Acta Cryst. (1953). **6**, 469

Locating the Principal Maxima of a Fourier Series

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(*Received 7 November* 1952)

A numerical method for locating the principal maxima of a multi-dimensional Fourier series is described which obviates the necessity for computing the function. The underlying postulate is that the most prominent maxima lie in those regions in which there occurs dense packing of the maxima of the individual terms of the series. The procedure has been adapted for use with I.B.M. equipment.

Introduction

The tedium and expense of computing multi-dimensional Fourier series are familiar problems. It therefore seemed desirable to develop a relatively rapid numerical procedure for locating the principal maxima of a Fourier series without computing the function at a prohibitively large number of points. This is particularly worthwhile for a Fourier series which contains more terms and higher frequencies than those usually dealt with in crystallographic computations; as occurs, for example, in the series expansion of the probability distribution for interatomic vectors (Hauptman & Karle, 1952, equation 58).

The procedure to be described depends upon the intuitive concept that the most prominent maxima of a Fourier series occur in those regions in which the degree of clustering of the maxima of the individual terms in the series is relatively high. In this way the smaller, unimportant maxima are automatically removed from consideration. The attempt to solve this problem by means of a first derivative not only leads to an impractical algebraic problem, but also offers no means for readily distinguishing between the principal maxima and the insignificant ones.

Basic concepts

In order to develop the basic ideas, we treat first the case for one dimension and consider the two-term series

$$S = A \cos 2\pi mx + B \cos 2\pi nx \,, \qquad (1)$$

where A and B are positive, and m and n are assumed to be relatively prime positive integers. The maxima of the term

$$S_1 = A \cos 2\pi mx \qquad (2)$$

occur at $x = u/m$, where u is any integer, and the maxima of

$$S_2 = B \cos 2\pi nx \qquad (3)$$

occur at $x = v/n$, where v is any integer. In accordance with the basic concept, it is postulated that the most prominent maximum of (1) occurs in the region in which a maximum of (2) is closest to some maximum of (3). Therefore, we consider the problem of minimizing the difference

$$\left|\frac{u}{m} - \frac{v}{n}\right| = \frac{|un - vm|}{mn} \,. \qquad (4)$$

Since $un - vm$ is an integer and m and n are assumed to be relatively prime, the minimum, non-trivial value of (4) is obtained by solving the diophantine equation

$$un - vm = \pm p \,, \qquad (5)$$

where $p = 1$, the solution of which is well known. Denoting by u_1, v_1 the fundamental solution (i.e. $0 < u_1/m \leq \frac{1}{2}$, $0 < v_1/n \leq \frac{1}{2}$) of (5) with $p = 1$, the most prominent maximum of (1) lies in the interval $u_1/m, v_1/n$, where the difference $|u_1/m - v_1/n|$ is equal to the small number $1/mn$.

The next step is to locate more accurately the point within the small region $u_1/m, v_1/n$ at which the maximum occurs. We replace S_1 and S_2 in (1) by the first two terms of their Taylor expansions at their respective maxima, u_1/m and v_1/n; and proceed to find the unique maximum of the resulting parabola for (1) by the usual method of equating the derivative to zero. In this way we find the position of the most prominent maximum of (1) to be very nearly

$$x = \frac{Amu_1 + Bnv_1}{Am^2 + Bn^2} = \frac{Am^2 . u_1/m + Bn^2 . v_1/n}{Am^2 + Bn^2} \,. \qquad (6)$$

The last term in (6) is seen to be a weighted average of the two maxima of (2) and (3) respectively which are closest together. The next most prominent maxima of (1) are obtained by permitting p in (5) to take on successively the values 2, 3, 4, ...

A simple numerical example will illustrate the principles involved. In (1), let $A = 3$, $B = 1$, $m = 7$ and $n = 17$. Since $17 \times 2 - 7 \times 5 = -1$, $u_1 = 2$ and $v_1 = 5$. Substitution into (6) yields

$$x = \frac{3 \times 7 \times 2 - 1 \times 17 \times 5}{3 \times 7^2 + 1 \times 17^2} = 0{\cdot}29128,$$

while the true position of the maximum is $x=0{\cdot}29127$.

In the case that either of the coefficients in (1) is negative or that one or both terms may be a sine, a slight modification of (5) is required. Equation (5) is replaced by

$$(u+\eta_1)n-(v+\eta_2)m = \pm p\,, \tag{7}$$

where

$$\eta_1 = 0 \quad \text{if} \quad S_1 = A\cos 2\pi mx,\ A>0\,, \tag{8}$$

$$\eta_1 = \tfrac{1}{4} \quad \text{if} \quad S_1 = A\sin 2\pi mx,\ A>0\,, \tag{9}$$

$$\eta_1 = \tfrac{1}{2} \quad \text{if} \quad S_1 = A\cos 2\pi mx,\ A<0\,, \tag{10}$$

$$\eta_1 = \tfrac{3}{4} \quad \text{if} \quad S_1 = A\sin 2\pi mx,\ A<0\,, \tag{11}$$

and similarly for η_2. In (7), p ranges over only those values for which the equation is solvable in integers u, v.

The procedure just described falls naturally into two steps: the determination of the approximate locations of the maxima and the refinement of these locations. In generalizing the procedure to series having many terms this two-step process is maintained. In carrying out the first step, only terms having the largest amplitudes (roughly the first 10%) need be used, and in the refinement procedure the entire series is used.

A reference frequency is chosen (not necessarily a frequency occurring in a given series) which is large enough to give sufficient resolution for the problem under consideration. An increased accuracy in the rough computation resulting from the choice of an even larger frequency is generally not sufficient to justify the increased amount of labor which would be required. The reference frequency divides a unit interval into a corresponding number of sub-intervals, the one dimensional lattice. From another point of view, the above procedure described for two terms is a method for determining those maxima of either term which lie closest to the lattice points determined by the frequency of the other term. Now, we use this method to determine those maxima of each term in the Fourier series which lie closest to the lattice points determined by the reference frequency. The most prominent maxima of the Fourier series are expected to be near those lattice points about which there occurs the densest clustering of the maxima from the individual terms.

Each lattice point in a region of clustering is given an approximate weight based on the contributions from the maxima of the individual terms. As suggested by (6), the contribution of each term to the total weight is proportional to its amplitude and the square of its frequency. In addition, a correction should be applied which measures the degree of cluster in a particular region. At this stage this is roughly accomplished by including a factor which depends upon the distance from a maximum of an individual term to the lattice point. Later in the procedure this weighting can be improved by replacing the lattice point by the refined position of the maximum of the Fourier series.

Although the discussion thus far has been concerned with the one-dimensional problem, the generalization to higher dimensions is not difficult. In two dimensions we consider first the series consisting of three terms. The positions of the maxima of each term consist of parallel straight lines rather than isolated points. Thus we obtain three families of straight lines and the most prominent maximum of the series lies in the triangle of smallest area so determined (Fig. 1).

In three dimensions the positions of the maxima of each term of the series consist of parallel planes. The most prominent maximum of the series containing four terms lies in the smallest tetrahedron determined by planes corresponding to these terms. For the general series a three-dimensional reference lattice is used, and the numerical procedure to be described is a simple generalization of the one outlined for one dimension.

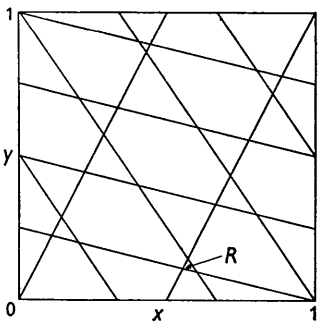

Fig. 1. Locating the principal maximum for the three-term series

$$A\cos 2\pi(x+4y)+B\cos 2\pi(2x-y)+C\cos 2\pi(3x+2y)\,,\quad A,B,C>0\,.$$

The biggest maximum occurs in the region R defined by the smallest triangle. The refined position of the maximum is found from (37).

Procedure

To find the prominent maxima of

$$S=\sum_{h,k,l} C_{hkl}\cos 2\pi(hx+ky+lz) + \sum_{h,k,l} C'_{hkl}\sin 2\pi(hx+ky+lz) \tag{12}$$

we first select three triples h_i, k_i, l_i, $i=1,2,3$ which determine the reference mesh or lattice and which may or may not occur among the triples appearing in (12). The numbers C_{hkl}, C'_{hkl} are arranged in decreasing numerical order

$$C_4 \geq C_5 \geq C_6 \geq \ldots \tag{13}$$

and for each $i=1,2,3,\ldots$

$$C_i = |C_{h_ik_il_i}| \quad \text{or} \quad |C'_{h_ik_il_i}|\,. \tag{14}$$

Approximately the first 10% of the terms of (12), as ordered by (13) and (14), are retained in the preliminary computation. We define

$$\eta_i = 0 \quad \text{if} \quad C_i = |C_{h_ik_il_i}| \quad \text{and} \quad C_{h_ik_il_i} > 0\,, \tag{15}$$

$$\eta_i = \tfrac{1}{4} \quad \text{if} \quad C_i = |C'_{h_ik_il_i}| \quad \text{and} \quad C'_{h_ik_il_i} > 0\,, \tag{16}$$

$$\eta_i = \tfrac{1}{2} \quad \text{if} \quad C_i = |C_{h_ik_il_i}| \quad \text{and} \quad C_{h_ik_il_i} < 0\,, \tag{17}$$

$$\eta_i = \tfrac{3}{4} \quad \text{if} \quad C_i = |C'_{h_ik_il_i}| \quad \text{and} \quad C'_{h_ik_il_i} < 0\,, \tag{18}$$

$$\Delta_i = \begin{vmatrix} m_1+\eta_1 & h_1 & k_1 & l_1 \\ m_3+\eta_2 & h_2 & k_2 & l_2 \\ m_3+\eta_3 & h_3 & k_3 & l_3 \\ n_i+\eta_i & h_i & k_i & l_i \end{vmatrix}\,, \tag{19}$$

$$\Delta_{\mu\nu\varrho} = \begin{vmatrix} h_\mu & k_\mu & l_\mu \\ h_\nu & k_\nu & l_\nu \\ h_\varrho & k_\varrho & l_\varrho \end{vmatrix}\,. \tag{20}$$

The volume of the tetrahedron defined by the four planes

$$h_\mu x+k_\mu y+l_\mu z = m_\mu+\eta_\mu,\ \mu = 1, 2, 3\,, \tag{21}$$

$$h_i x+k_i y+l_i z = n_i+\eta_i \tag{22}$$

is proportional to Δ_i^3. In order to locate the small tetrahedra, we equate Δ_i to a small number and therefore solve each of the solvable equations

$$\Delta_i = \pm\tfrac{1}{4}j, \qquad \begin{matrix} j = 0, 1, 2, \ldots, 4M_i\,, \\ i = 4, 5, 6, \ldots \end{matrix} \tag{23}$$

in integers $m_\mu = m_\mu(i, j)$, $\mu = 1, 2, 3$, $n_i = n_i(j)$, where M_i is the largest integer not exceeding any one of $|\tfrac{1}{4}\Delta_{123}|$, $|\tfrac{1}{4}\Delta_{12i}|$, $|\tfrac{1}{4}\Delta_{13i}|$, $|\tfrac{1}{4}\Delta_{23i}|$, and the solutions are such that

$$h_1x_{ij}+k_1y_{ij}+l_1z_{ij} = m_1+\eta_1\,, \tag{24}$$

$$h_2x_{ij}+k_2y_{ij}+l_2z_{ij} = m_2+\eta_2\,, \tag{25}$$

$$h_3x_{ij}+k_3y_{ij}+l_3z_{ij} = m_3+\eta_3\,, \tag{26}$$

$$0 \le x_{ij} < 1, \quad 0 \le y_{ij} < 1, \quad 0 \le z_{ij} < 1\,, \tag{27}$$

so that attention is restricted to the unit cube. If $C'_{hkl} = 0$ for every hkl, the additional restriction

$$0 \le x_{ij}+y_{ij}+z_{ij} \le \tfrac{3}{2} \tag{28}$$

is desirable. Equations (24), (25) and (26) thus determine the cartesian coordinates x_{ij}, y_{ij}, z_{ij} of the lattice point in the reference mesh which is a vertex of a small tetrahedron defined by (21) and (22).

After expanding (19) and collecting terms without multiplying by a numerical factor, equation (23) reduces to

$$a\xi+b\eta+c\zeta+d\omega = p\,, \tag{29}$$

where a, b, c, d are integers. Equation (29) is solvable in integers ξ, η, ζ, ω if, and only if, p is a multiple of the greatest common divisor (g.c.d.) of a, b, c, d. In order to simplify the computations performed on I.B.M. equipment we have treated only the case in which the g.c.d. of a, b, c, d is unity and $p \neq 0$. The reference mesh can always be chosen so that this condition is fulfilled by almost all equations (29). The solution to (29) is well known (Dickson, 1936, pp. 1, 2). In Table 1 an outline of the solution is given.

Next we solve

$$\left.\begin{aligned} h_1x+k_1y+l_1z &= \xi+\eta_1\,, \\ h_2x+k_2y+l_2z &= \eta+\eta_2\,, \\ h_3x+k_3y+l_3z &= \zeta+\eta_3 \end{aligned}\right\} \tag{30}$$

for x, y, z and set x_{ij}, y_{ij}, z_{ij} equal to the fractional parts of x, y, z respectively so that (27) is satisfied. In order to fulfill (28) if $C'_{hkl} = 0$ for every h, k, l, x_{ij}, y_{ij}, z_{ij} are left unaltered or x_{ij} is replaced by $1-x_{ij}$, y_{ij} by $1-y_{ij}$ and z_{ij} by $1-z_{ij}$ according as (28) is or is not satisfied. Finally, $m_1=m_1(i, j)$, $m_2=m_2(i, j)$, $m_3 = m_3(i, j)$ are determined by (24), (25) and (26). These integers, when substituted into the left side of (23), yield a value of j for which m_1, m_2, m_3 is the unique solution of (23) in integers satisfying also (24)–(27).

For each i and each j we write down the triples $m_1(i, j)+\eta_1$, $m_2(i, j)+\eta_2$, $m_3(i, j)+\eta_3$ and the corresponding weights

$$\begin{aligned} F_{ij} = C_i(h_i^2+k_i^2+l_i^2)(1-j^2/16M_i^2)\,, \\ i = 4, 5, 6, \ldots\,, \\ j = 0, 1, 2, \ldots, 4M_i\,, \end{aligned} \tag{31}$$

where the three factors on the right of (31) correspond to the amplitude, the square of the frequency and a rough measure of the degree of clustering, as measured by the volume of the tetrahedron bounded by (21) and (22). We find the values of

$$\Sigma F_{ij}, \qquad i = 4, 5, 6, \ldots \tag{32}$$

summed over those values of F_{ij} corresponding to each fixed value of the triple

$$m_1(i, j)+\eta_1,\ m_2(i, j)+\eta_2,\ m_3(i, j)+\eta_3\,. \tag{33}$$

For fixed i, the triples (33) are distinct for different values of j but various combinations of i and j will correspond to the same value of the triple m_1, m_2, m_3. The values of (32) are arranged in decreasing order and the corresponding values of the triples are written down:

$$m_1(\mu)+\eta_1,\ m_2(\mu)+\eta_2,\ m_3(\mu)+\eta_3,\ \mu=1, 2, 3, \ldots\,, \tag{34}$$

where

$$m_1(\mu)=m_1(i_\mu, j_\mu),\ \ m_2(\mu)=m_2(i_\mu, j_\mu),\ \ m_3(\mu)=m_3(i_\mu, j_\mu)\,.$$

For each fixed value of μ, the triple (34) when substituted into (21) determines the approximate position of a prominent maximum (x_μ, y_μ, z_μ) and the value of μ is a rough measure of the relative magnitude of this maximum.

The final step is to refine the approximate positions x_μ, y_μ, z_μ, of the maxima using all the terms in the

Table 1. *Flow diagram of procedure for locating maxima*

$C_1 = |C_{h_1 k_1 l_1}|$ or $|C'_{h_1 k_1 l_1}|$

$C_i \geq C_j$ if $i < j$

$$\Delta_{\mu\nu\rho} = \begin{vmatrix} h_\mu & k_\mu & l_\mu \\ h_\nu & k_\nu & l_\nu \\ h_\rho & k_\rho & l_\rho \end{vmatrix}$$

Δ_{123}, Δ_{12i}, Δ_{13i}, Δ_{23i}

$i = 4, 5, 6, \ldots$

M_i is the largest integer not exceeding any $\frac{1}{4}\Delta_{\mu\nu\rho}$.

$i = 4, 5, 6, \ldots$

$j = 0, 1, 2, \ldots, 4M_i$

$\eta_i = 0, \frac{1}{4}, \frac{1}{2}$, or $\frac{3}{4}$.

To find the g. c. d. of a,b,c,d use the Euclidean algorithm to find the g. c. d. $g(=a_n)$ of $a_1 = a$ and $a_2 = b$.

$a_1 = a_2q_1 + a_3$, $a_2 = a_3q_2 + a_4$, $a_3 = a_4q_3 + a_5$, $\ldots$, $a_{n-2} = a_{n-1}q_{n-2} + a_n$, $a_{n-1} = a_nq_{n-1}$.

Similarly find the g. c. d. h of g and c, and the g. c. d. k of h and d. We treat only the case that the g. c. d. k of a,b,c,d is unity.

$$F_{ij} = C_1\left(h_i^2 + k_i^2 + l_i^2\right)\left(1 - \frac{j^2}{16M_i^2}\right)$$

Find ΣF_{ij}, $i = 4, 5, 6, \ldots$ summed over those values of F_{ij} corresponding to a fixed value of the triple $m_\nu(i,j) + \eta_\nu$, $\nu = 1, 2, 3$, and arrange in decreasing order.

We obtain

$m_1(\mu) + \eta_1$, $m_2(\mu) + \eta_2$, $m_3(\mu) + \eta_3$, .

$\mu = 1, 2, 3, \ldots$

To solve $a\xi + b\eta + c\zeta + d\omega = p$ in integers ξ, η, ζ, ω first express g as a linear combination of a and b. Define

$r_0 = 0$	$s_0 = 1$
$r_1 = 1$	$s_1 = q_1$
$r_2 = q_2$	$s_2 = q_1q_2 + 1$
$r_3 = q_2q_3 + 1$	$s_3 = (q_1q_2 + 1)q_3 + q_1$
$r_i = r_{i-1}q_i + r_{i-2}$	$s_i = s_{i-1}q_i + s_{i-2}$

Then (if necessary by reversing the signs of r_{n-2} and s_{n-2}) we obtain $r_{n-2}a - s_{n-2}b = g$. Similarly find $h = r'_{n'-2}g - s'_{n'-2}c$ and $1 = r''_{n''-2}h - s''_{n''-2}d$. Combining these equations yields a solution of $a\xi' + b\eta' + c\zeta' + d\omega' = 1$. Then let $\xi = p\xi'$, $\eta = p\eta'$, $\zeta = p\zeta'$, $\omega = p\omega'$.

Solve

$$h_1x + k_1y + l_1z = \xi + \eta_1$$
$$h_2x + k_2y + l_2z = \eta + \eta_2$$
$$h_3x + k_3y + l_3z = \zeta + \eta_3$$

Let $'x_{ij} = x - [x]$ where $[x]$ is the largest integer not exceeding x, $y_{ij} = y - [y]$, $z_{ij} = z - [z]$.

If $C'_{hkl} = 0$ for every h,k,l, leave x_{ij}, y_{ij}, z_{ij} unaltered or replace x_{ij} by $1 - x_{ij}$, y_{ij} by $1 - y_{ij}$, z_{ij} by z_{ij} according as $x_{ij} + y_{ij} + z_{ij} \leq \frac{3}{2}$ or $> \frac{3}{2}$.

Finally determine m_1, m_2, m_3' by means of

$$h_1x_{ij} + k_1y_{ij} + l_1z_{ij} = m_1 + \eta_1$$
$$h_2x_{ij} + k_2y_{ij} + l_2z_{ij} = m_2 + \eta_2$$
$$h_3x_{ij} + k_3y_{ij} + l_3z_{ij} = m_3 + \eta_3$$

m_i is the integer nearest to $h_ix_\mu + k_iy_\mu + l_iz_\mu - \eta_i$

For each μ compute x,y,z by means of

$$x\sum_i C_ih_i^2 + y\sum_i C_ih_ik_i + z\sum_i C_ih_il_i = \sum_i C_ih_i(m_i + \eta_i)$$
$$x\sum_i C_ik_ih_i + y\sum_i C_ik_i^2 + z\sum_i C_ik_il_i = \sum_i C_ik_i(m_i + \eta_i)$$
$$x\sum_i C_il_ih_i + y\sum_i C_il_ik_i + z\sum_i C_il_i^2 = \sum_i C_il_i(m_i + \eta_i)$$

series. The procedure is a generalization of the one described for two terms in one dimension.*

Each term in the Fourier series determines an index i by means of (14). For a fixed μ and each such i, the number m_i is defined to be that integer which is nearest to

$$h_i x_\mu + k_i y_\mu + l_i z_\mu - \eta_i \,. \tag{35}$$

Consequently, the plane

$$h_i x + k_i y + l_i z = m_i + \eta_i \tag{36}$$

is that plane of the family (22) which passes nearest to the point x_μ, y_μ, z_μ, i.e. the maximum of

$$C_i \left\{ \begin{array}{l} \cos 2\pi(h_i x + k_i y + l_i z) \\ \sin 2\pi(h_i x + k_i y + l_i z) \end{array} \right\}$$

(the cosine or sine is used according as $C_i = |C_{h_i k_i l_i}|$ or $C_i = |C'_{h_i k_i l_i}|$) closest to x_μ, y_μ, z_μ is in the plane (36). As in one dimension, the term

$$C_i \left\{ \begin{array}{l} \cos 2\pi(h_i x + k_i y + l_i z) \\ \sin 2\pi(h_i x + k_i y + l_i z) \end{array} \right\}$$

is replaced by its Taylor expansion in the region of the plane (36) for each i, and the results substituted into (12). The unique maximum of the resulting function of the second degree is readily found by the standard method of partial differentiation to be the solution, x, y, z, of

$$\left.\begin{array}{l} x\sum_i C_i h_i^2 + y\sum_i C_i h_i k_i + z\sum_i C_i h_i l_i = \sum_i C_i h_i (m_i + \eta_i) \,, \\ x\sum_i C_i k_i h_i + y\sum_i C_i k_i^2 + z\sum_i C_i k_i l_i = \sum_i C_i k_i (m_i + \eta_i) \,, \\ x\sum_i C_i l_i h_i + y\sum_i C_i l_i k_i + z\sum_i C_i l_i^2 = \sum_i C_i l_i (m_i + \eta_i) \,, \\ i = 1, 2, 3, \ldots \,. \end{array}\right\} \tag{37}$$

Using the solution x, y, z of (37) instead of x_μ, y_μ, z_μ, the refinement procedure may be repeated to yield a still better approximation to the location of the maximum, and the cycle may be repeated again and again. This iterative process ordinarily converges within ten cycles. The final values of the triples x, y, z, so obtained, as μ ranges through the values 1, 2, 3, ..., are the coordinates of the most prominent maxima of (12), arranged approximately in decreasing order.

The procedure described herein has been programmed for I.B.M. equipment by Mr Peter O'Hara of the Computation Laboratory of the National Bureau of Standards. His excellent cooperation is deeply appreciated.

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* The refinement procedure may be applied no matter how the approximate locations x_μ, y_μ, z_μ have been obtained.

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Application of Statistical Methods to the Naphthalene Structure

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(*Received* 7 *November* 1952)

A method for locating the principal maxima of a Fourier series was applied to a function describing the probability distribution for interatomic vectors using the data of Abrahams, Robertson & White for naphthalene. A structure comparable to that found by Abrahams *et al.* was obtained. No attempt was, however, made to obtain the ultimate accuracy inherent in this method.

Introduction

This paper concerns the application of the statistical methods developed in a previous paper (Hauptman & Karle, 1952) in order to determine the structure of the carbon frame in naphthalene. The principal maxima of formula (58) (Hauptman & Karle, 1952) expressing the probability distribution for interatomic vectors, have been located by a method described previously (Hauptman & Karle, 1953). The validity of the results therefore constitutes a test not only of the statistical method, but also of the method for locating the principal maxima of a Fourier Series. Since the X-ray scattering data of Abrahams, Robertson & White (1949) were used, a comparison with their results is significant.

Treatment of data

The logarithm of equation (58) (Hauptman & Karle, 1952) may be expressed as the Fourier series