DECIPHERING A VECTOR SYSTEM FROM A SINGLE MULTIPLE PEAK

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

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

DECIPHERING A VECTOR SYSTEM FROM A SINGLE MULTIPLE PEAK

In ([1]) the fundamental possibility was shown of deciphering a point vector system (v.s.) from its multiple peaks. Earlier ([2], [3]) an algorithm was given for extracting the basic system (b.s.) from the vector one using two different multiple peaks of the v.s.

A particular case may be considered that in which the v.s.* has only one multiple peak of multiplicity N_1, with total number N of points in the b.s. At the first stage of decomposing the v.s. according to Buerger ([1]), $2N_1(N-1)$ equal and parallel segments are extracted, of which

$$\left\{2(N_1-1)(N-1)-2\sum_{n=2}^{N_1}(N-2n)\right\}=$$

$$=2(N-1)\left\{(N_1-1)-\sum_{n=2}^{N_1}\left(1-\frac{1-2n}{N-1}\right)\right\}$$

must systematically overlap.

At the second stage of extracting the b.s. ([2], [3]) we again turn to the same peak of multiplicity N_1 and, operating with it, extract $2N_1^2$ pairs of points connecting the vector N_1, among the points that have already once been fixed by the vector N_1. These $2N_1^2$ pairs of points are combined into $2N_1^2$ parallelograms (but not arbitrary quadrilaterals, as in ([2], [3])), in which one pair of sides $\parallel \overline{ON}_1$, while the other pair is arbitrary.

Table 1

Group	Number of copies of the b.s. extracted in the group at the parallelogram stage
I	1
I	.

Group	Number of copies of the b.s. extracted in the group at the parallelogram stage
I	.
I	.
I	$2N_1$
II	1
II	.
II	.
II	.
II	$2N_1$
.	.
.	.
.	.
N_1	1
N_1	.
N_1	.
N_1	.
N_1	$2N_1$

The use of one multiple peak in some sense broadens the possibilities of the method. However, it is necessary to draw attention to an essential difference of methodological order arising in this particular case (in comparison with the two-peak method ([2], [3])).

With initially one multiple peak, one is forced (at the second stage!) to deal with an aggregate of parallelograms (and not arbitrary quadrilaterals). The parallelograms fall into N_1 groups, and here there is a complete analogy with the previous algorithm ([2], [3]). But within its own group N_1 parallelograms already extract not one copy of a single b.s., as in the case of more arbitrary quadrilaterals, but two copies. Each parallelogram (by its vertices the points of the b.s. are arranged) in its group, by virtue of its own centrosymmetry, belongs simultaneously to two copies of the b.s.: the direct and the reflected—

* Here and below, unless this is specially stipulated, a point vector system is meant.

located at the center of symmetry of the parallelogram—and therefore any particular parallelogram* will at once pick out both copies of the o.s. from the v.s. ([1]) (Fig. 1).

Table 1 ([2,3]) undergoes changes: the number of groups, i.e., the number of copies of the o.s. displaced relative to one another, remains the same and equal to N_1, but within each group $2N_1$ copies of the o.s. are localized.

Thus the number of points singled out at this stage by means of parallelograms must be greater than the number of points in the copy of the o.s. singled out by means of arbitrary quadrilaterals, which complicates the process of decomposing the v.s. and may lead to an increase in the number of subsequent stages in extracting the "true" copy of the o.s. in comparison with that indicated in ([2,3]).** Rejection of one of two copies, as in the case of quadrilaterals, again occurs at the stage of pairwise merging of parallelograms into hexagons. For arbitrary quadrilaterals the ambiguity arising from the "left-handedness" and "right-handedness" of the quadrilaterals was eliminated. In the particular case of one multiple peak, because of the centrosymmetry of the parallelograms, the left and right copies of the o.s. singled out by them coincide, but at the same time two copies of the o.s. arise, related by the center of symmetry of the parallelogram itself. Hexagons, however, single out only one copy of the o.s., as is clearly shown by Table 2. The further process of enlarging hexagons into octagons, etc., is identical to that described earlier in ([3]).

Table 2

Group	Number of copies of the o.s. singled out in a group by hexagons	O.s.
I	1	I
I	.	I
I	.	I
I	.	I
I	N_1	I
II	1	II
II	.	II
II	.	II
II	.	II
II	N_1	II
.	.	.
.	.	.
.	.	.
N_1	1	N_1
N_1	.	N_1
N_1	.	N_1
N_1	.	N_1
N_1	N_1	N_1

In passing from a point v.s. to a real Patterson function with "smeared" peaks, no fundamental difficulties arise either; the effectiveness of the method increases with increasing multiplicity N_1 of the initial peak (one must not, of course, go to the absurdity of using a peak due to the presence of translations). The key moment in the case of one peak should be considered the analysis at the stage of combining parallelograms into hexagons—comparison of the points on the copies of the o.s. of each hexagon with all the other copies within its group (Table 2).

Fig. 1

Figure 1: Fig. 1

In order subsequently to exclude accidental coincidences (because of broadened maxima and superfluous points from both the direct and the inverted copies of the o.s. at the stage of parallelograms), one should discard those hexagons that single out copies with a number of points $< N/2$. The remaining hexagons are pairwise enlarged into octagons. The copy of the o.s. singled out by an octagon consists of the common points of the copies of the o.s. from the preceding stage plus those points which are represented on one of the combined copies, if the vectors between them and all the other points are found in the Patterson synthesis. A negative search result serves as the basis for rejecting points as accidental coincidences.

The second remark concerns the determination of the multiplicity of the initial (selected) peak in a point v.s. (the general case of an acentric triclinic o.s.).

Let the initial peak of the v.s. be double, generated by the presence in the o.s. of two such pairs of points with coordinates $x_1y_1z_1$, $x_2y_2z_2$ and $x_3y_3z_3$, $x_4y_4z_4$, that for them $\mathbf{r}_{12} = \mathbf{r}_{34}$. In this case a triplet of peaks arises in the v.s., lying

* It is precisely in this that the difference lies from the case of arbitrary quadrilaterals (two different peaks of multiplicities N_1 and N_2), each of which singles out from the v.s. only one copy of the o.s.

** We are not yet considering the appearance of rulers due to accidental coincidences.

on one line parallel to the vectors $\mathbf{r}_{12}$ and $\mathbf{r}_{34}$. In other words, in the v.s. there must exist a "segment" * of double length, parallel to the initial vector, which in the general case does not pass through the origin of coordinates**. It is convenient to specify each segment by the coordinates of its center, i.e., by the vectors $\mathbf{r}_{13} = \mathbf{r}_{24}$ (translated to the origin of coordinates of the vector system). The ends of the segment are easily found from the relations $\mathbf{r}_{23} = \mathbf{r}_{13} + \mathbf{r}_{21}$, $\mathbf{r}_{14} = \mathbf{r}_{12} + \mathbf{r}_{24}$.

Fig. 1. *a* –the basic system of 5 points. For the coordinates of points 1—2 and 3—4 the condition $\mathbf{r}_{12} = \mathbf{r}_{34}$ is satisfied. *b* –the vector system corresponding to the b.s. of Fig. 1*a*. The initial vectors *I* ($\mathbf{r}_{21} = \mathbf{r}_{43}$) and *II* ($\mathbf{r}_{53}$) and the segments parallel to vector *I* are indicated; the first segment $\mathbf{r}_{31} = \mathbf{r}_{42}$; the second, associated with it by the center of symmetry, $\mathbf{r}_{13} = \mathbf{r}_{24}$, and the third, passing through the origin of coordinates; *v* –parallelogram $O(22)$—21—23—24 and two copies of the b.s. selected with its aid, 1—2—3—4—5 and 1—2—3—4—5′; points 1—2—3—4 are common to both copies of the b.s. *g* –quadruple (22) = 0—21—53—23 and the single copy of

the b.s. $(5, 2, 1, 3, 4)$ selected with its aid. Point 5, not shown in Fig. v, is located symmetrically to point $5'$ as its reflection.

If in the b.s. there are three pairs of points with coordinates $x_1y_1z_1 \dots x_6y_6z_6$ such that $\mathbf{r}_{12} = \mathbf{r}_{34} = \mathbf{r}_{56}$, then in the v.s. there arise three segments not passing through the origin of coordinates (plus three inverted segments plus one segment passing through zero). Of the three segments under consideration, two will be independent, while the third is derived from them, i.e., the radius vector of its midpoint $\mathbf{r}_{15} = \mathbf{r}_{26} = \mathbf{r}_{13} + \mathbf{r}_{35} = \mathbf{r}_{24} + \mathbf{r}_{46}$ (equal to the sum of the radius vectors of the independent segments).

In the general case, for N_1 pairs of points of the b.s. with coordinates $x_1y_1z_1, x_2y_2z_2 \dots \dots x_{2N_1-1}y_{2N_1-1}z_{2N_1-1}, x_{2N_1}y_{2N_1}z_{2N_1}$, such that $\mathbf{r}_{12} = \dots = \mathbf{r}_{2N_1-1,2N_1}$, there arise in the v.s. $N_1(N_1-1)/2$ (in all $\{N_1(N_1-1)+1\}$) segments, of which (N_1-1) are independent, while the remaining $(N_1-1)(N_1-2)/2$ will be derived from the first ones.

Conversely, having fixed in the v.s. $M = N_1(N_1-1)+1$ "segments" and having selected among them the independent (N_1-1), we determine the multiplicity of the peak-generator of M segments (we note once again that the conclusion has been drawn for the ideal case, without allowance for accidental coincidences). From the multiplicity of the selected peak (or two ([2,5])) one can represent the number of steps of the successive

* A large number of points increases the probability that, when the v.s. is decomposed into b.s. at the subsequent stages, extraneous points of the stage will fall onto the lines of the parallelograms.

** For every two pairs of points of the b.s. connected by the relation $\mathbf{r}_{12} = \mathbf{r}_{34}$, strictly speaking, in the v.s. there correspond three parallel segments: one passing through the origin of coordinates, and two not passing through the origin but related by an inversion point coinciding with the origin of the v.s. ([4]). In what follows we shall always speak of one segment out of the three, bearing this remark in mind.

coarsening of points into polygons and the rank of the last polygon $(2+2N_2$ or $2+2N_1)$, which fixes only one copy of the o.s. within each group of Tables 1 and 2.

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Institute of Crystallography
Academy of Sciences of the USSR
Moscow

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