SEPARATION OF THE BASIC SYSTEM FROM A VECTORIAL ONE BY A PEAK OF MULTIPLICITY TWO (GENERAL CASE, FEDOROV GROUP \(P1\))

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Abstract

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É. A. KUZ' MIN, V. V. ILYUKHIN, Academician N. V. BELOV

SEPARATION OF THE BASIC SYSTEM FROM A VECTORIAL ONE BY A PEAK OF MULTIPLICITY TWO (GENERAL CASE, FEDOROV GROUP $P1$)

The algorithm for separating the basic system (b.s.) from the vectorial system (v.s.) by multiple peaks was given in ([1,2]), and it was indicated that separation of the b.s. is the more effective, the higher the multiplicity N_1 of the initial peak of the v.s. One may consider as the limiting and at the same time the simplest case that in which the multiplicity of the initial peak is the least and is equal to two ($N_1 = 2$)*, i.e., when in the point b.s. two pairs of points with coordinates $x_1 y_1 z_1 \dots x_4 y_4 z_4$ satisfy the condition

Figure 1 and Figure 2

Fig. 1. Basic system of 6 points. Points 1–4 satisfy condition (1)

Fig. 2. V.s. for the b.s. in Fig. 1. The vectors $\mathbf{r}_{12} = \mathbf{r}_{34}$ (I) and $\mathbf{r}_{13} = \mathbf{r}_{24}$ (II) are singled out

$$\mathbf{r}_{12} = \mathbf{r}_{34} \quad \text{(and, consequently, } \mathbf{r}_{13} = \mathbf{r}_{24}\text{)}. \tag{1}$$

In the corresponding v.s., regardless of whether the b.s. (N points) is acentric or centrosymmetric, there arise three line segments parallel to $\mathbf{r}_{12} \# \mathbf{r}_{34}$ and, at the same time, three more line segments parallel to $\mathbf{r}_{13} \# \mathbf{r}_{24}$ ([3,4]). The line segments not passing through the center form a parallelogram, at whose vertices the peaks are single, while at the midpoints of the sides they are double—they are located at the ends of two (doubled) line segments passing through the origin of coordinates. Thus, if, under the assumption that there exist in the b.s. two pairs of points satisfying (1), we succeed in isolating in the v.s. a "promising" parallelogram, then the peaks at the midpoints of its sides are double** (provided there are no accidental coincidences).

Let this parallelogram have been found in the v.s. (for the b.s. of 6 points—Fig. 1) (Fig. 2). We choose as the initial peak any one of the 4 double peaks at the midpoints of the sides of the parallelogram (vector I—Fig. 2). At the first stage of the algorithm ([1,2]) we obtain a system of points—the endpoints of vectors singled out by vector I (images of segment 1 according to ([5]))—Fig. 3. In this case there are contoured

* If the initial peak (or all peaks) of the v.s. is single, separation of the b.s. is accomplished sufficiently rapidl

** If the weights of the initial 4 points of the b.s. $Z_1, Z_2, Z_3, Z_4,$ then the weights of the peaks at the vertices

(the ends of vectors $\mathbf{r}_{14}$ and $\mathbf{r}_{41}$) and Z_2Z_3 (the ends of vectors $\mathbf{r}_{23}$ and $\mathbf{r}_{32}$), and at the midpoints of the sides $Z_1Z_2 + Z_3Z_4$ ($\mathbf{r}_{21} + \mathbf{r}_{43} = \mathbf{r}_{12} + \mathbf{r}_{34}$) and $Z_1Z_3 + Z_2Z_4$ ($\mathbf{r}_{13} + \mathbf{r}_{24} = \mathbf{r}_{31} + \mathbf{r}_{42}$).

$2N_1 = 4$ copies of the basic system, with the initial vector I remaining common to all copies (at the midpoint of segment I a center of symmetry arises, and the 4 copies of the basic system are connected by it in pairs). As the peak N_2 we likewise choose a double (not used earlier) peak at the middle of another side of the parallelogram (not parallel to the first) and carry out a shift along vector II of the points already selected by vector I. Thus, at the second stage, instead of arbitrary quadrilaterals ([1]), we turn to a parallelogram (not to be confused with the parallelogram described in ([2]), where the latter arises because $N_2 = N_1$). In this displacement along vector II, the center of symmetry* from the midpoint of vector I (Fig. 3)—by the elementary theorem on the product of a symmetry element (operation) with a translation—moves to the center of the "small" parallelogram, with sides equal and parallel to vectors I and II, and thereby this operation selects at once two copies of the basic system, while the points at the vertices of the marked "small" parallelogram will be common to the direct and inverted copies of the basic system (by virtue of the centrosymmetry of the parallelogram).

Figure 3 and Figure 4 diagrams

Fig. 3. First stage of extracting the basic system from the vector system. *a*—$N_1 = \mathbf{r}_{13}$ (I); *b*—$N_1 = \mathbf{r}_{12}$ (II)

Fig. 4. Two copies of the basic system, extracted by vectors N_1 (I) and N_2 (II) (or by N_1 (II) and N_2 (I))

This is the exceptional nature of the present case of the method of a multiple (parallel) peak ([2]). By specifying a parallelogram**, we at once obtain the common part of two (left and right) basic systems, and it is immaterial which, since a centrosymmetric part of the basic system is selected (see ([2])). To obtain a discrete basic system, it is sufficient to take and add to our parallelogram either of the two points (5 or 5′—Fig. 4) located outside the parallelogram but related by inversion in its center. The vectors $\mathbf{r}_{51}, \mathbf{r}_{52}, \mathbf{r}_{53}, \mathbf{r}_{54}$ will necessarily be present in the point vector system. For each subsequent point that we add to a copy of the basic system from among the points selected by N_1 and N_2, we check for the presence of vectors between this point and the remaining points of the basic system. In our example (Figs. 1-4), to the points 1—5 one can add only point 6, but not point 6′, since in the vector system we find the vectors $\mathbf{r}_{56}$ and $\mathbf{r}_{65}$, but not the vectors $\mathbf{r}_{56'}$ and $\mathbf{r}_{6'5}$.

* Under ordinary minimization by two unit vectors, both of the selected M_2 functions are centrosymmetric, but M_3 no longer has a center of symmetry. In the algorithm under consideration, by vector II we immediately obtain M_4; however, the center of symmetry is preserved because of the specificity of the choice of vectors I and II.

** In the general case, in order to extract the most purified copy of the basic system ([1,2]), it is necessary to perform N_2 stages of successive unification of points into polygons, the last of which, fixing only one copy of the basic system, will be a $(2 + 2N_2)$-gon. For $N_2 = 2$, the number of quadrilaterals will be $2!/(2-1)!1! = 2$, and the number of hexagons $2!/0!2! = 1$. In the proposed algorithm, both quadrilaterals degenerate into a parallelogram and coincide with one another, thereby making the stage of hexagons superfluous.

The algorithm just described is illustrated by a matrix (algebraic) description according to Buerger ([5]). Retaining the notation for the points of the basic system adopted above, we have, for the vector system, the matrix

$$\begin{matrix} 11 & 12 & 13 & 14 & 15 & 16 \\ 21 & 22 & 23 & 24 & 25 & 26 \\ \vdots & & & & & \vdots \\ 61 & 62 & 63 & 64 & 65 & 66 \end{matrix} \tag{2}$$

Under the condition of equality of the segments $\mathbf{r}_{12}\#\mathbf{r}_{34}$, the shift by the vector $\mathbf{r}_{12}$ is demonstrated by

$$\begin{matrix} 11 & 12 & 13 & 14 & 15 & 16 \\ 21 & 22 & 23 & 24 & 25 & 26 \\ 31 & 32 & 33 & 34 & 35 & 36 \\ 41 & 42 & 43 & 44 & 45 & 46 \\ 51 & 52 & 53 & 54 & 55 & 56 \\ 61 & 62 & 63 & 64 & 65 & 66 \end{matrix} \tag{3}$$

In the case of a double peak, 4 basic systems are selected—2 along the segment $\mathbf{r}_{12}$ (outlined by a rectangle) and 2 along the segment $\mathbf{r}_{34}$ (oblique and vertical hatching) (4). In this quadruple of copies of the basic system, each pair (A and B; A and Γ; B and B; B and Γ) has common points (listed last in (5) and (6); see also Fig. 3). Moreover, all four copies have a common segment $\mathbf{r}_{12} = \mathbf{r}_{34}$.

Since condition (1) is satisfied in the basic system, selection along the vector $\mathbf{r}_{13} = \mathbf{r}_{24}$ is equally effective, which is reflected by the matrix (7), analogous to (4) (see Fig. 3).

$$\begin{array}{cccccc} 11 & 12 & 13 & 14 & 15 & 16 \\ 21 & 22 & 23 & 24 & 25 & 26 \\ 31 & 32 & 33 & 34 & 35 & 36 \\ 41 & 42 & 43 & 44 & 45 & 46 \\ 51 & 52 & 53 & 54 & 55 & 56 \\ 61 & 62 & 63 & 64 & 65 & 66 \end{array} \quad \begin{array}{c} A \\ \\ B \end{array} \tag{4}$$

Here also two pairs of copies of the basic system are selected. In each pair, again, 4 common points and 2 points proper to each copy are fixed.

The successive shift of the vector system by the vector $\mathbf{r}_{12}$ (I) and then by $\mathbf{r}_{13}$ (II) corresponds in the matrices to the superposition of all pairs: (5), (6), (7), and (8)

$$\begin{array}{cccccc} 64 & 54 & 44 & 34 & 24 & 14 \\ 16 & 15 & 11 & 12 & 13 & 14 \end{array} \tag{5}$$

$$\begin{array}{cccccc} 36 & 35 & 34 & 33 & 32 & 31 \\ 62 & 52 & 12 & 22 & 32 & 42 \end{array} \tag{6}$$

Diagram labeled (7)

$$\begin{array}{cccccc} 64 & 54 & 44 & 34 & 24 & 14 \\ 16 & 15 & 11 & 12 & 13 & 14 \end{array} \tag{8}$$

$$\begin{array}{cccccc} 63 & 53 & 43 & 33 & 23 & 13 \\ 26 & 25 & 21 & 22 & 23 & 24 \end{array} \tag{9}$$

in which only the coincident pairs are singled out, i.e. $64, 54, 44, 34, 24, 14$ and $16, 15, 11, 12, 13, 14$ (10). Thus we obtain two copies of the b.s. of points with common points $44 \equiv 11$, $34 \equiv 12$, $24 \equiv 13$, $14 \equiv 14$—the vertices of a quadrilateral; moreover, by virtue of condition (1), this latter must always be a parallelogram with its inherent center of symmetry at its center.

Gorky State University
named after N. I. Lobachevsky

Institute of Crystallography
Academy of Sciences of the USSR
Moscow

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(1) E. A. Kuz' min, V. V. Ilyukhin, N. V. Belov, DAN, **182**, 1067 (1968).
(2) E. A. Kuz' min, V. V. Ilyukhin, N. V. Belov, DAN, **189**, No. 4 (1969).
(3) Kh. S. Mamedov, N. V. Belov, DAN, **106**, 462 (1956).
(4) E. A. Kuz' min, V. V. Ilyukhin, N. V. Belov, *Crystallography*, **14**, 1059 (1969).
(5) M. Buerger, *Crystal Structure and Vector Space*, IL, 1961.

Note: Figure translations are in progress. See original paper for figures.