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Approximating Convolution Products Better than the DFT while Keeping the FFT

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In recent years there has been considerable interest in the use of the Fast Fourier Transform Algorithm (FFT) to calculate the Discrete Fourier Transform (DFT), allowing—in particular—for the fast computation of convolution products of finite sequences of numbers. Generalizations of the DFT and FFT to dimensions $n = 2, 3,...$ are immediate, but their use in dimensions $n > 1$ to (approximately) calculate convolution integrals appears quite limited, even though integral equations involving multi-dimensional convolutions are common in physics. Most likely this situation is due to the fact that the quadrature formulas for approximating multi-dimensional convolution integrals obtained via the DFT are quite poor if $n > 1$. It is shown how the FFT can be used to calculate each of a whole class of newly defined transforms, the LPT or Lattice Point Transforms (hence, each LPT has a "fast algorithm" implementation). In a manner analogous to the n-dimensional DFT, each n-dimensional LPT allows one to (approximately) compute n-dimensional convolution integrals. Some of the quadrature formulas so obtained are exceptionally good. Such quadrature formulas correspond to LPTs generated by "good lattice points." The cataloguing of "good lattice points" represents an area of research in present day multi-dimensional integration theory. Where N_1 denotes the number of points of functional evaluation used, the expected error of the quadrature formulas arising through the use of the DFT is $O(N_1^{-1/n})$, while the expected error of the quadrature formulas arising through the use of LPTs generated by "good lattice points" is only slightly larger than $O(N_1^{-1})$. Applications to integral equations are discussed.

I. INTRODUCTION

We denote by L_N^n the set of points in the n-dimensional unit cube having coordinates $(j_1 N^{-1},..., j_n N^{-1})$, where $N > 1$ is an integer and $j_1,..., j_n$ each independently assume the values $0, 1,..., N-1$. The n-dimensional Discrete Fourier Transform (DFT) is a linear transformation (on the vector space of all complex functions f defined on L_N^n) which transforms each f into $\hat{f}$ given by

$$\hat{f}(\bar{x}) = N^{-n} \sum_{\bar{y} \in L_N^n} f(\bar{y}) \exp(2\pi i N \bar{y} \cdot \bar{x}). \tag{1}$$

The FFT (Fast Fourier Transform) is an algorithm which permits the calculation of (1) in $O(N^n \log N)$ steps if N is a power of 2. The implied constant is independent of N. The inverse DFT is given by

$$f(\bar{y}) = \sum_{\bar{x} \in L_N^n} \hat{f}(\bar{x}) \exp(-2\pi i N \bar{x} \cdot \bar{y}), \tag{2}$$

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and it can be calculated in $O(N^n \log N)$ steps also. (Note $N^n\hat{\hat{f}}(\bar{x}) = f(-\bar{x})$.) As is well known (and will be shown later) one may use the FFT to calculate the convolution product, $f_1 * f_2$, of any two complex functions f_1 and f_2 defined on L_N^n in $O(N^n \log N)$ steps, where

$$(f_1 * f_2)(\bar{x}) = N^{-n} \sum_{\bar{l} \in L_N^n} f_1(\bar{x} - \bar{l})\, f_2(\bar{l}). \tag{3}$$

We shall show how $f_1 * f_2$ arises naturally in the study of numerical solutions to certain integral equations; we shall see the drawbacks of using $f_1 * f_2$ to approximate numerically convolution integrals; and we shall produce a new class of transformations (each capable of being calculated via the FFT) some of which give rise *to much better integration formulas for approximating convolution integrals*, when $n > 1$, than does $f_1 * f_2$.

II. Integral Equations

Many problems in physics give rise to the consideration of n-dimensional integral equation of the type

$$f(\bar{x}) = \int k_1(\bar{t})\, k_2(\bar{x} - \bar{t})\, f(\bar{t})\, d\bar{t} + h(\bar{x}), \tag{4}$$

where k_1, k_2, and h are each known functions, and $\bar{x}$ and $\bar{t}$ are points in n-dimensional real space. In (4) the range of integration has been deleted; it may be all of n-dimensional space, but it can often be approximated by all values of $\bar{t}$ in an n-dimensional cube having sides parallel to the coordinate axes. A fairly usual technique of integral equations is to pick points $\bar{x}_1,\ldots, \bar{x}_{N_1}$ (where $N_1 \geqslant 1$) which are such that

$$N_1^{-1} \sum_{l=1}^{N_1} k_1(\bar{x}_l)\, k_2(\bar{x}_j - \bar{x}_l)\, f(\bar{x}_l)$$

is a good approximation to

$$\int k_1(\bar{t})\, k_2(\bar{x} - \bar{t})\, f(\bar{t})\, d\bar{t},$$

when $\bar{x}$ equals $\bar{x}_j$.

Then, instead of (4), one considers the system of linear equations

$$f(\bar{x}_j) = N_1^{-1} \sum_{l=1}^{N_1} k_1(\bar{x}_l)\, k_2(\bar{x}_j - \bar{x}_l)\, f(\bar{x}_l) + h(\bar{x}_j), \tag{5}$$

for $j = 1, 2,\ldots, N_1$.

N. N. Bojarski, in particular, has dealt with computational aspects of solving systems such as (5). (See [1].) Bojarski noted that many Green's functions are of the form $k_1(\bar{t})\,k_2(\bar{x}-\bar{t})$, where generally $k_1(\bar{t})\,k_2(\bar{x}-\bar{t})$ *does* have singularities. There are techniques which can often be used to remove the singularities. Often the cost of removing a singular part of $k_1(\bar{t})\,k_2(\bar{x}-\bar{t})$ is to add a linear term in $f(\bar{x}_{l_1})$ to the right hand side of (5), for some $\bar{x}_{l_1}$ in n-dimensional real space. If $\bar{x}_{l_1}$ is an $\bar{x}_j$, this leads to a small variation on the problem appearing in (5). We shall sketch an argument using the FFT in the case that $k_1(\bar{t})\,k_2(\bar{x}-\bar{t})$ has no singularities.

Since (5) is a system of N_1 linear equations in N_1 unknowns one could solve it by inverting an $N_1 \times N_1$ matrix, if this matrix is nonsingular. Such an inversion takes $O(N_1^3)$ steps in general. The coefficient matrix in (5) is of the form $I-M$ where I is the identity matrix. Thus, formally, its inverse is $I+M+M^2+\cdots$. Using a number of terms of this series is apparently equivalent to an iterative scheme in which the right hand side of (5) is repeatedly substituted back for f in the right hand side of (5). If K iterations are felt to be enough to ensure the accuracy desired then a solution takes $O(KN_1^2)$ steps to calculate accurately. This labor can often be reduced to $O(KN_1 \log N_1)$ steps via the FFT algorithm, as we shall now see.

One obvious choice of N_1 is N_2^n for some integer N_2 which is a positive integral power of 2. After rescaling, we can choose the $\bar{x}_l$ to be the vectors $(j_1 N_2^{-1},\ldots, j_n N_2^{-1})$, where each $j_l = 0, 1,\ldots, N_2 - 1$ for $l = 1, 2,\ldots, n$. These points all lie in the unit cube in n-dimensional real space, which shall be denoted by $([0,1])^n$. If $k_1 f$ and k_2 are periodic functions with period 1 in each variable the FFT may be used to calculate the right side of (5) in $O(N_2^n \log N_2)$ steps. The periodicity condition is often unrealistic, but it can sometimes be forced to hold. For example: suppose f and k_2 are approximately zero outside of $([-\frac{1}{4},\frac{1}{4}])^n$. Since we are then not concerned with using (5) to determine f for $\bar{x}_l$ outside of $([-\frac{1}{4},\frac{1}{4}])^n$ we might as well redefine $f(\bar{x})$, $k_1(\bar{x})$, and $h(\bar{x})$ to: (i) equal their old values if $\bar{x}$ is in $([-\frac{1}{4},\frac{1}{4}])^n$; (ii) be periodic with period 1 in each variable separately; (iii) vanish where not defined by (i) or (ii). The set of equations in (5) resulting from this redefinition should give usable values of $f(\bar{x})$ only if $\bar{x}$ is in $([-\frac{1}{4},\frac{1}{4}])^n$, but the economy in computation that results from using the DFT can justify having to throw away some of the computed values of $f(\bar{x})$. [Bojarski mentioned in a private conversation that he has developed a technique, applicable to problems of electromagnetic and acoustical scattering, which produces smooth integrands having compact support (so no discontinuities need be introduced in applying the above redefinition). This could increase accuracy considerably; see Section VI.]

III. The DFT, LPT, and the FFT

The DFT can be defined for all complex functions f defined on L_N^n. The DFT transforms each such function $f(\bar{x})$ into a complex function $\hat{f}(\bar{x})$ on L_N^n defined by

$$\hat{f}(\bar{x}) = N^{-n} \sum_{\bar{y}\in L_N^n} f(\bar{y}) \exp(2\pi i N \bar{y}\cdot\bar{x}) \tag{6}$$

for all $\bar{x}$ in L_N^n.

A derivation of the DFT which proves to be a good guide to defining other transforms is the following: Consider the inner product defined for all pairs of complex functions f_1 and f_2 on L_N^n by

$$\langle f_1, f_2 \rangle = \sum_{\bar{x} \in L_N^n} f_1(\bar{x}) \bar{f}_2(\bar{x}).$$

(Here the bar over f_2 denotes complex conjugation.) The N^n functions $N^{-n/2} \exp(-2\pi i N\bar{x} \cdot \bar{y})$ are orthonormal under the above inner product; it follows that they are also complete. Then for all complex functions f defined on L_N^n

$$\begin{aligned} f(\bar{y}) &= \sum_{\bar{x} \in L_N^n} N^{-n}(\langle f(\bar{x}), \exp(-2\pi i N\bar{y} \cdot \bar{x})\rangle) \exp(-2\pi i N\bar{y} \cdot \bar{x}) \\ &= \sum_{\bar{x} \in L_N^n} \hat{f}(\bar{x}) \exp(-2\pi i N\bar{y} \cdot \bar{x}), \end{aligned} \tag{7}$$

for all $\bar{y}$ in L_N^n. Equation (7) is the basic identity associated with the DFT.

In (6) substitute first f_1 then f_2 for f and multiply corresponding sides of the resulting equation together obtaining

$$\hat{f}_1(\bar{x}) \hat{f}_2(\bar{x}) = N^{-n} \sum_{\bar{y} \in L_N^n} \left(N^{-n} \sum_{\bar{l} \in L_N^n} f_1(\bar{y} - \bar{l}) f_2(\bar{l}) \right) \exp(2\pi i N\bar{y} \cdot \bar{x}). \tag{8}$$

It follows that the inverse DFT of $\hat{f}_1(\bar{x}) \hat{f}_2(\bar{x})$ is

$$N^{-n} \sum_{\bar{y} \in L_N^n} f_1(\bar{x} - \bar{l}) f_2(\bar{l}), \tag{9}$$

which we define to be $f_1 * f_2$. We note, also that

$$\hat{f}(x) = N^{-n}\langle f(\bar{y}), \exp(-2\pi i N\bar{y} \cdot \bar{x})\rangle. \tag{10}$$

In effect, above, one is doing part of the theory of square summable functions on a set of N^n well distributed points in the unit cube. The purpose of this "abstract harmonic analysis" is, from our present standpoint, to approximate numerically some of the corresponding quantities for complex functions defined on $([0, 1])^n$. Notice that L_N^n is an Abelian group under component-wise addition followed by reduction modulo one. Reasonable questions are: Why choose the group L_N^n? Why is L_N^n so special?

The idea behind defining the lattice point transforms is this: from the theory of multi-dimensional integration it is known that very well distributed subgroups G of L_N^n exist which have many fewer elements than L_N^n, but which are such that the *average value on* G of each of a large class of integrands can be expected to be nearly as close to the value of the integral as is the average value on L_N^n. The ability to deal with fewer points of evaluation in order to (approximately) solve (4) reduces the labor greatly.

Also, for integral equation such as (4), there is an additional advantage in solving for values of f at the points of a subgroup G of L_N^n. Set M equal to N^n divided by the order of G. Let the factor group L_N^n modulo G be represented by the cosets $\bar{a}_j + G$, where $j = 1, 2, \ldots, M$. Then for each $\bar{g}_k$ in G the following approximate identity holds:

$$f(\bar{a}_j + \bar{g}_k) \cong (\text{order of } G)^{-1} \sum_{\bar{g}_l \in G} k_1(\bar{g}_l)\, f(\bar{g}_l)\, f(\bar{g}_l)\, k_2(\bar{a}_j + \bar{g}_k - \bar{g}_l) + h(\bar{a}_j + \bar{g}_k).$$

This relation allows for an interpolation of f (supposed to be determined accurately on G) onto all of the points L_N^n. (One reason for requiring G to be a subgroup of L_N^n is that the minimal number of translates of G covers L_N^n.)

Let $\bar{v}$ be any element of L_N^n such that $\bar{0}, \bar{v}, \ldots, (N-1)\bar{v}$ are distinct; i.e., the cyclic group $C(\bar{v})$ generated by $\bar{v}$ is of order N and $C(\bar{v})$ is therefore isomorphic to L_N^1 (as a group) under the mapping $k\bar{v} \to kN^{-1}$. We proceed making definitions motivated by this isomorphism. An inner product can be defined for all complex functions $f_1(\bar{y})$ and $f_2(\bar{y})$ defined on $C(\bar{v})$ by

$$\langle f_1, f_2 \rangle = \sum_{\bar{y} \in C(\bar{v})} f_1(\bar{y})\, \bar{f}_2(\bar{y}).$$

Set $|v|^2 = \bar{v} \cdot \bar{v}$. The N functions, $N^{-1/2} \exp(-2\pi i N^{-1} |\bar{v}|^{-2} \bar{x} \cdot \bar{y})$, for each $\bar{x}$ in $C(\bar{v})$, are a complete orthonormal set of functions defined on $C(\bar{v})$. Recalling (10) we define a transformation on the complex functions defined on $C(\bar{v})$ by

$$\tilde{f}(x) = N^{-1} \langle f(\bar{y}), \exp(-2\pi i N^{-1} |v|^{-2} \bar{x} \cdot \bar{y}) \rangle. \tag{11}$$

Writing this out we see

$$\tilde{f}(k\bar{v}) = N^{-1} \sum_{l=0}^{N-1} f(l\bar{v}) \exp(2\pi i N^{-1} lk). \tag{12}$$

The Lattice Point Transform (LPT) of f with respect to $\bar{v}$. We call the $\tilde{f}$ given in (11) and (12) the Lattice Point Transform (of complex functions f defined on $C(\bar{v})$). If f is a complex function having a domain which includes $C(\bar{v})$, the Lattice Point Transform of f with respect to $\bar{v}$ is the (uniquely defined) Lattice Point Transform of the function f restricted to $C(\bar{v})$.

Suppose that f is a complex function on $C(\bar{v})$. Defining functions g and h on L_N^1 by

$$g(kN^{-1}) = f(k\bar{v}) \qquad \text{and} \qquad h(lN^{-1}) = \tilde{f}(l\bar{v}),$$

it becomes apparent that $h(lN^{-1}) = \tilde{f}(l\bar{v})$ is the 1-dimensional DFT of $g(kN^{-1})$. Thus the *Lattice Point Transform* has an inverse and the 1-dimensional FFT algorithm can be used to calculate $\tilde{f}$ in $O(N \log N)$ steps if N is a power of 2. Given two complex functions f_1 and f_2 defined on $C(\bar{v})$, define g_1 and g_2 in analogy with g above. From (12) we see that

$$\begin{aligned} \tilde{f}_1(\bar{x})\, \tilde{f}_2(\bar{x}) &= \hat{g}_1(kN^{-1})\, \hat{g}_2(kN^{-1}) \\ &= N^{-1} \sum_{l=0}^{N-1} \left(\left(N^{-1} \sum_{k=0}^{N-1} g_1(lN^{-1} - kN^{-1}) \right) g_2(kN^{-1}) \right) \exp(2\pi i N^{-1} lk); \end{aligned} \tag{13}$$

thus, the inverse Lattice Point Transform of $\tilde{f}_1 \tilde{f}_2$ is

$$N^{-1} \sum_{k=0}^{N-1} f_1((l-k)\bar{v})\, f_2(k\bar{v}).$$

DEFINITIONS. For any pair of complex functions f_1 and f_2 defined on $C(\bar{v})$ we define $f_1 \circledast f_2$ by

$$(f_1 \circledast f_2)(\bar{y}) = N^{-1} \sum_{\bar{x} \in C(\bar{v})} f_1(\bar{y} - \bar{x})\, f_2(\bar{x}).$$

If f_1 and f_2 each have a domain including $C(\bar{v})$ then $f_1 \circledast f_2$ is defined to be the $\circledast$ product of the respective restrictions to $C(\bar{v})$.

From what has been said $f_1 \circledast f_2$ can be calculated in $O(N \log N)$ steps if N is a power of 2. In what follows we shall present the case for regarding $f_1 \circledast f_2$, for appropriate $\bar{v}$, as a good quadrature formula for approximately calculating the convolution integral of f_1 and f_2. *Note $\circledast$ depends upon the choice of $\bar{v}$.*

IV. A BACKGROUND ON n-DIMENSIONAL INTEGRATION

This section gives a sketch of that part of n-dimensional integration theory which motivated the definitions of the Lattice Point Transforms. Let S denote the class of all subsets of $([0, 1])^n$ of the form

$$R = R(a_1, b_1, \ldots, a_j, b_j, \ldots, a_n, b_n) = \prod_{j=1}^{n} [a_j, b_j],$$

where, for $j = 1, 2, \ldots, n$, the a_j's and the b_j's satisfy $0 \leqslant a_j \leqslant b_j \leqslant 1$ and where $\prod$ denotes the Cartesian product. For any finite set X, let $|X|$ denote the number of elements in X.

DEFINITION. The discrepancy of a nonempty finite subset X of $I^n = ([0, 1])^n$ is the supremum over all R in S with $a_1 = a_2 = \cdots = a_n = 0$ of

$$\left| \prod_{j=1}^{n} (b_j - a_j) - |X \cap R|(|X|)^{-1} \right|.$$

The discrepancy of a set X is therefore a real number and we denote it by $D(X)$.

Clearly $0 < D(X) \leqslant 1$. The discrepancy of X is a measure of how well distributed X is in I^n. The lower the discrepancy the better distributed X is considered to be.

For complex valued functions F defined in $([0, 1])^n$ there is a concept called the Vitali variation $V^{(n)}(F)$ of F. (See [2, p. 147].) If $n = 1$ the Vitali variation agrees with the ordinary definition of the total variation of F on $[0, 1]$. We say that a function F is of bounded Vitali variation on $([0, 1])^n$ if $V^{(n)}(F) < +\infty$. A function F is said to be of bounded variation in the sense of Hardy and Krause if the Vitali variation of F on $([0, 1])^n$ is finite *and* if the Vitali variations of F restricted to each k-dimensional face of $([0, 1])^n$ are finite, for $k = 1, 2, \ldots, n-1$. We shall denote the sum of these variations by $V(F)$.

LEMMA. *Suppose F is defined on an open subset U of n-dimensional space which contains some R in S (cf. the definition of discrepancy). Then if each*

$$\frac{\partial}{\partial x_{j(1)}} \cdots \frac{\partial}{\partial x_{j(k)}} F$$

is continuous on U whenever $1 \leqslant j(1) < j(2) < \cdots < j(k) \leqslant n$, the function which agrees with F on R and which is identically zero on the complement of R in $([0, 1])^n$ is of bounded Hardy–Krause variation on $([0, 1])^n$. Also, the Hardy–Krause variations of the truncations of F, corresponding to each R_1 in S such that $R_1 \subseteq R$, are uniformly-bounded.

The proof of this technical lemma is omitted here. (A more detailed report is available from the author.)

The basic result connecting the concepts of numerical integration, $V(F)$, and $D(X)$ is:

THEOREM I. *For all nonempty finite sets $X \subset ([0, 1])^n = I^n$*

$$\left| \int_{I^n} F(\bar{y})\, d\bar{y} - |X|^{-1} \sum_{\bar{x} \in X} F(\bar{x}) \right| \leqslant D(X)\, V(F).$$

For a proof of Theorem I see [2, p. 151]. (The result there is sharper, as may be seen by noting that the discrepancy, in $([0, 1])^n$, of the projection of X onto a k-dimensional face of $([0, 1]^n$ is less than or equal to $D(X)$, for $k = 1, 2, \ldots, n-1$.)

We next see that the set L_N^n has discrepancy at least N^{-1}. This follows since for each ε satisfying $0 < \varepsilon < (2N)^{-1}$, $R(\varepsilon, BN^{-1} - \varepsilon, 0, 1, \ldots, 0, 1)$ has volume $N^{-1} - 2\varepsilon$ and contains no points of L_N^n. Notice L_N^n has N^n points. *It is known that there are sets S of exactly N points in $([0, 1])^n$ having discrepancy not much larger than N^{-1}.* Some of these sets having low discrepancy are sets of the form $C(\bar{v}) \subseteq L_N^n$. We shall next discuss such vectors $\bar{v}$; they are called "good lattice points." S. K. Zaremba has been very active in these investigations regarding good lattice points: see [3–8].

V. Good Lattice Points

A few preliminary comments: there appear to be several defintions of "good lattice points" in the literature. The basic requirement of course is that, where $X = C(\bar{v})$, $D(X)$ must be small if $\bar{v}$ is to be a good lattice point. A disappointment is that there is, in general, no formula for producing good lattice points. Computer searches are common and tables have been produced, see [9]. Much effort has been expended upon showing the existence of good lattice points, so that we know ahead of time that the computer search will be fruitful. For many physical applications probably n should equal 2 or 3 and N should ideally be a power of 2. The cases $n = 2$ and 3 have been investigated, but the principal interest has been in dimensions $n \geqslant 5$ where even Monte Carlo integration requires very many points. (Some applications in theoretical chemistry involve this many dimensions and more.) The values of N and $\bar{v}$ chosen for tables are usually picked so as to produce a sequence of optimally small values of $D(C(\bar{v}))$; as it turns out, those N which are powers of 2 are usually not listed. Dr. S. Haber of the National Bureau of Standards has calculated a table of higher-dimensional good lattice points where each N is a power of 2. Haber's table is in the Appendix. (In [3] it is shown that good lattice points exist for all integers N. Here we have assumed that N is a power of 2 because the FFT algorithms are most efficient in this case. If the restriction of N to be a power of 2 should turn out to increase the integration error unacceptably it is possible, using algebraic tricks, to compute $f \circledast g$ even when N is not a power of 2, as values of a convolution of two sequences each of length to a power of 2. Thus the computation can still be carried out using the FFT.) For more about good lattice points see [10, 11].

DEFINITION. In [2], a definition of a good lattice point is given for the integer N and the dimension n. Provisionally we define a good lattice point for the integer N and the dimension n to be a vector $\bar{v}$ in L_N^n such that the discrepancies of $C(\bar{v})$ and each of its translates (i.e., every set of the form $\bar{x} + C(\bar{v})$ for all n-dimensional vectors $\bar{x}$) are less than

$$c_n(\log N)^n N^{-1}, \tag{14}$$

where, if $N \geqslant 3$,

$$c_n \leqslant (4n^2 3^{n+1})(5^n + 1). \tag{15}$$

The actual definition will be given in the Section VI where the definition will be better motivated. (The provisional definition is a consequence of the ultimate definition. The bound in (15) is obtained by following through the proof of our Theorem I given in [2] and using the bound on the constant in the Erdös Turan Koksma Theorem on page 116 of [2]. Professor Niederreiter has recently informed me that some of his newer results would improve these estimates, see [12–14].

VI. PERIODIC INTEGRANDS

Good lattice points were apparently first discovered in an attempt to (numerically) integrate functions which are periodic with period one in each variable and are quite smooth. Suppose $f = \sum_{\bar{k}} a_{\bar{k}} \exp(2\pi i \bar{k} \cdot \bar{x})$, where $\bar{x} = (x_1, ..., x_n)$, $\bar{k}$ runs over all n-tuples with integral coordinates, each $a_{\bar{k}}$ is a complex number, and $\sum_{\bar{k}} |a_{\bar{k}}| < \infty$. Let

I^n denote $([0, 1])^n$. Since f is Lebesgue integrable on I^n $\int_{I_n} f(\bar{x})\,d\bar{x} = a_0$. Using $\sum_{\bar{k}} |a_{\bar{k}}| < \infty$, it is easily seen that

$$\int_{I^n} f(\bar{x})\,d\bar{x} - \frac{1}{N}\sum_{j=1}^{N-1} f(j\bar{v}) = \sum{}' a_{\bar{k}},$$

where the prime indicates that the sum is over all nonzero $\bar{k}$ such that $\bar{v} \cdot \bar{k}$ is an integer. Obviously, a bound for the absolute value of the error in numerical integration is $\sum' |a_{\bar{k}}|$.

DEFINITION. For each n-vector of integers, $\bar{k}$, set,

$$R(\bar{k}) = \prod_{j=1}^{n} (\max\{1, |k_j|\}).$$

Let α be an integer, $\alpha > 1$. If enough partial derivatives of f with respect to $x_1,\ldots, x_n$ exist and are continuous on I^n, then each $|a_{\bar{k}}| \leqslant c(\alpha)(R(\bar{k}))^{-\alpha}$, where $c(\alpha) > 0$, is independent of $\bar{k}$. In these cases one should apparently choose $\bar{v}$ such that

$$\sum_{\bar{k}}{}' (R(\bar{k}))^{-\alpha}$$

is small (the prime has the same meaning as before). One approach is to find vectors $\bar{v}$ such that $\bar{k} \cdot \bar{v}$ is an integer implies that either $\bar{k} = \bar{0}$ or $R(\bar{k})$ is comparatively large, i.e., $R(\bar{k}) > \phi(N)$, where $\phi(N)$ has order of growth close to that of the function N.

S. K. Zaremba defines good lattice points to be vectors $\bar{v}$ for which the associated number $\phi(N)$ is at least as large as $(n-1)!\,N(2\log N)^{1-n}$. We now give the definition of a good lattice point from inequality (5.32) of [2].

DEFINITION. The vector $\bar{v}$ in L_N^n is a good lattice point if

$$\sum_{\bar{k}}{}'' (R(\bar{k}))^{-1} < 2N^{-1}(5\log N)^n,$$

where the double prime indicates that we sum only over those nonzero k such that each component of $\bar{k}$ has absolute value less than N and also $\bar{k} \cdot \bar{v}$ is an integer.

(From this definition, inequalities (14) and (15) can be shown to follow. In this case, as with the Zaremba definition, good lattice points to be good for the integration of periodic functions. Obviously using Zaremba's definition of a good lattice point $\sum''(R(\bar{k}))^{-1}$ is small, so the two concepts are close.)

Suppose that f is of the form $f = \sum_{\bar{k}} a_{\bar{k}} \exp(2\pi i\bar{k} \cdot \bar{x})$, where $\bar{k}$ varies over all n-tuples of integers and where $|a_{\bar{k}}| < M(R(\bar{k}))^{-\alpha}$ for two real constants $M > 0$ and $\alpha > 1$. It is shown on page 157 of [2] that:

THEOREM II. *If $\bar{v}$ is a good lattice point in our sense, then*

$$\left| N^{-1} \sum_{j=0}^{N-1} f(j\bar{v}) - \int_{I^n} f(\bar{x})\, d\bar{x} \right| < M(1 + 2\zeta(\alpha))^n (1 + 2^\alpha (5 \log N)^{\alpha n})\, N^{-\alpha},$$

where ζ denotes the Riemann Zeta Function.

Thus, the numerical integration of periodic functions using good lattice points exploits the "amount of differentiability" actually present in f, *whatever that amount may be*. For the sake of comparison consider that

$$\int_{I^n} f(\bar{x})\, d\bar{x} - N^{-n} \sum_{\bar{y} \in L_N^n} f(\bar{y}) = -\sum_{\bar{k} \neq \bar{0}} aN_{\bar{k}},$$

where $N\bar{k} = (Nk_1, \ldots, Nk_n)$. The integration error is then potentially at least as large as

$$MN^{-\alpha}$$

using N^n points. *The error using a good lattice point is* $O((\log N)^n N^{-1})^\alpha$ using only N points!

VII. INTEGRATION ERRORS AND INTEGRAL EQUATIONS

Suppose that $\bar{v} \in L_N^n$ is a good lattice point. Suppose that $f_1(\bar{x}) = h_1(\bar{x} + (\frac{1}{2}, \ldots, \frac{1}{2}))$ and $f_2(\bar{x}) = h_2(\bar{x} + (\frac{1}{2}, \ldots, \frac{1}{2}))$, where h_1 and h_2 are functions defined on n-dimensional real space each of which satisfies the hypotheses on F in the Lemma of this paper, for all R in S having each $a_j \geqslant \frac{1}{4}$ and every $b_j \leqslant \frac{3}{4}$, for $j = 1, 2, \ldots, n$. Consider from now on instead of f_1 and f_2 truncations of f_1 and f_2 to $([-\frac{1}{4}, \frac{1}{4}])^n$. Then h_1 and h_2 are truncated to $([\frac{1}{4}, \frac{3}{4}])^n$. We further change h_1 and h_2 by keeping their (new) definitions on I^n but extending then from I^n to all of n-dimensional real space so as to make them periodic with period one in each variable. By a change of variables

$$\int_{([-1/4, 1/4])^n} f_1(\bar{t})\, f_2(x - \bar{t})\, d\bar{t} = \int_{I^n} h_1(\bar{t})\, h_2(\bar{x} - \bar{t})\, d\bar{t}$$

for each $\bar{x}$ in I^n.

Each integrand on the right side of the equation above vanishes outside of some $R_k \subseteq ([\frac{1}{4}, \frac{3}{4}])^n$, where R_k is in S. By the Lemma, there exists $M > 0$ such that M is a bound for the Hardy–Krause variation of these integrands. It follows, using Theorem I, that

$$\left| h_1 * h_2(k\bar{v}) - \int_{I^n} h_1(\bar{t})\, h_2(k\bar{v} - \bar{t})\, d\bar{t} \right| < M \cdot D(C(\bar{v})), \tag{16}$$

for $k = 0, 1, \ldots, N - 1$.

Similarly,

$$\left| h_1 * h_2(\bar{x}) - \int_{I^n} h_1(\bar{t})\, h_2(\bar{x} - \bar{t})\, d\bar{t} \right| < MD(L_N^n), \tag{17}$$

for all $\bar{x}$ in L_N^n. Recall $D(L_N^n) \geqslant N^{-1}$.

As in Section III let the $\bar{a}_j + C(\bar{v})$ be a set of representatives for the cosets of L_N^n modulo $C(\bar{v})$, for $j = 1, 2, \ldots, N^{n-1}$.

Suppose that one approximately solves an integral equation of type (4) by using the method outlined in Section II where: (i) for some $\bar{v}$ in L_N^n the $\bar{x}_l$ in (5) are the vectors of the form $\bar{c} - (\frac{1}{2}, \ldots, \frac{1}{2})$ for all $\bar{c}$ in $C(\bar{v})$; (ii) $f_1 = k_1 f$; and (iii) $f_2 = k_2$. If K iterations are felt to be necessary, the number of steps required to approximately calculate f at all of the points $\bar{x}_l$ is $O(KN \log N)$. If after this calculation one wishes to know f at all of the points of the form $\bar{l} - (\frac{1}{2}, \ldots, \frac{1}{2})$, where $\bar{l}$ is in L_N^n, one may take $f_1 = k_1 f$ and set $f_2(\bar{t})$ equal successively to $k_2(\bar{a}_j + \bar{t})$ for $j = 1, 2, \ldots, N^{n-1}$. Since to compute $h_1 * h_2$ takes $O(N \log N)$ steps, to approximately compute the integrals in (16) for all N^n values of $\bar{a}_j + k\bar{v}$ takes $O(N^n \log N)$ steps. For K much less than N^{n-1}, this says that one can approximate f at all of the points $\bar{l} - (\frac{1}{2}, \ldots, \frac{1}{2})$ in $O(N^n \log N)$ steps instead of $O(KN^n \log N)$ steps, with what should be close to the same accuracy as is obtained using the DFT.

VIII. Periodic Integrands in Integral Equations

If the integrand is periodic the previous analysis holds except that the accuracy of both sets of integration formulas (using $C(\bar{v})$ and using L_N^n) is enhanced. Therefore, it may be possible to obtain good accuracy while using fewer than N points of evaluation. How might one determine f at fewer than N points and then extend this determination of f to all of L_N^n?

Notice that $L_{2^m}^n \subseteq L_{2^{m+1}}^n \subseteq \cdots$. Using a good lattice point in $L_{2^m}^n$ one could, after a number of iterations, approximately calculate f first at all points of $L_{2^m}^n - (\frac{1}{2}, \ldots, \frac{1}{2})$ and then at all points of $L_{2^m}^n - (1/2^{m+1}, \ldots, 1/2^{m+1}) - (\frac{1}{2}, \ldots, \frac{1}{2})$ using the techniques of the previous section. Together these two sets of points comprise $L_{2^{m+1}}^n - (\frac{1}{2}, \ldots, \frac{1}{2})$. Continuing, one could approximate f at the points of $L_{2^{m+j}}^n - (\frac{1}{2}, \ldots, \frac{1}{2})$. for any j. The method discussed at the end of Section VII takes $O(N^n \log N + KN \log N)$ steps. The method just described takes $O(N^n \log N + KN_1 \log N_1)$ steps, where the K iterations are each carried out using $N_1 \leqslant N$ points. When $K > N^{n-1}$, the savings in the number of steps could be important.

Appendix: Haber's Calculation of Some Good Lattice Points

S. Haber conducted a computer search for good lattice points in dimensions 2 to 8 when N is a power of 2. Haber looked only at vectors of the form $(1, a, a^2, \ldots, a^{n-1})$

as potential good lattice points. Reproduced below are the best values of a which he found for each pair (n, N) considered.

The table below is self-explanatory, except for the columns labeled error. The error in these tables is the maximal integration error which could occur in integrating any function of the form $\sum_{\bar{k}} a_{\bar{k}} \exp(2\pi i \bar{k} \cdot \bar{x})$ with each $|a_{\bar{k}}| \leqslant (R(\bar{k}))^{-2}$, using the lattice point $(1, a, a^2, ..., a^{n-1})$. The last two digits in the error columns refer to a factor of 10 to the indicated power.

The author has available a report with slightly more details. He is interested in obtaining feedback about applications of the method, especially since the method should be capable of greater refinement in specific circumstances.

N	a	Error	N	a	Error
	$n=2$			$n=3$	
4	1	0.387805+01	4	1	0.187716+02
8	3	0.108049+01	8	3	0.856411+01
16	7	0.372186+00	16	5	0.350605+01
32	9	0.123207+00	32	11	0.141611+01
64	27	0.315720–01	64	5	0.563185+00
128	29	0.952037–02	128	41	0.175298+00
256	99	0.248180–02	256	37	0.590787–01
512	189	0.721157–03	512	123	0.196052–01
1024	399	0.214383–03	1024	173	0.669393–02
2048	849	0.688732–04	2048	753	0.203153–02
4096	1787	0.165999–04	4096	1271	0.884861–03
8192	3453	0.439584–05	8192	2835	0.210598–03
16384	6279	0.119209–05	16384	1163	0.799447–04
32768	5133	0.402331–06	32768	8655	0.205934–04
65536	27627	0.119209–06	65536	22201	0.591576–05
131072	34613	0.298023–07	131072	42445	0.233948–05
	$n=4$			$n=5$	
4	1	0.837706+02	4	1	0.362219+03
8	3	0.416424+02	8	3	0.180840+03
16	5	0.202653+02	16	5	0.898656+02
32	3	0.981764+01	32	5	0.433930+02
64	21	0.382833+01	64	13	0.201308+02
128	21	0.154038+01	128	3	0.962822+01
256	39	0.613026+00	256	21	0.405588+01
512	107	0.252041+00	512	151	0.181237+01
1024	493	0.912730–01	1024	363	0.734556+00
2048	941	0.384578–01	2048	659	0.303642+00
4096	2023	0.131653–01	4096	661	0.133277+00
8192	539	0.395443–02	8192	3333	0.482314–01
16384	2037	0.157484–02	16384	2705	0.205285–01
32768	11579	0.618219–03	32768	145	0.880437–02
65536	18793	0.189885–03	65536	18351	0.303666–02
131072	2771	0.645667–04	131072	2771	0.108038–02

Table continued

N	a	Error	N	a	Error
	$n=6$			$n=7$	
4	1	0.155717+04	4	1	0.668317+04
8	3	0.777900+03	8	3	0.334092+04
16	5	0.388402+03	16	5	0.166999+04
32	3	0.193766+03	32	5	0.834552+03
64	11	0.937380+02	64	11	0.414317+03
128	5	0.441573+02	128	5	0.204352+03
256	123	0.217294+01	256	99	0.997137+02
512	3	0.963975+01	512	93	0.490582+02
1024	491	0.461733+01	1024	141	0.225562+02
2048	443	0.212211+01	2048	683	0.104945+02
4096	1271	0.894023+00	4096	1159	0.507417+01
8192	67	0.355784+00	8192	3091	0.237492+01
16384	7011	0.161691+00	16384	2037	0.113009+01
32768	4335	0.670017+01	32768	453	0.457384+00
65536	24565	0.294434–01	65536	4855	0.193287+00
131072	33269	0.139112–01	131072	33269	0.926493–01
	$n=8$				
4	1	0.286732+05			
8	3	0.143362+05			
16	5	0.716763+04			
32	5	0.358321+04			
64	11	0.178947+04			
128	35	0.894503+03			
256	99	0.448897+03			
512	93	0.216616+03			
1024	141	0.102948+03			
2048	443	0.503627+02			
4096	595	0.253335+02			
8192	2153	0.114092+02			
16384	6957	0.563589+01			
32768	453	0.244354+01			
65536	25219	0.120873+01			
131073	11495	0.586658+00			

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