A plot of the relation between N_U and N_H is given in Figure 3.

Figure 3

4. IMPLEMENTATION

The confluence of mathematics and precision engineering has yet many bridges to be established. In his article [18], R. Hocken reports that there needs to be characterization of errors in the kinematics and dynamics of the CMM, lobing errors in the probe of the CMM, and the uncertainty in the manufacturing processes that create the workpiece. As the characterization of machine by machine, probe by probe, and workpiece by workpiece can be precise but laborious, the classical mathematization of manufacturing as random processes [19] seems once again attractive.

Not only because random processes offer first order (mean), second order (variance) and higher order statistics [20] that capture ensemble behavior of manufactured surfaces, evidenced in a beautiful catalog of machined surfaces [21], it turns out that random processes also provide a crucial link to Roth's bound and Hammersley's sequence [22, 23]. It is in this connection that the measurement for the roughness of a machined surface, modeled as Wiener, Gaussian or any process, permits the employment of discrepancy [24] hence the Hammersley and other sequences [25].

A number of experiments have been conducted to assess the accuracy of the Hammersley points for coordinate measurement. The number of samples range from 16 to 15,625 -- for two reasons. First, the uniform distribution of N_U = 10x10, 25x25, 50x50 and 125x125 = 15,625 points are used as benchmark. Secondly, the Hammersley points are chosen at N_H = 16, 32, 64 and 128 to approximate the reduction in (19).

Machined surfaces are simulated with two models: Wiener and Gaussian. For each of the two surface models, the uniform and the Hammerslsy points are used as samples so that their (respective) accuracies can be assessed. to give meaning to the notion of discrepancy (11,14), the roughness of a surface is measured, such that the average heights h at a point (s,t) on a surface is aproximated by N discrete measurements:

$$\int_0^1 \int_0^1 |h(s,t)|\, ds\, dt \cong \frac{1}{N} \sum_{i=1}^{N} |h(p_{is}, p_{it})| \qquad (20)$$

where p_{is} are the s-coordinates of the ith point in a sequence of N points. (Absolute value is taken on h(s,t) in (20) so as to ensure that the asperities do

not cancel out.) the similarity between (20) and (9) may be noted here. Calling the difference between the two sides of (20) as the error:

$$\epsilon(s,t,N,\mathbf{p_i}) = \int_0^1 \int_0^1 |h(s,t)| ds\, dt - \frac{1}{N} \sum_{i=1}^N |h(\mathbf{p_{is}}, \mathbf{p_{it}})| \tag{21}$$

the *root-mean-square error* in surface measurement ϵ_{RMS}, by invoking the L_2 metric, is simply:

$$\epsilon_{RMS} = \left\{ \int_0^1 \int_0^1 [\epsilon(s,t,N,\mathbf{p_i})]^2 \, f(s,t) ds\, dt \right\}^{1/2} \tag{22}$$

where $f(s,t)$ is the probability density function (for the Wiener and the Gaussian distributions). Again, note the similarity between (22) and (11).

Figure 4 shows thirty-two Hammersley points superimposed on a Wiener surface and on a Gaussian surface. It may be seen that the Wiener surface is smooth and periodic, simulating single-point cutting with a rotary tool. The Gaussian surface is more textured, simulating such processes as electro-discharge machining or sand-blasting.

Figure 4

Twenty runs are made for each of the Wiener and the Gaussain surface models and the RMS error in using the Hammersley points versus the uniform points are calculated based on (22). Table 1 shows the experimental results, on the RMS errors for the Wiener surfaces, with approximate correspondences in the equivalent number of sample points.

uniform		Hammersley	
number	RMS error	number	RMS error
50x50	0.01414	64	0.00678
25x25	0.03295	32	0.01081
10x10	0.09469	16	0.01407

Table 1. RMS Error on Wiener Surfaces

Table 1 shows that, for approximately a quadratic reduction in the numbr of points, the Hammersley samples are more accurate that uniform sampling. Results on the twenty Gaussian surfaces are given in Table 2.

uniform		Hammersley	
number	RMS error	number	RMS error
125x125	0.02254	128	0.01766
50x50	0.08092	64	0.04398
25x25	0.06107	32	0.05453
10x10	0.52517	16	0.08300

Table 2. RMS Error on Gaussian Surfaces

For approximately a quadratic reduction in the number, the Hammerslay points are of the same order in accuracy as the uniform points, as shown in Table 2, with the possible exception of the last row.

5. CONCLUSION

This work introduces the application of the Hammersley sequence to coordinate measurement, hence bringing some convergence to sampling methods. The basis upon which the Hammersley sequence applies is that it exhibits a discrepancy approaching the number theoretic limit asserted by Roth. And disrepancy is related to the RMS error in measuring surface roughness.

For point sampling, users of the CMM may wish to examine the reported strategy, over random or uniform sampling. For line sampling, practitioners in computer vision may take heart that a scan of 500 x 500 points can now be dramatically compacted [26]. And likewise for plane sampling, such as in computer tomography, a similar saving in data storage is in hand.

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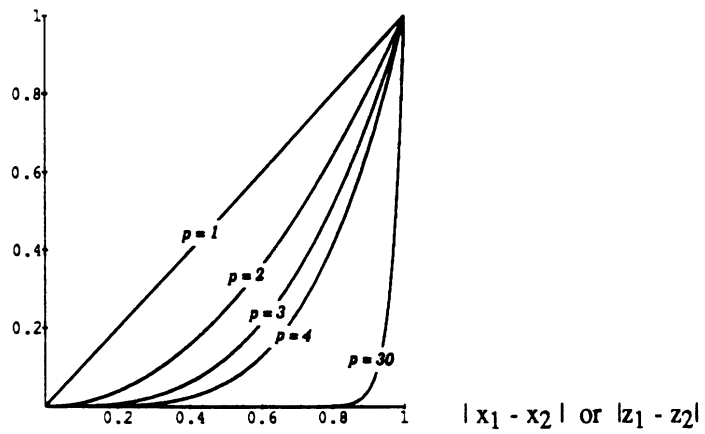
$| x_1 - x_2 |^p$ or $|z_1 - z_2|^p$

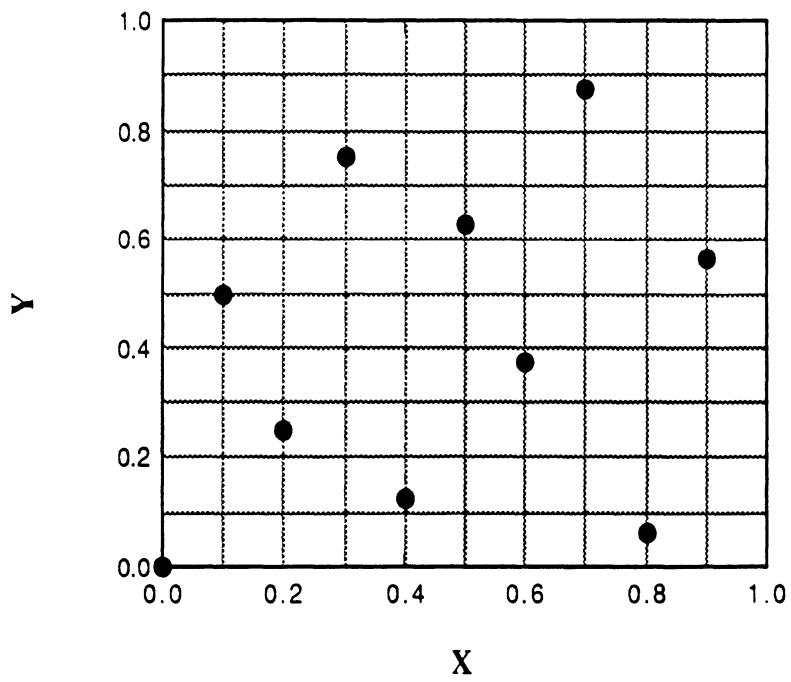Figure 1 Relative Importance of the individual items in (4) for different p

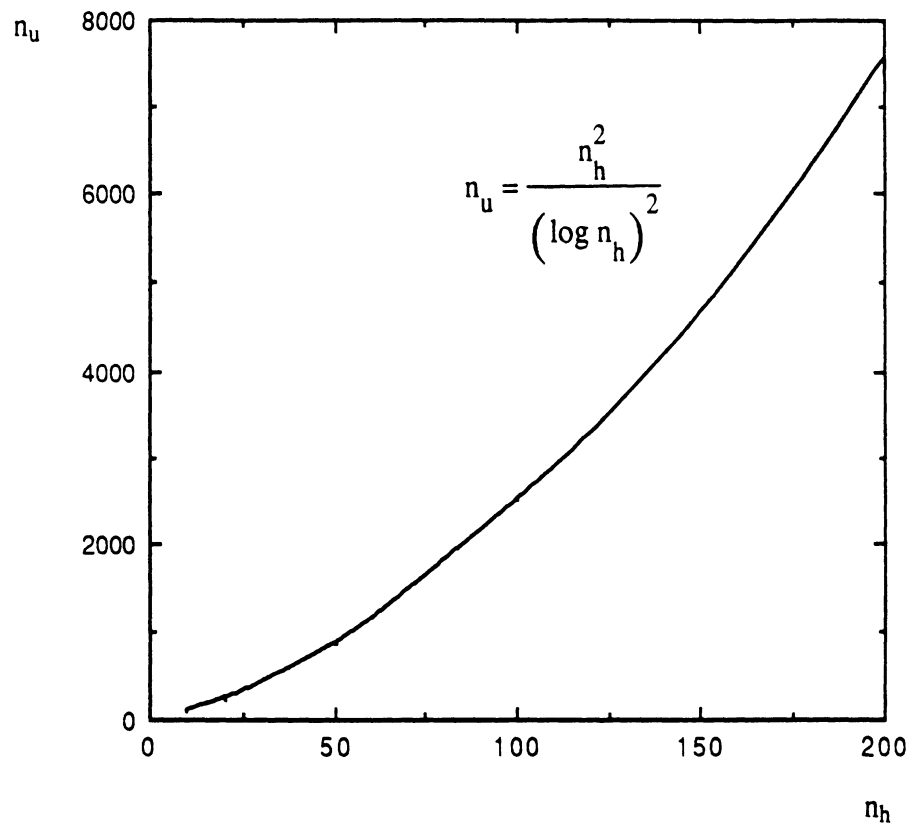Figure 2 The Distribution of Ten Hammersley Points

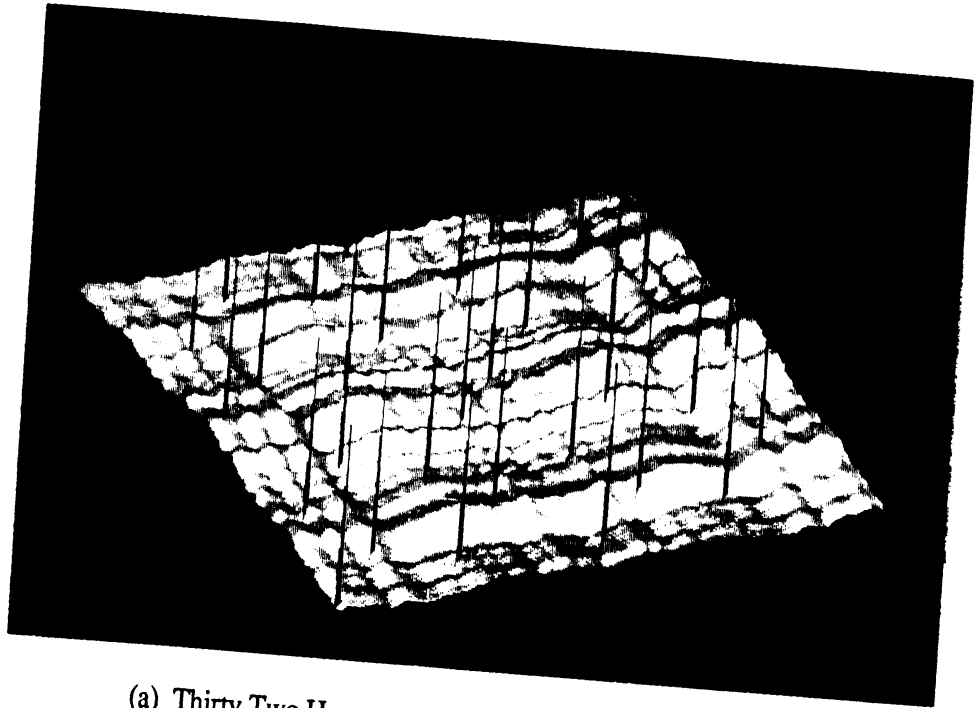$$n_u = \frac{n_h^2}{\left(\log n_h\right)^2}$$
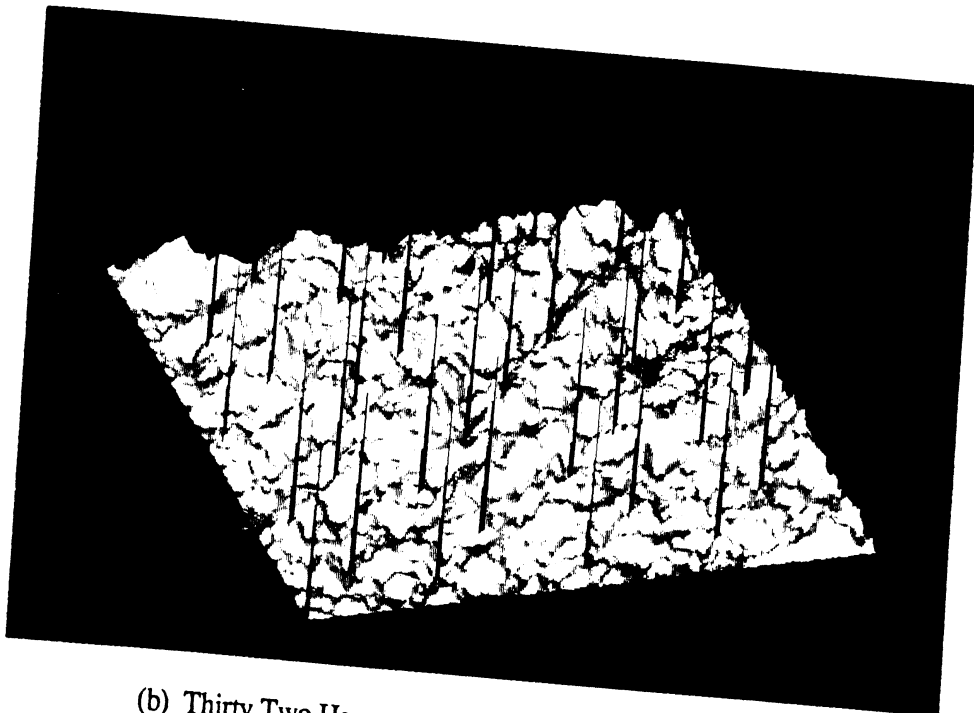
Figure 3   Hammersley Points (n_h) vs Uniform Points (n_u) under the Same Accuracy

(a) Thirty Two Hammersley Points on a Modified Wiener Surface

(b) Thirty Two Hammersley Points on a Gaussian Surface

Figure 4 Hammersley Points on Wiener and Gaussian Surfaces