сообщения
объединенного
института
ядерных
исследований
дубна



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V.Gadjokov

# NUMERICAL GENERATION OF ORTHONORMAL POLYNOMIALS IN MANY DIMENSIONS

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## 1. INTRODUCTION

In a previous paper [1] we described an algorithm which generates a polynomial family whose members are orthonormal over a finite real one-dimensional discrete point set. No limitation on the spacing of points in the set was imposed. Some applications of such polynomials to the problem of data fitting in physics are discussed in ref. [2]. The present study aims at presenting a generalization of the technique referred to in the case of generating sets in a space of more than one dimension.

The following section 2 gives the basic definition and the mathematical foundations of the method. Section 3 presents an algorithm of numerical generation of orthonormal polynomials. Specific considerations on the algorithm implementation in two dimensions are given in section 4. In section 5 a package of five FORTRAN-IV codes is described which carry out all the steps of the above-mentioned two-dimensional algorithm.
A numerical example and some results from using the codes are described in the last section 6.

## 2. DEFINITIONS, NOTATIONS AND PROOFS

2.1. It appears opportune to start by citing an entire excerpt from M.Weisfeld's paper [3] which we endorse in full:

"Let $D$ be a set bearing a non-negative measure $\mu$. Given two mappings $f$ and $g$ of $D$ into the reals, their <u>scalar product</u> $(f,g)$ is defined to be $\int_D fg\,d\mu$, where $(fg)(x)=f(x)g(x)$ for all $x \in D$. A set of real valued mappings of $D$ is <u>orthogonal</u> if and only if $(f,g)=0$ for each $f$ and $g$, $f \neq g$, in the set, and <u>independent</u> if and only if no nontrivial finite linear combination of elements in the set is zero almost everywhere. Let $\Phi=\{\phi_j \mid j \in J\}$ be an ordered independent square-integrable set of real-valued mappings of $D$. An <u>orthogonalization</u> of $\Phi$ is an ordered orthogonal set $\Psi=\{\psi_j \mid j \in J\}$ of real-valued mappings of $D$ such that for each $i \in J$, $\phi_i$ can be written as a finite linear combination of elements of the set $\{\phi_k \mid k \in J, k \leq i\}$.

We consider the case of D being a subset of $R^n$ , the Cartesian product of n real lines, J being the set of n - tuplets of non-negative integers; and $\Phi$ , the set on monomials in the co-ordinate variables; that is, if $j = (j_1, \ldots, j_n)$ and $x_1, \ldots, x_n$ represent coordinates, $\phi_j = x_1^{j_1} x_2^{j_2} \ldots x_n^{j_n}$ . Define $\sigma(j) = j_1 + \ldots + j_n$ . Order J as follows: $i < j$ if and only if (a) $\sigma(i) < \sigma(j)$ or (b) $\sigma(i) = \sigma(j)$ and for some $k \leq n$ $i_k + \ldots + i_n < j_k + \ldots + j_n$ . This induces an order in $\Phi$".

In addition, we shall call an orthogonalization $\Psi$ normalized if and only if $(\psi_j, \psi_j) = 1$ for each $j \in J$ . Accordingly, the polynomials $\psi \in \Psi$ will be termed orthonormal.

Throughout this paper D will be supposed to be both finite and discrete, i.e., consisting of distinct ordered points $P_i \in D$ , $i = 1, 2, \ldots, M$ . The measure $\mu$ is manifested by attributing to each point $P_i$ a finite positive weight $w_i$ . Hence, the scalar product is expressed as

$$(f, g) = \int_D fg \, d\mu = \sum_{i=1}^{M} f(P_i) w_i \, g(P_i), \tag{2.1}$$

and the relation of orthonormalization takes the form

$$\sum_{i=1}^{M} \psi_j(P_i) \, w_i \, \psi_k(P_i) = \delta_{jk} \, . \tag{2.2}$$

Obviously, the co-ordinates of $P_i$ are $(x_1^{(i)}, x_2^{(i)}, \ldots, x_n^{(i)})$.

Note that the order induced in $\Phi$ is unique, i.e., there exists a single-valued positive integer function N of n integer arguments $j_1, \ldots, j_n$ . Thus, at given N one can calculate the distribution of degrees over the variables $x_1, \ldots, x_n$ and vice versa (see 3.2). The integer $\sigma(j)$ will be further referred to as overall degree of the respective monomials.

2.2. Supposing that the generating set D , the number function $N(j_1, \ldots, j_n)$ and its inverse $(j_1, \ldots, j_n) = J(L)$ are known, an orthonormalization of $\Phi$ can be built as follows:

(a) Introduce formally

$$N(\sigma = -1) = 0 \tag{2.3}$$

and

$$\psi_0(P) \equiv 0; \tag{2.4}$$

as in[4] and [1] $\psi_0$ does not belong to the orthonormalized set (in particular, it cannot be normalized) and is only needed for starting up a recurrency (see below).

(b) Define

$$N(0,0,\ldots,0)=1 \tag{2.5}$$

and

$$\psi_1(P)=\left(\sum_{i=1}^{M} w_i\right)^{-1/2} = \text{const.} \tag{2.6}$$

(c) For each $L\geq 2$ define the degree distribution

$$(j_1,\ldots,j_n)=J(L) \tag{2.7}$$

and compute

$$\sigma_L = j_1+j_2+\ldots+j_n \ . \tag{2.8}$$

(d) Define from (2.7) and (2.8) a unique $k$ such that

$$\sigma_L = j_1+\ldots+j_k \tag{2.9}$$

and

$$j_{k+1}=\ldots=j_n=0. \tag{2.10}$$

Evidently,

$$1\leq k\leq n \ . \tag{2.11}$$

(e) Calculate

$$K=N(j_1,j_2,\ldots,j_k-1,\ j_{k+1},\ldots,j_n) \tag{2.12}$$

and

$$I=N(\sigma_L-2,0,\ldots,0). \tag{2.13}$$

Note that for $L=2,\ldots,n+1$ $\sigma_L-2=-1$ and, accordingly, $I=0$ .

(f) Define

$$\psi_L = c_L\left[(x_k-\beta_{L-1})\psi_k - \sum_{\substack{m=I\\ m\neq k}}^{L-1} \alpha_L^m \psi_m\right], \tag{2.14}$$

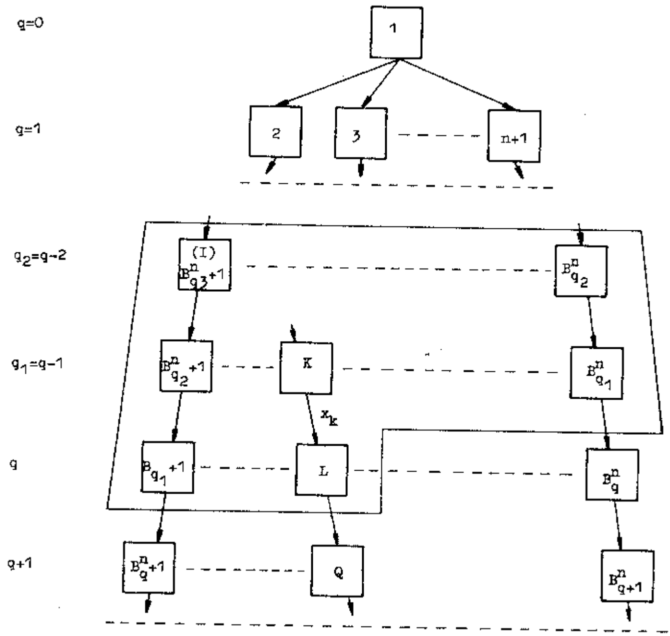


Fig.1. Fraction of a polynomial pyramide. Ordinary numbers are given within squares each representing a polynomial (monomial). A recursion family is framed; the grand-daughter term $\psi_Q$ is otside the frame.

where

$$\beta_{L-1} = (x_k \psi_k , \psi_k), \tag{2.15}$$

$$\alpha_L^m = (x_k \psi_k , \psi_m), \tag{2.16}$$

and

$$c_L = [(x_k \psi_k , x_k \psi_k) - \beta_{L-1}^2 - \sum_{\substack{m=I \\ m \neq K}}^{L-1} (\alpha_L^m)^2]^{-1/2}. \tag{2.17}$$

The scalar product of the two sides of (2.14) reveals the useful relation

$$c_L = 1/\alpha_Q^k , \tag{2.18}$$

where

$$Q = N(j_1, j_2, \dots, j_k+1, j_k, \dots, j_n). \qquad (2.19)$$

When the construction of the orthonormal set $\Psi_{L_{max}} = \{\psi_L \mid L = 1,\dots,L_{max}\}$ has been carried out up to a certain $L_{max}$ we can totally ignore the assumption made in (a) above. Due to the mode of building $\Psi_{L_{max}}$ each $\psi_L \in \Psi_{L_{max}}$ contains a leading term proportional to $\phi_L \in \Phi_{L_{max}}$, all the remaining terms being of the type $\phi_\ell$, $\ell < L$, i.e., $\psi_L$ are ordered in accordance with their leading terms.

2.3. The orthogonality of the set $\Psi_{L_{max}}$ is proved by Weisfeld[3] in slightly different notations for the case $c_L = 1$, $L = 1,2,\dots,L_{max}$. As this proof is based on the implicit assumption that all $\psi_L \in \Psi_{L_{max}}$ have nonzero finite norms and these, in turn, ensure the computability of $c_L$, we do not deem it necessary to repeat the proof here.

The normalization of the set $\Psi_{L_{max}}$ can be checked by substituting (2.17) into (2.14) and by calculating the scalar product of the right-hand side. Again, the computability of $c_L$, i.e., the requirement that inequality.

$$(x_k\psi_k, x_k\psi_k) - \beta^2_{L-1} - \sum_{\substack{m=1 \\ m \neq K}}^{L-1} (\alpha_L^m)^2 > 0 \qquad (2.20)$$

holds for all $L \in [1, L_{max}]$ is a conditio sine qua non.

The maximum number $L_{max}$ of orthonormal polynomials $\psi_L \in \Psi_{L_{max}}$ is related to the spacing of points $P_i \in D$, $i = 1,2,\dots,M$. When these points lie on no algebraic hypersurface of order $q \leq M$, then $L_{max} = M$, since the determinant of the matrix

$$A = \begin{matrix} \phi_1(P_1), & \phi_2(P_1),\dots, & \phi_M(P_1) \\ \phi_1(P_2), & \phi_2(P_2),\dots, & \phi_M(P_2) \\ \text{-----} & \text{-----} & \text{-----} \\ \phi_1(P_M), & \phi_2(P_M),\dots, & \phi_M(P_M) \end{matrix} \qquad (2.21)$$

differs from zero and an orthogonalization of $\Phi_M = \{\phi_i \mid i \leq M\}$ is possible (see[5], chapter 21). If, however, $\det A = 0$, then $L_{max}$ coincides with the number of linearly independent columns in (2.21) counted from left to right. The position of these columns is stressed as the procedure of building the orthogonal set $\Psi_{L_{max}}$ is based on (2.14) and, therefore, breaks at the first apparence of linear dependence in A rather than when reaching its rank. In a numerical implementation inequality (2.20) can constitute a practical guide of whether or not the orthogonalization is to be continued towards higher numbers L .

The completeness of $\Psi_{L_{max}}$ with respect to the class of functions f(P) which are non-singular at all the points $P_i \in D$ and have no more than $L_{max}$ different values at these points may be proved in a way similar to that used in[1], and a repetition does not seem justified.

## 3. ALGORITHM OF NUMERICAL GENERATION

3.1. To implement numerically the orthonormalization described we need a closer look at the relationship among members of $\Psi_{L_{max}}$. As $\Phi_{L_{max}}$ and $\Psi_{L_{max}}$ are isomorphous, we can base our discussion on either of them.

All the monomials $\phi_L$ (and, accordingly, all the polynomials $\psi_L$ classified by their leading terms) may be thought of as constituting a pyramide-like structure (Fig.1) resembling the Pasquale triangle. The top of the pyramide consists of $\phi_1$, the next floor of n monomials $\phi_2, \phi_3, \dots, \phi_{n+1}$ each of overall degree $\sigma = 1$, etc. Generally, the q-th row contains all the monomials of overall degree $\sigma = q-1$ in the appropriate order, the numbering going from top to bottom and, along the rows, from left to right. Combinatorial considerations[5] (chapter 21) yield that the first (q+1) rows contain the total of

$$B_q^n = \frac{(n+q)!}{n!\,q!} \tag{3.1}$$

independent monomials, while the amount of members in the (q+1)-th row only is

$$b_q^n = \frac{(n+q-1)!}{(n-1)!\,q!}\,, \tag{3.2}$$

where n is as before the number of dimensions in $R^n$ .

It can be seen that the recurrency (2.14) encompasses (a) all the terms on the left of $\psi_L$ in the same row and (b) all the terms in the two adjacent rows above that of $\psi_L$. All these may be said to represent a recurrence family where $\psi_L$ is the daughter-term, $\psi_k$ is the mother term, and the remaining ones are relative-terms. The grand-daughter term $\psi_Q$, although not a member of the family, is also related to it through the normalizing coefficient of (2.18). The leading terms of polynomials $\psi_k$, $\psi_L$ and $\psi_Q$ are of the same degree in all variables but $x$ wherein their degrees are $j_k-1$, $j_k$ and $j_k+1$, respectively. These considerations may contribute to a better understanding of the algorithm described in 3.4.

It can be seen that each mother-term $\psi_k$ gives rise to $n-k+1$ new members of the orthonormal set through variables $x_k,\dots,x_n$. Hence, the first polynomial in a row with degrees $(q,0,\dots,0)$ generates $n$ new polynomials in the next row while the last polynomial in the same row with degrees $(0,0,\dots,q)$ generates only one.

3.2. In a numerical implementation it is essential to have either an analytical expression for $L=N(j_1,\dots,j_n)$ and its inverse $(j_1,\dots,j_n)=J(L)$ or combinatorial algorithms for their computation. The former may be rather cumbersome and even non-existent for $n\geq 5$; the latter, as we shall show below, are always feasible.

(a) Let us note that due to the very way of ordering introduced in 2.1. the polynomials in the $(q+1)$th row of Fig.1 are arranged with respect to variables $x_2,\dots,x_n$ exactly as polynomials of $n-1$ variables should be ordered. This means that

$$N_n(j_1,\dots,j_n)=B^n_{q-1}+N_{n-1}(j_2,\dots,j_n), \tag{3.3}$$

where $N_n$ and $N_{n-1}$ are the number functions for $n$ and $n-1$ dimensions respectively, and $q=j_1+\dots+j_n$. This relation suggests a recursive approach to computing $N_n$. Indeed, since

$$N_1(j_n)=j_n+1, \tag{3.4}$$

we can compute $N_n$ for as many dimensions as necessary.

(b) An analogous approach may also be used to compute the inverse $J(L)=(j_1,\dots,j_n)$. The problem here is slightly less transparent as both $q$ and $(j_1,\dots,j_n)$ are unknown initially. Nevertheless, $q$ is easily defined as the only integer satisfying the inequality

$$B^n_{q-1} + 1 \leq L \leq B^n_q \quad . \tag{3.5}$$

Now, the difference $L - B^n_{q-1}$ is clearly the ordinary number of our polynomial in the $(q+1)$th row, i.e.,

$$B^{n-1}_{q'-1} + 1 \leq L - B^n_{q-1} \leq B^{n-1}_{q'} \quad , \tag{3.6}$$

where $q' = j_2 + \ldots + j_n$ and, accordingly,

$$j_1 = q - q' \tag{3.7}$$

Repeating (3.5)-(3.7) $n-1$ times we find $j_1, \ldots, j_{n-1}$ whereupon

$$j_n = q - j_1 - \ldots - j_{n-1} \quad . \tag{3.8}$$

(c) The method described is in principle suitable to any $n$ . In two dimensions, however, the use of simple analytical expressions (see 4) may prove faster and more convenient.

3.3. Before describing the generating algorithm we should formulate clearly its goal. Ascher and Forsythe pointed out /6/ that "to find a polynomial" (or, in our case, a set of polynomials) may be given at least three meanings:

- to find the values of all the coefficients involved;
- to have a sufficiently large and detailed table of polynomial values for various arguments;
- to set the constants in a computer code capable of computing the values of polynomials for any set of admissible arguments.

We shall adhere to the latter definition; in other words, our algorithm aims at calculating the recurrence factors in (2.14) and the normalizing factors (2.17). Then, using the recurrency, we can compute any polynomial $\psi_L \in \Psi_{L_{max}}$ at any point $P$ . Note that when $c_L$ , $\beta_{L-1}$ and $\alpha^m_L$ are known the polynomials $\psi_L$ are defined everywhere in $R^n$ , although the orthonormalization holds in $D$ only.

3.4. Suppose that the co-ordinates $x^{(i)}_1, \ldots, x^{(i)}_n$ of all $P_i \in D$ are given together with the positive weights $\{w_i\}$ , $i = 1, 2, \ldots, M$ . Without loss of generality we can assume that $-1 \leq x^{(i)}_j \leq +1$ holds for all admissible $i$ and $j$ . Suppose also that the number function $N(j_1, \ldots, j_n)$ and its inverse $J(L)$ are known. Then the algorithm computing $c_L$ , $\beta_{L-1}$ and $\alpha^m_L$ consists of the following steps:

(a) Set $L_{max} \leq M$ .

(a) Set $L_{max} \leq M$ .

(b) Calculate

$$c_1 = \psi_1 = (\sum_{i=1}^{M} w_i)^{-1/2}.$$

(c) Calculate

$$\beta_1 = (x_1\psi_1, \psi_1),$$

$$c_2 = [(x_1\psi_1, x_1\psi_1) - \beta_1^2]^{-1/2},$$

and

$$\psi_2 = c_2[x_1 - \beta_1]\psi_1 .$$

(d) Set $L=3$ and $k=2$ .

(e) Calculate

$$\beta_{L-1} = (x_k\psi_1, \psi_1)$$

$$\alpha_L^m = (x_k\psi_1, \psi_m) \qquad m=2,3,\ldots,L-1,$$

$$c_L = [(x_k\psi_1, x_k\psi_1) - \beta_{L-1}^2 - \sum_{m=2}^{L-1}(\alpha_L^m)^2]^{-1/2}$$

and

$$\psi_L = c_L[(x_k - \beta_{L-1})\psi_1 - \sum_{m=2}^{L-1}\alpha_L^m \psi_m].$$

(f) Set $L=L+1$ and $k=k+1$ .

(g) If $L \leq n+1$ return to (e); else go to next step (h).

(h) Define:

$$(j_1, \ldots, j_n) = J(L),$$

$$\sigma = j_1 + \ldots + j_n ;$$

k such that

$$\sigma = j_1 + \ldots + j_k$$

$$j_{k+1} = \ldots = j_n = 0,$$

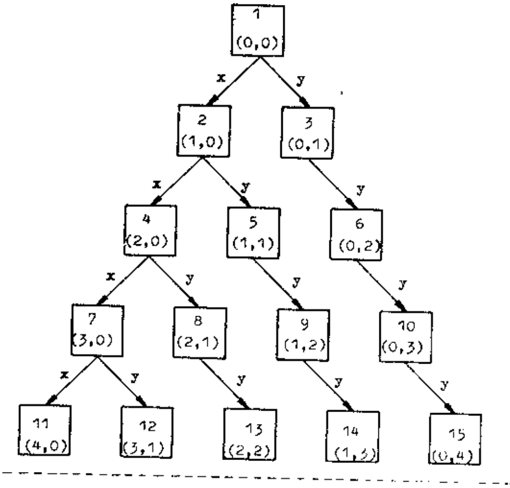


Fig.2. Relationship among members of set $\Psi$ in the case of $n = 2$. Each square represents a polynomial $\psi_L$, the ordinary number L and the $(x,y)$ -degrees being given within it. The x variable is x when arrows point to the left and y when they point to the right.

and

$$K = N(j_1,\ldots, j_k - 1, j_{k+1},\ldots,j_n)$$

and

$$I = N(\sigma - 2, 0,\ldots,0).$$

(i) Compute:

$$\beta_{L-1} = (x_k \psi_k, \psi_k)$$

$$\alpha_L^m = (x_k \psi_k, \psi_m), \quad m = I,\ldots,L-1, \; m \neq k$$

and

$$c_L^{-2} = (x_k \psi_k, x_k \psi_k) - \beta_{L-1}^2 - \sum_{\substack{m=I \\ m \neq K}}^{L-1} (\alpha_L^m)^2.$$

(j) If $c_L^{-2} > 0$ continue to next step (k); else skip to (n)

(k) Compute

$$c_L = (c_L^{-2})^{-1/2}$$

and

$$\psi_L = c_L [(x_k - \beta_{L-1})\psi_k - \sum_{\substack{m=I \\ m \neq K}}^{L-1} \alpha_L^m \psi_m].$$

(l) Set $L = L+1$ .

(m) If $L \leq L_{max}$ return to (h); else skip to (o).

(n) Modify $L_{max} = L-1$ . Print a warning and the new value of $L_{max}$ .

(o) Stop. The recurrence and normalizing factors are ready to use.

## 4. CASE OF TWO DIMENSIONS

In this section $n = 2$ ; we renounce the notations $(x_1,\dots,x_n)$ and $(j_1,\dots,j_n)$ in favour of the usual $(x,y)$ and $(j_x,j_y)$ respectively. The pyramide-like structure of Fig.1 becomes much simpler (Fig.2) and contains in its q-th row exactly q members of the orthonormal set $\Psi$ , each of them of overall degree $q-1$ . Formulae (3.1) and (3.2) yield respectively

$$B_q^2 = (q+1)(q+2)/2 \tag{4.1}$$

and

$$b_q^2 = q+1. \tag{4.2}$$

Therefore, the number function $N(j_x, j_y)$ takes the form

$$N(j_x, j_y) = \frac{(j_x+j_y)(j_x+j_y+1)}{2} + 1 + j_y \quad , \tag{4.3}$$

where the first two terms correspond to the number of the first polynomial in the $(q+1)$ th row of Fig.2, provided that $j_x + j_y = q$ .

To derive the inverse $(j_x, j_y) = J(L)$ we proceed as follows:

(a) The substitution of (4.1) into (3.5) leads to the inequality chain

$$(q^2+q+2)/2 \leq L \leq (q^2+3q+2)/2. \tag{4.4}$$

(b) This, in turn, gives rise to two limiting equations

$$q^2+q+2(1-L) = 0 \tag{4.5}$$

$$q^2+3q+2(1-L) = 0 \tag{4.6}$$

whose positive roots are respectively

$$q_1 = \sqrt{2L - 7/4} - 1/2 \tag{4.7}$$

and

$$q_2 = \sqrt{2L + 1/4} - 3/2, \tag{4.8}$$

while (4.4) takes the form

$$q_1 \geq q \geq q_2 \ . \tag{4.9}$$

(c) An elementary investigation shows that both $q_1$ and $q_2$ are real for each $L = 1, 2, \ldots$ ; moreover

$$q_1 > q_2 \tag{4.10}$$

and

$$q_1 - q_2 < 1. \tag{4.11}$$

(d) It follows from (4.9)-(4.11) that the closed interval $[q_2, q_1]$ contains a single integer, i.e., the overall degree $q$ is uniquely defined as the larger of the two integers obtained when trunkating the fractions of $q_1$ and $q_2$.

(e) Once the $q$ has been found we may solve (4.3) with respect to $j_y$

$$j_y = L - \frac{q(q+1)}{2} - 1 \tag{4.12}$$

and, finally,

$$j_x = q - j_y \ . \tag{4.13}$$

The procedure outlined is programmed in a FORTRAN-IV subroutine DEG2; formula (4.3) is implemented in an integer function NUMB2.

Clearly, the number of normalizing factors $c_L$ and that of recurrence factors $\beta_{L-1}$ are directly linked to $L_{max}$ . Alpha-type recurrence factors are more numerous, and knowledge of their precise quantity may be of help in allocating the memory available. Direct computation yields:

– a single polynomial $\psi_L$ of overall degree $q = j_x + j_y$ needs

$$A_L = 2(q-1) + j_y \tag{4.14}$$

alphas;

- all the polynomials of overall degree q need

$$A_q = \frac{(q+1)(5q-4)}{2} \qquad (4.15)$$

alphas;

- all the polynomials of overall degrees $0 \leq q \leq J$ need

$$A_J = \frac{(J-1)(5J^2+14J+6)}{6} \qquad (4.16)$$

recurrence factors of the alpha-type.
Naturally, both (4.15) and (4.16) give precise integer values.

## 5. FORTRAN-IV IMPLEMENTATION

The algorithm described in section 3 has been implemented with $n=2$ as in 4. The full FORTRAN-IV texts of the codes are available from the author. In this section a brief description of the package is given and certain details of its usage are reported.

The package consists of five codes: two principal subroutines ØRTHN2 and PRERF2, two auxiliary ones DEG2 and ERR2, and an integer function NUMB2. The principal subroutines contain a named CØMMØN /LINKS/ where the recurrence factors and some auxiliary variables are recorded; this must also be declared in any calling program which makes use of the package. The present size of /LINKS/ allows for overall degrees as high as 16 and for $L_{max} = (16+1)(16+2)/2 = 153$ . Computational needs and/or current memory restrictions may impose changes of the array dimensions in /LINKS/.

5.1. Subroutine ØRTHN2(NUMBNX,X,Y,POLY) computes the values of all the polynomials $\psi_L(x,y)$ , where $1 \leq L \leq L_r$. The list of formal arguments includes:

NUMBMX - the value of $L_r$ ;

X and Y - the co-ordinates of point $P(x,y)$ , where $\psi_L$ are calculated; this point is not bound to belong to D , however both x and y undergo the same linear transform which maps D onto $[-1, +1]$ square;

PØLY - one-dimensional array of results; at the exit from ØRTHN2 PØLY(1) contains $\psi_1$, etc., up to PØLY (NUMBMX) which contains $\psi_{L_r}$ . Core allocation for PØLY should be ensured by the main (calling) program.

5.2. Subroutine PRERF2(M,MAXD,X,Y,PØLY) computes the recurrence factors in a single call which, accordingly, must precede any working call of ØRTHN2. The arguments have the following meaning:

M — the number of points $P_i \in D$ ;

MAXD — the maximum overall degree for which recurrence factors are computed. The actual number $L_{max}$ is defined from (4.1) with $q = MAXD$;

X and Y — two one-dimensional arrays containing the co-ordinates of points $P_i \in D$ . Again, co-ordinates are given in their natural (physical) units and mapped internally onto a $-1$ , $+1$ -square.

PØLY — the same as in ØRTHN2, used here as scratch-pad storage.

The output from PREPF2 goes to the /LINKS/-common block. Core allocation for X,Y and PØLY should be ensured by the calling program. When computing $\beta_{L-1}$, $\alpha_L^m$ and $c_L$ PRERF2 makes successive recursive calls to ØRTHN2 with NUMBMX = L-1, then L is incremented, etc., - until $L_{max}$ is reached.

Since the computation of recurrence factors may be time consuming, PRERF2 provides for their recording on a peripheral device (tape or disk) in binary form and for reading of prerecorded recurrence factors in case of repetitive use of generated polynomials. This is controlled by means of IRP (Integer Regime Parameter) which is entered in I1 format and may have values within the range 0 to 7 (IRP > 7 will be accepted but actually its modulo 7 will be used). IRP is treated by PRERF2 as an octal with the following meaning of bits:

- high bit
  - 1 compute recurrence factors;
  - 0 read prerecorded binary values;
- middle bit
  - 1 write on a spare file binary values computed of read;
  - 0 skip binary writing;
- low bit
  - 1 control print of values computed or read;
  - 0 skip control printing.

5.3. Subroutine DEG2(N,J,JX,JY) calculates at given polynomial number N the overall degree of the leading term J, the degree in $x$-variable JX and that in $y$-variable JY. To avoid round-off errors when computing the roots (4.7) and (4.8) these are complemented with a small additive ($10^{-5}$) before truncating the fractions.

5.4. The integer function NUMB2(JX,JY) returns at given JX and JY the ordinary number of polynomial with that particular structure of the leading term.

5.5. Subroutine ERR2(KE) prints out error messages in case of necessity. The argument KE is the message number and is set by PRERF2 and ØRTHN2; messages may appear after irregular calls and are self explaining.

## 6. EXAMPLES OF USE

6.1. We shall consider first as a simple illustration the case of an eight-point generating set for which all the computations may be checked analytically. Let M = 8 and the point co-ordinates be

$$x_i = -1,\ 1,\ -1/2,\ 1/2,\ -1/2,\ 1/2,\ -1,\ 1;$$

$$y_i = 1,\ 1,\ 1/2,\ 1/2,\ -1/2,\ -1/2,\ -1,\ -1;$$

with respective weights

$$w_i = 1/9,\ 2/9,\ 1/9,\ 1/9,\ 1/9,\ 1/9,\ 1/9,\ 1/9.$$

These points lay on a surface formed by a rotating parabola and we cannot expect to reach $L_{max} = 8$ when generating the orthonormal set. Indeed, matrix (2.21) takes the form

$$A = \begin{pmatrix} 1 & -1 & 1 & 1 & -1 & 1 & -1 & 1 \\ 1 & 1 & 1 & 1 & 1 & 1 & 1 & 1 \\ 1 & -1/2 & 1/2 & 1/4 & -1/4 & 1/4 & -1/8 & 1/8 \\ 1 & 1/2 & 1/2 & 1/4 & 1/4 & 1/4 & 1/8 & 1/8 \\ 1 & -1/2 & -1/2 & 1/4 & 1/4 & 1/4 & -1/8 & -1/8 \\ 1 & 1/2 & -1/2 & 1/4 & -1/4 & 1/4 & 1/8 & -1/8 \\ 1 & -1 & -1 & 1 & 1 & 1 & -1 & -1 \\ 1 & 1 & -1 & 1 & -1 & 1 & 1 & -1 \end{pmatrix},$$

where the fourth column (corresponding to $x^2$) is repeated also in the sixth position (corresponding to $y^2$). Hence, five orthonormal polynomials may only be generated. These are

$$\psi_1 = 1,$$

$$\psi_2 = \frac{1}{\sqrt{53}}(9x-1) \quad ,$$

$$\psi_3 = \frac{3}{\sqrt{16165}}(53y-8x-5),$$

$$\psi_4 = \frac{2}{4293\sqrt{2013}}[61(477x+26)(9x-1)-243(53y-8x-5)-171349],$$

$$\psi_5 = \frac{2}{4293\sqrt{21153}}[(9x-1)(47223y-9540x-6856)-81(53y-8x-5)+14201].$$

The sixth member of the set comes proportional to $y^2-x^2$ and, having eight zeroes at the generating-set points, cannot be normalized. Numerical execution of these calculations yields the same results within the limits of machine accuracy ($10^{-7}$-$10^{-6}$ in our case).

6.2. We use the codes described and the technique explained in detail in /2/ for approximating data on crystal orientation measured at various temperatures ( x ) and layer thickness ( y ). Over a D-set of 334 points 55 orthonormal polynomials were generated (MAXD = 9). Optimum length of fitting series fell on L = 38 which was selected according to the minimum $\chi^2$ per degree of freedom. Smooth fitting surface was obtained for the entire range of x and y involved.

6.3. The same codes are presently being used for fitting the distortion residuals when computing the parameters of a large optical system. Gratifying results are being obtained when the selection of optimum fitting length is based on smoothness criteria which turns out more suitable in this particular case.

## 7. CONCLUSIONS

The algorithm described can be implemented within limited hardware resources and does not require double-precision computations. In combination with the technique reported in /2/ it is a powerfull tool of data fitting when multidimensional polynomial models suit the phenomena studied. The recursive approach to orthonormalization renders it more universal and more economic than direct matrix diagonalization /7/. Moreover, the discrete orthogonality relation and the normalization to unity help to avoid matrix inversion at all which cannot be done under different conditions as, e.g., in ref. /8/.

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