Acta Cryst. (1961). **14**, 257

On Homometric Sets. I. Some General Theorems

BY R. K. BULLOUGH*

The School of Chemistry, The University, Leeds, 2, England

(*Received 20 October* 1959 *and in revised form* 24 *February* 1960)

Hosemann & Bagchi (1954) have shown that it is possible to generate homometric point sets from subsets of points. Their theorem is here sharpened and a series of analogous and related theorems are given. The theorems are illustrated by several examples, and the properties of one of these are such as to merit a special investigation of this type of homometric pair. Some very general pairs are so discovered, and from these it is possible to derive explicitly sets of homometric r-tuplets ($r > 2$). Various preliminary definitions and theorems are given as a basis for later work.

Some definitions

The existence of pairs of point sets which have the same weighted vector set has been demonstrated by Pauling & Shappell (1930), by Patterson (1939, 1944), by Hosemann & Bagchi (1954) and by other workers. Patterson (1944) was the first to demonstrate the existence of triplets, quadruplets, etc. of distinct point sets which yield the same weighted vector set; he calls such pairs, triplets, etc. homometric pairs, triplets, etc. and this name is now generally accepted. In this series of papers I shall call any set which, together with one or more different sets, forms a homometric pair, triplet, etc. a homometric set (h.s.). Before giving anything like a formal definition of a h.s., however, it is necessary to develop some preliminaries. Some of the terminology of Number Theory is useful in the investigation of h.s. and I shall therefore use the general reference (H.W., n) to indicate page n of Hardy & Wright (1954) in all papers of this series.

The choice of the origin of the coordinates of a point set is arbitrary and if the set shows no symmetry it may be chosen for convenience coincident with the position of one of the N points in the set: the positions of the remaining members of the point set are then specified by $N-1$ coordinate (vector) parameters $\mathbf{x}_i$. In general the weights, z_i, of the N points must also be specified, but, since in a single set only relative weights are of interest, one can choose integral z_i such that†

$$(z_0, z_1, \ldots, z_{N_1-1}) = 1 , \tag{1}$$

where we use $(p, q, \ldots, t) = d$ to mean that d is the highest common divisor of $p, q, \ldots, t$ (H.W. 20).

$$S = S(0, \mathbf{x}_1, \ldots, \mathbf{x}_{N-1}: z_0, z_1, \ldots, z_{N-1}) \tag{2}$$

is then a general point set.

The result, $\widehat{g_1 g_2}$, of convolutions on sets g_1 and g_2 is defined by

$$\widehat{g_1 g_2} = \int g_1(\mathbf{y}) g_2(\mathbf{x}-\mathbf{y}) d\tau , \tag{3}$$

where $d\tau = dy_1 dy_2 \ldots dy_m$ in m-dimensions.* The range of integration is all of the m-dimensional space, if g_1 and g_2 are not periodic, or is the unit of repeat which can always be taken as unity in each of m dimensions. We can in principle consider also m-dimensional sets periodic in $q < m$ dimensions.

Sets of points like S in (2) can be represented by N m-dimensional δ-functions each of weight z_i; periodic sets are representable by periodic δ-functions of period unity. The convolution $\widehat{S_1 S_2}$ of two such sets is defined by (3).

From (3) if $\bar{S}_1 = S_1(-\mathbf{x})$,

$$\widehat{S_1 \bar{S}_1} = \int S_1(\mathbf{y}) S_1(\mathbf{y}-\mathbf{x}) d\tau$$

$$= \int S_1(\mathbf{x}+\mathbf{z}) S_1(\mathbf{z}) d\tau$$

and $\widehat{S_1 \bar{S}_1}$ is the vector set associated with the point set S_1. Obviously $\widehat{S_1 \bar{S}_1}$ is also the vector set associated with $\bar{S}_1$. A necessary condition that two sets, S_1 and S_2, be homometric is

$$\widehat{S_1 \bar{S}_1} = \widehat{S_2 \bar{S}_2} .$$

This condition is unfortunately not sufficient. Some sufficient conditions are developed below, notably Theorems 3–9. It has not proved possible to find useful conditions which are both necessary and sufficient.

It is necessary to distinguish between three cases in which S_1 and S_2 yield the same weighted vector set. In what follows below and throughout this whole series of papers we use the symbol $\rightarrow$ (H.W. viii) to denote 'implies': '$a = b \rightarrow c = d$' is to be read as 'a equal to b' implies $c = d$: if $p \rightarrow q$ and $q \rightarrow r$, $p \rightarrow r$. We also

* Now at the Dept. of Mathematics, The College of Science and Technology, Manchester 1, England.

† We exclude the case of irrational weights.

* Because of Lemma 1 we can always use orthogonal axes.

use $\nrightarrow$ to denote 'does not imply', the relation contrary to $\rightarrow$: '$a=b \nrightarrow c=d$' is to be read as 'a equal to b does not imply $c=d$'. Finally if $p \rightarrow q$ and $q \rightarrow p$ we write $p \leftrightarrow q$ or $q \leftrightarrow p$: if $p \leftrightarrow q$ and $q \leftrightarrow r$, both $p \rightarrow r$ and $r \rightarrow p$, so that $p \leftrightarrow r$.

Definition 1. The set S_1 is identical with the set S_2, in symbols $S_1 \equiv S_2$, if S_1 is transformed into S_2 by simple translation. $S_1 \not\equiv S_2$ indicates that S_1 is not identical with S_2.

Identity is an equivalence relation, for it is reflexive, $S_1 \equiv S_1$: symmetric, $S_1 \equiv S_2 \leftrightarrow S_2 \equiv S_1$: and transitive, $S_1 \equiv S_2$, $S_2 \equiv S_3 \rightarrow S_1 \equiv S_3$.

The definition of identity we have adopted is perhaps a little anomalous for it is less stringent than equality: $S_1 = S_2 \rightarrow S_1 \equiv S_2$ but $S_1 \equiv S_2 \nrightarrow S_1 = S_2$ because of the arbitrary translation permitted in the identity relation. If $S_1 \equiv S_2$ and, after translation of S_1 by $\mathbf{c}$, $S_1 = S_2$, then we shall write $S_1 + \mathbf{c} = S_2$.

Definition 2. The set S_1 is enantiomorphic to the set S_2, in symbols $S_1 \sim S_2$ if $S_1(\mathbf{x}) \equiv S_2(-\mathbf{x})$, that is $S_1 \equiv \bar{S}_2$. $S_1 \nsim S_2$ means that S_1 is not enantiomorphic to S_2.

If $S_1 \equiv S_2$, $S_1 \nsim S_2$ unless $S_2 \equiv \bar{S}_2$: if $S_2 \equiv \bar{S}_2$ we shall define the relation between S_1 and S_2 as identity and exclude it from enantiomorphism. Then if $S_1 \equiv S_2$, $S_1 \nsim S_2$: if $S_1 \sim S_2$, $S_1 \not\equiv S_2$. Enantiomorphism is not an equivalence relation because $S_1 \nsim S_1$, and if $S_1 \sim S_2$ and $S_2 \sim S_3$, then $S_1 \equiv S_3$: but $S_1 \sim S_2 \rightarrow S_2 \sim S_1$.

Definition 3. The set S_1 is homometric with the set S_2, in symbols $S_1 \,)(\, S_2$, if both S_1 and S_2 yield the same weighted vector set, i.e. $\widehat{S_1\bar{S}_1} = \widehat{S_2\bar{S}_2}$, and $S_1 \not\equiv S_2$, $S_1 \nsim S_2$. $S_1 \,)\!\not(\, S_2$ means that S_1 is not homometric to S_2.

$)($ is not an equivalence relation: $S_1 \,)\!\not(\, S_1$ since $S_1 \equiv S_1$: $S_1 \,)(\, S_2$, $S_2 \,)(\, S_3 \nrightarrow S_1 \,)(\, S_3$ since, although $\widehat{S_1\bar{S}_1} = \widehat{S_3\bar{S}_3}$, either $S_1 \equiv S_3$, or $S_1 \sim S_3$, or $S_1 \,)(\, S_3$: but $S_1 \,)(\, S_2 \rightarrow S_2 \,)(\, S_1$.

If $S_1 \equiv S_2$, then $S_1 \,)(\, S_3 \rightarrow S_2 \,)(\, S_3$: if $S_1 \sim S_2$, then $S_1 \,)(\, S_3 \rightarrow S_2 \,)(\, S_3$. For in the second proposition $\widehat{S_1\bar{S}_1} = \widehat{S_2\bar{S}_2} = \widehat{S_3\bar{S}_3}$; and if $S_2 \equiv S_3$, $S_1 \sim S_3$: and if $S_2 \sim S_3$, $S_1 \equiv S_3$.

One homometric pair is a member of a family of equivalent homometric pairs. For suppose T is a non-singular affine transformation such that, under T, $\mathbf{x}$ becomes $\mathsf{T}\mathbf{x} = \mathbf{b} + \mathsf{A}.\mathbf{x}$ where A is a non-singular m-dimensional square matrix. By $S^* = \mathsf{T}S$ we mean that set which is obtained from S by subjecting each of the $\mathbf{x}_i$ to the transformation: $\mathbf{x}_i$ becomes $\mathsf{T}\mathbf{x}_i = \mathbf{b} + \mathsf{A}.\mathbf{x}_i$.

If $S_1 \equiv S_2$, $S_1 = S_2 + \mathbf{c}$, where $\mathbf{c}$ is arbitrary. Then

$$\mathsf{T}S_1 = \mathsf{T}S_2 + \mathsf{T}\mathbf{c}: \quad \text{or} \quad S_1^* \equiv S_2^* \,.$$

Because T is non-singular, i.e. $\det \mathsf{A} \neq 0$, there exists a T^{-1} such that

$$\mathsf{T}^{-1}\mathsf{T}\mathbf{x} = \mathbf{x}$$

(Birkhoff & MacLane, 1953). It then follows in a similar way that $S_1^* \equiv S_2^* \rightarrow \mathsf{T}^{-1}S_1^* \equiv \mathsf{T}^{-1}S_2^* \rightarrow S_1 \equiv S_2$. Thus

$$S_1 \equiv S_2 \leftrightarrow S_1^* \equiv S_2^* \,. \tag{4}$$

Similarly since $S_1 \sim S_2 \leftrightarrow S_1 \equiv \bar{S}_2$,

$$S_1 \sim S_2 \leftrightarrow S_1^* \sim S_2^* \,. \tag{5}$$

Further

$$\begin{aligned} \mathsf{T}(\widehat{S_1\bar{S}_1}) &= \int S_1(\mathbf{y})S_1(\mathbf{y} - \mathsf{T}^{-1}\mathbf{x})d\tau \\ &= |(\det \mathsf{A})^{-1}| \int S_1(\mathsf{T}^{-1}\mathbf{y})S_1(\mathsf{T}^{-1}\mathbf{y} - \mathsf{T}^{-1}\mathbf{x})d\tau \\ &= |(\det \mathsf{A})^{-1}| \widehat{S_1^*\bar{S}_1^*} \,. \end{aligned} \tag{6}$$

Since $\det \mathsf{A} \neq 0$, it follows that

$$\widehat{S_1\bar{S}_1} = \widehat{S_2\bar{S}_2} \leftrightarrow \widehat{S_1^*\bar{S}_1^*} = \widehat{S_2^*\bar{S}_2^*} \,. \tag{7}$$

From (4), (5) and (7) there follows the lemma:

Lemma 1:

$$S_1 \,)(\, S_2 \leftrightarrow S_1^* \,)(\, S_2^*$$

and it is sufficient to consider one homometric pair in order to consider the whole family of pairs generated by the non-singular affine transformations T.

By (6) the operations $\frown$ and T commute for unimodular T: since (6) is true for $\mathbf{b} = \mathbf{0}$ and

$$\mathsf{A} = \operatorname{diag}(-1, 1, \ldots, 1) \,,$$

Lemma 1 holds for the limited enantiomorphism

$$S_1 \equiv \mathsf{T}S_2 = S_2(-x_1, x_2, \ldots, x_m)$$

in $m > 1$ dimensions. It holds also for the full enantiomorphism $S_1 \equiv \mathsf{T}S_2 = S_2(-\mathbf{x}) = \bar{S}_2$, whilst from (6) $\frown$ and $^{-}$ commute.

Because of Lemma 1 it is convenient to call the whole family of pairs related by transformations T *one* homometric pair. But this does not adequately define the most general distinct homometric pair. It happens in general that $S_1 \,)(\, S_2$ for a range of values of the $\mathbf{x}_i^{(1)}$, $z_i^{(1)}$ in S_1 and the corresponding $\mathbf{x}_i^{(2)}$, $z_i^{(2)}$ in S_2. Nor is it necessary, as Hosemann & Bagchi (1954) have shown, that the number of points, N_1, in S_1 should be the same as the number, N_2, in S_2. However, the total weight of points in S_1 and S_2 is necessarily the same: for

$$\widehat{S_1\bar{S}_1} = \widehat{S_2\bar{S}_2} \rightarrow \left(\sum_{i=0}^{N_1-1} z_i^{(1)}\right)^2 = \left(\sum_{i=0}^{N_2-1} z_i^{(2)}\right)^2$$

and we always choose positive weights z_i. More precisely if (1) is true for both S_1 and S_2

$$\sum_{i=0}^{N_1-1} z_i^{(1)} = w \sum_{i=0}^{N_2-1} z_i^{(2)} \,,$$

where w is an integer > 0: and S_2 may be normalized so that

$$(z_0^{(2)}, z_1^{(2)}, \ldots, z_{N_2-1}^{(2)}) = w\,.$$

Now if $S_1 \,)\!-\!(\, S_2$ for a range of the $\mathbf{x}_i$ and z_i, then the correspondence $)\!-\!($ is specified by parameters $\mathbf{a}, \mathbf{b}, \ldots, \mathbf{g}$ defining the coordinates, and parameters $p, q, \ldots, t$ defining the weights. These parameters are common to both S_1 and S_2. S_1 (or S_2) is then completely specified by further constant vectors $\mathbf{n}_1^{(1)}, \mathbf{n}_2^{(1)}, \ldots, \mathbf{n}_r^{(1)}$ (or $\mathbf{n}_1^{(2)}, \mathbf{n}_2^{(2)}, \ldots, \mathbf{n}_{r'}^{(2)}$) and constants $m_1^{(1)}, m_2^{(1)}, \ldots, m_s^{(1)}$ (or $m_1^{(2)}, m_2^{(2)}, \ldots, m_{s'}^{(2)}$): $r, s \le N_1$; $r', s' \le N_2$; and the $\mathbf{n}_i^{(1)}, m_i^{(1)}$ necessarily differ from the $\mathbf{n}_i^{(2)}, m_i^{(2)}$. It is convenient to call the whole family of correspondences $S_1 \,)\!-\!(\, S_2$ specified by $\mathbf{a}, \mathbf{b}, \ldots, \mathbf{g}$; $p, q, \ldots, t$; *one* homometric pair and to call S_1 and S_2 each *one* homometric set (h.s.).

DEFINITION 4. If

$$S_1 = S_1(\mathbf{n}_i^{(1)}, \mathbf{a}, \mathbf{b}, \ldots, \mathbf{g};\; m_i^{(1)}, p, q, \ldots, t)$$
$$S_2 = S_2(\mathbf{n}_{i'}^{(2)}, \mathbf{a}, \mathbf{b}, \ldots, \mathbf{g};\; m_{i'}^{(2)}, p, q, \ldots, t)$$

and $S_1 \,)\!-\!(\, S_2$ for some $\mathbf{a}, \mathbf{b}, \ldots, \mathbf{g}$; $p, q, \ldots, t$; then S_1 (together with its equivalents $\mathsf{T}S_1$) and S_2 (together with its equivalents $\mathsf{T}S_2$) are each one homometric set, and S_1 and S_2 together constitute one homometric pair.

In the definition we have adopted there is still a possible uncertainty. If $S \,)\!-\!(\, \mathsf{T}'S$ where T' is some non-singular affine transformation, $\mathsf{T}S \,)\!-\!(\, \mathsf{T}\mathsf{T}'S$ is some pair of h.s. for general T. But T' itself may be so simple that it could seem unreasonable to call S and $\mathsf{T}'S$ distinct sets. An example is given by Hosemann & Bagchi (1954) from a private communication by Dr Patterson (their Figs. 1 and 2).

Hosemann & Bagchi (*HB*) have called pairs of sets of the type of this example 'pseudohomometric'. According to their definition two sets S_1 and S_2 are pseudohomometric either (*a*) if $\mathsf{T}S_1 \,)\!-\!(\, \mathsf{T}S_2$ and $S_2 = \mathsf{T}^*S_1$ with T^* a congruence or an enantiomorphism; or (*b*) $S_1 \,)\!-\!(\, S_2$ if and only if S_1 and S_2 are infinite (and therefore almost certainly periodic) sets. For our purposes the distinction in (*b*) between infinite and finite h.s. is unnecessary since, if $S_1 \,)\!-\!(\, S_2$ and S_1 and S_2 are finite (and therefore non-periodic) sets, the sets S_1 and S_2 can be assigned to a unit cell of a periodic lattice to give infinite (periodic) sets S_1' and S_2' with the property $S_1' \,)\!-\!(\, S_2'$. Thus the class of all infinite periodic sets includes as a sub-class the class of all finite non-periodic sets; and except for the as-yet-unexplored case of infinite non-periodic h.s. it is sufficient to investigate all periodic h.s. in order to investigate all h.s.

For our purposes the distinction in (*a*) between general h.s. S_1 related to others S_2 by $\mathsf{T}S_1 \,)\!-\!(\, \mathsf{T}S_2$, and a sub-class of h.s. for which both $\mathsf{T}S_1 \,)\!-\!(\, \mathsf{T}S_2$ and $S_2 = \mathsf{T}^*S_1$, is also unnecessary. According to the definition of *HB*(6), S_1 and S_2 are congruent if T^* is a combination of translation and rotation. According to our Definition 1, if T^* is a congruence in *HB*'s sense, $S_2 \equiv \mathsf{T}^\dagger S_1$ where $\mathsf{T}^\dagger$ is a rotation. The definition of enantiomorphy given by *HB*(7) is identical with our Definition 2: but from (5)

$$S_1 \sim S_2 \leftrightarrow \mathsf{T}S_1 \sim \mathsf{T}S_2$$

so that there are no h.s. obeying $\mathsf{T}S_1 \,)\!-\!(\, \mathsf{T}S_2$, $S_2 \equiv \mathsf{T}^\ddagger S_1$ with $\mathsf{T}^\ddagger$ an enantiomorphism. However, from *HB*'s example after Patterson, *HB* Figs. 1 and 2, by the enantiomorphism $\mathsf{T}^\ddagger$ they must mean a limited enantiomorphism (reflection) in m-dimensions of the type

$$\mathsf{T}^\ddagger = \mathrm{diag}\,(-1, 1, \ldots, 1), \qquad m \ge 2\,;$$

or again

$$\mathsf{T}^\ddagger = \mathrm{diag}\,(-1, 1, -1, \ldots, 1), \quad m \ge 3\,;$$

or indeed any enantiomorphism but the full enantiomorphism

$$\mathsf{T} = \mathrm{diag}\,(-1, -1, \ldots, -1)\,.$$

By 'enantiomorphism' we shall always mean 'full enantiomorphism': enantiomorphism's $\mathsf{T}^\ddagger$ which are not full we refer to as 'limited enantiomorphisms'.

The example of *HB* Figs. 1 and 2 means that sets satisfying $\mathsf{T}S_1 \,)\!-\!(\, \mathsf{T}S_2$, $S_2 \equiv \mathsf{T}^\ddagger S_1$, with $\mathsf{T}^\ddagger$ a limited enantiomorphism, exist. In this 2-dimensional example

$$\mathsf{T}^\ddagger = \begin{bmatrix} 0 & 1 \\ 1 & 0 \end{bmatrix}$$

and if the reference system is rotated through 45° (so that both sets are rotated equally relative to the reference system)

$$\mathsf{T}^\ddagger = \mathrm{diag}\,(-1, 1)$$

in the new system. Patterson has emphasized, in lecturing on the sets of *HB* Figs. 1 and 2, that if two sets S_1 and S_2 satisfy $\mathsf{T}S_1 \,)\!-\!(\, \mathsf{T}S_2$ for some T, and $S_2 \equiv \mathsf{T}^\ddagger S_1$, then, despite the simplicity of $\mathsf{T}^\ddagger$, the fact that S_1 and $\mathsf{T}^\ddagger S_1$ have the same vector set is not trivial. This view accords with that of the author, for if $S_2 \equiv \mathsf{T}^\ddagger S_1$ we should expect according to (6) that $\widehat{S_2\bar{S}_2} = \mathsf{T}^\ddagger \widehat{S_1\bar{S}_1}$ rather than $\widehat{S_2\bar{S}_2} = \widehat{S_1\bar{S}_1}$. Indeed, when $S_2 \equiv \mathsf{T}^\dagger S_1$ with $\mathsf{T}^\dagger$ a rotation we should also expect $\widehat{S_2\bar{S}_2} = \mathsf{T}^\dagger \widehat{S_1\bar{S}_1}$ rather than $\widehat{S_2\bar{S}_2} = \widehat{S_1\bar{S}_1}$.

Thus, if $\mathsf{T}S_1 \,)\!-\!(\, \mathsf{T}S_2$ and $S_2 \equiv \mathsf{T}'S$ with T' either a rotation or a limited enantiomorphism, we can still write within the terms of Definition 3 that $S_1 \,)\!-\!(\, \mathsf{T}'S_1$. It is here that uncertainty arises however: for if $\mathsf{T}'\mathsf{T}'$ is the identical transformation (as for the limited enantiomorphism for example) $\mathsf{T}'S_1 \,)\!-\!(\, \mathsf{T}'\mathsf{T}'S_1$ and $\mathsf{T}'S_1$ is one of the equivalents of S_1 under T'. Nevertheless, because $S_1 \,)\!-\!(\, \mathsf{T}'S_1$ is a valid relation we treat S_1 and $\mathsf{T}'S_1$ so related as distinct h.s.

Finally, we must remark that if $S_1 \,)\!-\!(\, S_2$ and $\mathsf{V}S_1 \,)\!-\!(\, \mathsf{V}S_2$ with V a singular affine transformation then, until we have more information on the point, we shall treat S_1 and $\mathsf{V}S_1$ as the same h.s.: an example of h.s. which remain h.s. under V appears in *HB* Figs. 2 and 3 (after Patterson). A difficulty associated with this choice is that it will not in general be clear to what family a given h.s. belongs; but Patterson (1944) has already shown that sets in one dimension have their counterpart in $m>1$ dimensions, and that these sets become 1-dimensional in $m(>1)$-dimensions for particular 1-dimensional sets of parameters. It would be unreasonable to isolate this set of parameters from the more general m-dimensional set. We shall always count h.s. in m-dimensional space as distinct from h.s. in m'-dimensional space if $m \neq m'$, however.

By analogy with Definition 4, the definition of different homometric n-tuplets is now obvious unless there exist n-tuplets which break down into sets of pairs for some values of the parameters!

Some theorems on the generation of h.s. from subsets

Hosemann & Bagchi (1954) have provided a very powerful means of generating h.s. Expressed in our notation, the relation $HB(10)$ is the theorem:

'If $S_1 \sim S_2$ and $S_3 \sim S_4$, then $\widehat{S_1S_3}$)-($\widehat{S_1S_4}$' [α].

The proviso $S_1 \sim S_2$ means that $S_1 \not\equiv \bar{S}_1$. The debt which the theorems of this paper owe to Hosemann & Bagchi will be apparent from the manner of their proofs. But HB in fact proved only the theorem:

'If $S_1 \sim S_2$ and $S_3 \sim S_4$, then $\widehat{S_1S_3}$ and $\widehat{S_1S_4}$ have the same weighted vector set' [β].

Whilst the difference between the theorem as asserted and the theorem as proved seems slight, consider the one-dimensional sets of unit period containing all points of equal weight:

$S_1 = 0,\ 1/12,\ 1/4,\ 1/2;\ \ S_3 = 1/13,\ 1/12,\ 5/12,\ 3/4,\ 12/13;$
$S_4 = \bar{S}_3 = 1/13,\ 1/4,\ 7/12,\ 11/12,\ 12/13.$

S_1 is not centrosymmetrical so that $S_1 \not\equiv \bar{S}_1$: nor is $S_3 \equiv \bar{S}_3$. Yet it is easily verified that

$\widehat{S_1S_3} = \widehat{S_1\bar{S}_3} = 0,\ 1/12-1/13,\ 1/13,\ 1/12,\ 1/12+1/13,\ 1/6,$
$1/4-1/13,\ 1/4,\ 1/4+1/13,\ 1/3,\ 5/12,\ 1/2-1/13,$
$1/2,\ 1/2+1/13,\ 7/12,\ 2/3,\ 3/4,\ 5/6,\ 11/12,\ 12/13;$

in which again all points are of equal weights.

We therefore take HB's theorem in the form of [β] and our Theorem 3 is then HB's assertion [α] with some provisos on the subsets—namely that $R_1 \neq 0$ for all $\mathbf{h}$ and $R_3 \neq 0$ for all $\mathbf{h}$, where the Fourier Transform, R, of S is defined below. Since $\widehat{S_2S_4} \sim \widehat{S_1S_3}$ and $\widehat{S_2S_3} \sim \widehat{S_1S_4}$ (since $\widehat{S_1S_4} \sim \overline{\widehat{S_1S_4}} \equiv \widehat{\bar{S}_1\bar{S}_4}$) we cannot obtain combinations which can hope to generate different homometric pairs.

We define the Fourier Transform of $S(\mathbf{x})$ (which is defined for all $\mathbf{h}$ for non-periodic sets and for all $\mathbf{h}$ with integral components for periodic sets) by

$$R(\mathbf{h}) = \int S(\mathbf{x}) \exp 2\pi i (\mathbf{h}.\mathbf{x}) d\tau\ ,$$

where the region of integration is as for $\widehat{g_1g_2}$ defined in (3) previously. If $S_1 \equiv S_2$ such that $S_1(\mathbf{x}) = S_2(\mathbf{x}-\mathbf{c}) = S_2(\mathbf{x})+\mathbf{c}$

$$R_1(\mathbf{h}) = R_2(\mathbf{h}) \exp\{-2\pi i \mathbf{h}.\mathbf{c}\}\ ,$$

which we write $R_1 \equiv R_2$. Then $S_1 \equiv S_2 \leftrightarrow R_1 \equiv R_2$ because of the Fourier Inversion Theorem.

We can now prove Lemma 2.

LEMMA 2: A sufficient condition that $\widehat{S_1S_2} \equiv \widehat{S_1S_3}$ is $S_2 \equiv S_3$. Providing $R_1(\mathbf{h})$ is never zero, a necessary condition is that $S_2 \equiv S_3$.

The condition is obviously sufficient, and further

$$\widehat{S_1S_2} \equiv \widehat{S_1S_3} \rightarrow R_1R_2 \equiv R_1R_3 \rightarrow R_2 \equiv R_3$$
$$(\text{since } R_1 \neq 0) \rightarrow S_2 \equiv S_3\ .$$

THEOREM 3: If $S_1 \sim S_2$ and $S_3 \sim S_4$, and R_1 and R_2 are never zero then $\widehat{S_1S_3}$)-($\widehat{S_1S_4}$.

Since $\widehat{S_1S_3} \sim \widehat{S_2S_4}$ the theorem $\rightarrow \widehat{S_2S_4}$)-($\widehat{S_1S_4}$: we therefore write the full Th. 3 as asserting

$S_1 \sim S_2$ and $S_3 \sim S_4$, with $R_1, R_2 \neq 0$
for all $\mathbf{h} \rightarrow \widehat{S_1S_3} \sim \widehat{S_2S_4}$)-($\widehat{S_2S_3} \sim \widehat{S_1S_4}$.

Firstly, following Hosemann & Bagchi (1954),

$$(\widehat{S_1S_3})(\overline{\widehat{S_1S_3}}) = \widehat{S_1S_3}\widehat{\bar{S}_1\bar{S}_3} = \widehat{S_1\bar{S}_1}\widehat{S_3\bar{S}_3}$$
$$= \widehat{S_1\bar{S}_1}\widehat{S_4\bar{S}_4} = \widehat{S_1S_4}\widehat{\bar{S}_1\bar{S}_4} = (\widehat{S_1S_4})(\overline{\widehat{S_1S_4}})\ .$$

We can now prove the theorem providing $\widehat{S_1S_3} \not\equiv \widehat{S_1S_4}$ and $\widehat{S_1S_3} \nsim S_1S_4$. By Lemma 2, $\widehat{S_1S_3} \equiv \widehat{S_1S_4} \rightarrow S_3 \equiv S_4$ (since $R_1 \neq 0$). But $S_3 \sim S_4$. Further, if $\widehat{S_1S_3} \sim \widehat{S_1S_4}$, then $\widehat{S_1S_3} \equiv \widehat{\bar{S}_1\bar{S}_4} \equiv \widehat{\bar{S}_1S_3}$, whence, by Lemma 2, $S_1 \equiv \bar{S}_1 \equiv S_2$ (since $R_3 \neq 0$). But $S_1 \sim S_2$.

COROLLARY: If S_1, S_2 and S_3 are three point sets and $R_1 \neq 0$, $R_2 \neq 0$, $R_3 \neq 0$, for all $\mathbf{h}$, then

$$\widehat{S_1}\widehat{S_2}\widehat{S_3}\ \text{)-(}\ \widehat{S_1}\widehat{S_2}\widehat{\bar{S}_3}\ \text{)-(}\ \widehat{S_1}\widehat{\bar{S}_2}\widehat{S_3}\ \text{)-(}\ \widehat{S_1}\widehat{\bar{S}_2}\widehat{\bar{S}_3}$$

with (here))-(used transitively.

The four sets are a homometric quadruplet.

THEOREM 4: If $S_1 \sim S_2$, then $\widehat{S_1S_1}$)-($\widehat{S_1S_2}$.

For

$$\widehat{S_1S_1} \equiv \widehat{S_1S_2} \rightarrow R_1R_1 \equiv R_1R_2\ ,$$
$$\widehat{S_1S_1} \sim \widehat{S_1S_2} \rightarrow R_1R_1 \equiv R_2R_1:$$

and $R_1 = 0 \rightarrow R_2 = 0$. Whence in either case $S_1 \equiv S_2$, contra hyp.

THEOREM 5: If S_1)-(S_2 and S_3)-(S_4, then $\widehat{S_1S_3}$, $\widehat{S_1S_4}$, $\widehat{S_2S_3}$, $\widehat{S_2S_4}$, $\widehat{S_1\bar{S}_3}$, $\widehat{S_1\bar{S}_4}$, $\widehat{S_2\bar{S}_3}$ and $\widehat{S_2\bar{S}_4}$ have the same weighted vector set.

For

$$(\widehat{S_1S_3})(\widehat{\bar{S}_1\bar{S}_3}) = \widehat{S_1\bar{S}_1}\widehat{S_3\bar{S}_3}$$
$$= \widehat{S_1\bar{S}_1}\widehat{S_4\bar{S}_4} = \widehat{S_1S_4}\widehat{\bar{S}_1\bar{S}_4} = (\widehat{S_1S_4})(\widehat{\bar{S}_1\bar{S}_4}) .$$

The other cases are similar.

In view of Th. 5 with $S_3 \equiv S_1$, $S_4 \equiv S_2$, it is tempting now to prove that with suitable provisos

$$S_1 \;)\!-\!(\; S_2 \rightarrow \widehat{S_1S_1} \;)\!-\!(\; \widehat{S_1S_2} ,$$

analogous to Th. 4. Certainly, if

$$R_1 \neq 0,\ \widehat{S_1S_1} \equiv \widehat{S_1S_2} \rightarrow S_1 \equiv S_2 .$$

But if $\widehat{S_1S_1} \sim \widehat{S_1S_2}$ we have Th. 6:

THEOREM 6: If $\widehat{S_1S_1} \sim \widehat{S_1S_2}$ and $S_1 \;)\!-\!(\; S_2$, and $R_1 \neq 0$, $R_2 \neq 0$ for all $\mathbf{h}$, then $\widehat{S_1S_1} \;)\!-\!(\; \widehat{\bar{S}_1S_2}$.

$$\widehat{S_1S_1} \sim \widehat{S_1S_2} \rightarrow \widehat{S_1S_1} \equiv \widehat{\bar{S}_1\bar{S}_2} \;)\!-\!(\; \widehat{\bar{S}_1S_2} \text{ (by Th. 3).}$$

And because identity is an equivalence relation this implies

$$\widehat{S_1S_1} \;)\!-\!(\; \widehat{\bar{S}_1S_2} .$$

But because $)\!-\!($ is not an equivalence relation $\widehat{\bar{S}_1S_2} \;)\!-\!(\; \widehat{S_1S_3} \nleftrightarrow \widehat{S_1S_1} \sim \widehat{S_1S_2}$ so that $\widehat{S_1S_1} \;)\!-\!(\; \widehat{\bar{S}_1S_2} \nrightarrow \widehat{S_1S_1} \;)\!\not-\!(\; \widehat{S_1S_2}$. We therefore have:

THEOREM 7: If $S_1 \;)\!-\!(\; S_2$, and $R_1 \neq 0$ and $R_2 \neq 0$ for all $\mathbf{h}$, then either $\widehat{S_1S_1} \;)\!-\!(\; \widehat{S_1S_2}$, or $\widehat{S_1S_1} \;)\!-\!(\; \widehat{\bar{S}_1S_2}$, or $\widehat{S_1S_1} \;)\!-\!(\; \widehat{S_1S_2} \;)\!-\!(\; \widehat{\bar{S}_1S_2}$ with $)\!-\!($ used transitively. If $\widehat{S_1S_1} \;)\!\not-\!(\; \widehat{S_1S_2}$, $\widehat{S_1S_1} \sim \widehat{S_1S_2}$; if

$$\widehat{S_1S_1} \;)\!\not-\!(\; \widehat{\bar{S}_1S_2},\ \widehat{S_1S_1} \equiv \widehat{\bar{S}_1S_2} .$$

THEOREM 8: If $S_1 \;)\!-\!(\; S_2$, $S_1 \not\equiv \bar{S}_1$, and $R_1 \neq 0$ for all $\mathbf{h}$, then $\widehat{S_1\bar{S}_1}$ is homometric with each of $\widehat{S_1S_1}$, $\widehat{S_1S_2}$ and $\widehat{\bar{S}_1S_2}$.

$$\widehat{S_1\bar{S}_1} \;)\!-\!(\; \widehat{S_1S_1} \text{ is Th. 4.}$$
$$\widehat{S_1\bar{S}_1} \equiv \widehat{S_1S_2} \rightarrow S_2 \sim S_1;\ \widehat{S_1\bar{S}_1} \equiv \widehat{\bar{S}_1S_2} \rightarrow S_1 \equiv S_2$$

by Lemma 2; etc.

Theorems 7 and 8 together assert that $\widehat{S_1\bar{S}_1}$, $\widehat{S_1S_1}$ and one or other of $\widehat{S_1S_2}$ or $\widehat{\bar{S}_1S_2}$ form a homometric triplet providing $S_1 \not\equiv \bar{S}_1$, $S_1 \;)\!-\!(\; S_2$ and $R_1 \neq 0$, $R_2 \neq 0$ for all $\mathbf{h}$. They may also form a homometric quadruplet if $\widehat{S_1S_1} \;)\!-\!(\; \widehat{S_1S_2} \;)\!-\!(\; \widehat{\bar{S}_1S_2}$ (transitive $)\!-\!($). It is impossible to obtain more than a homometric quintuplet from the homometric pair S_1 and S_2. For we can have at most

$$\widehat{S_1S_1} \;)\!-\!(\; \widehat{S_1\bar{S}_1} (\equiv \widehat{S_2\bar{S}_2}) \;)\!-\!(\; \widehat{\bar{S}_1S_2}$$
$$(\sim \widehat{S_1\bar{S}_2}) \;)\!-\!(\; \widehat{S_1S_2} \;)\!-\!(\; \widehat{S_2S_2} ,$$

where $)\!-\!($ is used transitively.

A convenient illustration of Ths. 7 and 8 is provided by the one-dimensional periodic sets containing four points of equal weight

$$S_1 = 0,\ a,\ 1/4,\ 1/2+a;\ S_2 = 0,\ a,\ 1/4+a,\ 1/2;$$
$$\bar{S}_1 = 0,\ 1/2-a,\ 3/4,\ 1-a;\ \bar{S}_2 = 0,\ 1/2,\ 3/4-a,\ 1-a; \quad (8)$$

given originally by Patterson (1944).

It is easily verified that

$\widehat{S_1S_1} = (0,\ a,\ 2a,\ 1/4,\ 1/4+a,\ 1/2,\ 1/2+a,\ 1/2+2a,\ 3/4+a;\ 1,\ 2,\ 2,\ 2,\ 2,\ 1,\ 2,\ 2,\ 2)$,

$\widehat{S_1\bar{S}_1} = (0,\ a,\ 1/4-a,\ 1/4,\ 1/4+a,\ 1/2-a,\ 1/2,\ 1/2+a,\ 3/4-a,\ 3/4,\ 3/4+a,\ 1-a;\ 4,\ 1,\ 1,\ 1,\ 1,\ 1,\ 2,\ 1,\ 1,\ 1,\ 1,\ 1)$,

$\widehat{S_1S_2} = (0,\ a,\ 2a,\ 1/4,\ 1/4+a,\ 1/4+2a,\ 1/2,\ 1/2+a,\ 1/2+2a,\ 3/4,\ 3/4+2a;\ 1,\ 3,\ 1,\ 1,\ 2,\ 1,\ 1,\ 3,\ 1,\ 1,\ 1)$,

$\widehat{S_1\bar{S}_2} = (0,\ a,\ 1/4-a,\ 1/4,\ 1/2,\ 1/2+a,\ 3/4-a,\ 3/4,\ 3/4+a,\ 1-a;\ 2,\ 1,\ 1,\ 2,\ 2,\ 2,\ 1,\ 2,\ 1,\ 2)$,

and that

$$\widehat{S_1S_1} \sim \widehat{S_2S_2}:\ \widehat{S_1S_1} \;)\!-\!(\; \widehat{S_1\bar{S}_1} \;)\!-\!(\; \widehat{S_1S_2} \;)\!-\!(\; \widehat{S_1\bar{S}_2}$$

with $)\!-\!($ transitive.

A homometric quintuplet is generated by the two 4-sets

$$S_1 = 0,\ 1/13,\ 4/13,\ 6/13;\quad S_2 = 0,\ 1/13,\ 3/13,\ 9/13;$$
$$\bar{S}_1 = 0,\ 7/13,\ 9/13,\ 12/13;\ \bar{S}_2 = 0,\ 4/13,\ 10/13,\ 12/13;$$

containing again four points of equal weight. S_1 and S_2 were not mentioned by Patterson explicitly but can only be his cyclotomic sets for $n = 13$ as we shall show later.* For these sets

$\widehat{S_1S_1} = (0,\ 1/13,\ 2/13,\ 4/13,\ 5/13,\ 6/13,\ 7/13,\ 8/13,\ 10/13,\ 12/13;\ 1,\ 2,\ 1,\ 2,\ 2,\ 2,\ 2,\ 1,\ 2,\ 1)$,

$\widehat{S_2S_2} = (0,\ 1/13,\ 2/13,\ 3/13,\ 4/13,\ 5/13,\ 6/13,\ 9/13,\ 10/13,\ 12/13;\ 1,\ 2,\ 1,\ 2,\ 2,\ 1,\ 1,\ 2,\ 2,\ 2)$,

$\widehat{S_1S_2} = (0,\ 1/13,\ 2/13,\ 3/13,\ 4/13,\ 5/13,\ 6/13,\ 7/13,\ 9/13,\ 10/13;\ 2,\ 2,\ 2,\ 1,\ 2,\ 1,\ 1,\ 2,\ 2,\ 1)$,

$\widehat{S_1\bar{S}_2} = (0,\ 1/13,\ 3/13,\ 4/13,\ 5/13,\ 6/13,\ 8/13,\ 10/13,\ 11/13,\ 12/13;\ 2,\ 2,\ 2,\ 2,\ 2,\ 1,\ 1,\ 2,\ 1,\ 1)$,

$\widehat{S_1\bar{S}_1} = (0,\ 1/13,\ 2/13,\ 3/13,\ 4/13,\ 5/13,\ 6/13,\ 7/13,\ 8/13,\ 9/13,\ 10/13,\ 11/13,\ 12/13;\ 4,\ 1,\ 1,\ 1,\ 1,\ 1,\ 1,\ 1,\ 1,\ 1,\ 1,\ 1,\ 1)$.

Th. 7 is the restricted form of the more general Th. 9.

* These sets have been given explicitly by Menzer (1949).

THEOREM 9: If $S_1)(S_2$, $S_3)(S_4$, and neither $R_1=0$, nor $R_2=0$, nor $R_3=0$, nor $R_4=0$ for some **h**, then either $\widehat{S_1S_3})(\widehat{S_1S_4}$ or $\widehat{S_1S_3})(\widehat{\bar{S}_1S_4}$ or

$$\widehat{S_1S_3})(\widehat{S_1S_4})(\widehat{\bar{S}_1S_4} \,( )(\, \text{transitive}) .$$

Because of Th. 5 it is sufficient to prove that either $\widehat{S_1S_3} \not\equiv \widehat{S_1S_4}$ and $\widehat{S_1S_3} \sim \widehat{S_1S_4}$, or that

$$\widehat{S_1S_3} \sim \widehat{S_1S_4} \to \widehat{S_1S_3})(\widehat{\bar{S}_1S_4} .$$

The proof is identical to that of Th. 6.

$\widehat{S_1S_3} \equiv \widehat{S_1S_4} \to S_3 \equiv S_4$; $\widehat{S_1S_3} \sim \widehat{\bar{S}_1S_4} \to S_3 \equiv \bar{S}_4$. If $\widehat{S_1S_3} \sim \widehat{S_1S_4}$, $\widehat{S_1S_3} \equiv \widehat{\bar{S}_1\bar{S}_4})(\widehat{\bar{S}_1S_4}$ (by Th. 3). If $\widehat{S_1S_3} \equiv \widehat{\bar{S}_1S_4}$, $\widehat{S_1S_3})(\widehat{S_1S_4}$ (by Th. 3).

If $S_1)(S_2$ and $S_3)(S_4$, a complete set of sets generated by the four h.s. is

$$\widehat{S_1S_3},\ \widehat{S_1S_4},\ \widehat{S_2S_3},\ \widehat{S_2S_4},\ \widehat{S_1\bar{S}_3},\ \widehat{S_1\bar{S}_4},\ \widehat{S_2\bar{S}_3},\ \widehat{S_2\bar{S}_4} .$$

Of these, by Th. 3, $\widehat{S_1S_3})(\widehat{S_1\bar{S}_3}$, $\widehat{S_1S_4})(\widehat{S_1\bar{S}_4}$; and similarly when S_2 replaces S_1. That they do not necessarily form a homometric octuplet is already suggested by Th. 9. Indeed, if

$$\begin{aligned} &S_1=0,\ a,\ 1/4,\ 1/2+a; && S_2=0,\ a,\ 1/4+a,\ 1/2;\\ &S_3=0,\ b,\ 1/4,\ 1/2+b; && S_4=0,\ b,\ 1/4+b,\ 1/2;\\ &\bar{S}_3=0,\ 1/2-b,\ 3/4,\ 1-b; && \bar{S}_4=0,\ 1/2,\ 3/4-b,\ 1-b;\\ & && \text{with } b>a . \qquad (8')\end{aligned}$$

$\widehat{S_1S_3}=(0,\ a,\ b,\ a+b,\ 1/4,\ 1/4+a,\ 1/4+b,\ 1/2,\ 1/2+a,\ 1/2+b,\ 1/2+a+b,\ 3/4+a,\ 3/4+b;\ 1,\ 1,\ 1,\ 2,\ 2,\ 1,\ 1,\ 1,\ 1,\ 1,\ 2,\ 1,\ 1)$,

$\widehat{S_1S_4}=(0,\ a,\ b,\ a+b,\ 1/4,\ 1/4+b,\ 1/4+a+b,\ 1/2,\ 1/2+a,\ 1/2+b,\ 1/2+a+b,\ 3/4,\ 3/4+a+b;\ 1,\ 2,\ 1,\ 1,\ 1,\ 2,\ 1,\ 1,\ 2,\ 1,\ 1,\ 1,\ 1)$,

$\widehat{S_2S_3}=(0,\ a,\ b,\ a+b,\ 1/4,\ 1/4+a,\ 1/4+a+b,\ 1/2,\ 1/2+b,\ 1/2+a+b,\ 3/4+a,\ 3/4+b;\ 1,\ 1,\ 1,\ 2,\ 1,\ 2,\ 1,\ 2,\ 2,\ 1,\ 1,\ 1)$,

$\widehat{S_1\bar{S}_3}=(0,\ a,\ 1/4-b,\ 1/4,\ 1/4+a,\ 1/2-b,\ 1/2+a-b,\ 1/2+a,\ 3/4-b,\ 3/4,\ 3/4+a,\ 1-b,\ 1+a-b;\ 2,\ 1,\ 1,\ 1,\ 1,\ 1,\ 2,\ 1,\ 1,\ 1,\ 1,\ 1,\ 2)$,

$\widehat{S_1\bar{S}_4}=(0,\ a,\ 1/4-b,\ 1/4+a-b,\ 1/4,\ 1/2+a-b,\ 1/2,\ 1/2+a,\ 3/4-b,\ 3/4-b+a,\ 3/4,\ 1-b,\ 1-b+a;\ 1,\ 2,\ 1,\ 1,\ 1,\ 1,\ 1,\ 2,\ 1,\ 1,\ 1,\ 2,\ 1)$

and $\widehat{S_2S_4} \sim \widehat{S_1S_3}$, $\widehat{S_2\bar{S}_3} \sim \widehat{S_1\bar{S}_4}$, $\widehat{S_2\bar{S}_4} \sim \widehat{S_1\bar{S}_3}$. These three degenerate relations are actually different from those suggested by Th. 9, for that theorem suggests degenerate relations of the type $\widehat{S_1S_3} \sim \widehat{S_1S_4}$ *or* $\widehat{S_1S_3} \sim \widehat{\bar{S}_1S_4}$; $\widehat{\bar{S}_1S_3} \sim \widehat{\bar{S}_1S_4}$ *or* $\widehat{\bar{S}_1S_3} \sim \widehat{S_1S_4}$; etc. It may be that Th. 9 can be sharpened to assert that if $S_1)(S_2$ and $S_3)(S_4$, with R_1, R_2, R_3 and $R_4 \neq 0$, then

$$\widehat{S_1S_3})(\widehat{\bar{S}_1S_3})(\widehat{S_1S_4})(\widehat{\bar{S}_1S_4} \,( )(\, \text{transitive}).$$

Equivalently therefore we should have (omitting the $\frown$ for convenience)

$$\begin{aligned} &S_2S_3)(\bar{S}_2S_3)(S_2S_4)(\bar{S}_2S_4\\ &S_3S_1)(\bar{S}_3S_1)(S_3S_2)(\bar{S}_3S_2\\ &S_4S_1)(\bar{S}_4S_1)(S_4S_2)(\bar{S}_4S_2 .\end{aligned}$$

However, we have been unable to *prove* that there is even a homometric triplet amongst the eight sets generated by S_1 or S_2 and S_3 or S_4 or $\bar{S}_3$ or $\bar{S}_4$. But, if there is not, the sets must obey a formidable array of conditions: by Th. 9 we can always choose S_3 and S_4 so that $\widehat{S_1S_3})(\widehat{S_1S_4}$, and by Th. 3 $\widehat{S_1S_3})(\widehat{S_1\bar{S}_3}$ and $\widehat{S_1S_4})(\widehat{S_1\bar{S}_4}$. If now $\widehat{S_1S_3}$, $\widehat{S_1S_4}$ and $\widehat{S_1\bar{S}_3}$ do not form a triplet, $\widehat{S_1S_4})\not(\widehat{S_1\bar{S}_3} \to \widehat{S_1S_4} \equiv \widehat{S_1\bar{S}_3}$ or $\widehat{S_1S_4} \sim \widehat{S_1\bar{S}_3}$, and by Lemma 2 only $\widehat{S_1S_4} \sim \widehat{S_1\bar{S}_3}$ is possible. Similarly, $\widehat{S_1S_3})\not(\widehat{S_1\bar{S}_4} \to \widehat{S_1\bar{S}_4} \equiv \widehat{\bar{S}_1\bar{S}_3}$. We now have $\widehat{S_1S_4} \equiv \widehat{\bar{S}_1S_3}$, $\widehat{S_1\bar{S}_4} \equiv \widehat{\bar{S}_1\bar{S}_3}$. Since $\widehat{S_3\bar{S}_3} \equiv \widehat{S_4\bar{S}_4}$ we have from Lemma 2, $\widehat{S_1S_1} \equiv \widehat{\bar{S}_1\bar{S}_1} \to R_1 = \pm \bar{R}_1$.

By Th. 9 we can also choose S_2 so that $\widehat{S_1S_3})(\widehat{S_2S_3}$ and since by Th. 3 $\widehat{S_3S_2})(\widehat{S_3\bar{S}_2}$ and $\widehat{S_3S_1})(\widehat{S_3\bar{S}_1}$, we must have $\widehat{S_3S_3} \equiv \widehat{\bar{S}_3\bar{S}_3}$. Also $\widehat{S_1S_3}$, $\widehat{S_2S_3}$ and $\widehat{S_1S_4}$ form a triplet unless $\widehat{S_2S_3})\not(\widehat{S_1S_4} \to \widehat{S_2S_3})\not(\widehat{\bar{S}_1S_3}$ (since $\widehat{S_1S_4} \equiv \widehat{\bar{S}_1S_3}$ above). If $\widehat{S_2S_3})\not(\widehat{\bar{S}_1S_3}$,

$$\widehat{S_2S_3} \equiv \widehat{S_1\bar{S}_3} \to \widehat{S_2S_2}\widehat{S_3S_3} \equiv \widehat{S_1S_1}\widehat{\bar{S}_3\bar{S}_3} \to \widehat{S_1S_1} \equiv \widehat{S_2S_2}$$

(since $\widehat{S_3S_3} \equiv \widehat{\bar{S}_3\bar{S}_3}$ and $R_3 \neq 0$).

The relations $\widehat{S_1S_1} \equiv \widehat{S_2S_2}$ (with $S_1)(S_2$) is a possible one, however, as we prove in Th. 10 below; and sets obeying $\widehat{S_1S_1} \equiv \widehat{\bar{S}_1\bar{S}_1}$ require only that $\widehat{S_1S_1}$ be centro-symmetric.

If there is no triplet amongst the eight sets generated by S_1 or S_2 and S_3 or $\bar{S}_3$ or S_4 or $\bar{S}_4$, we must have also (again omitting $\frown$)

$$\begin{aligned} &S_1S_3)(S_1S_4,\ S_1S_3)(S_1\bar{S}_3,\ S_1S_3)(S_2S_3,\\ &S_2S_3)(S_2\bar{S}_3,\ S_1S_4)(S_1\bar{S}_4,\ S_2S_4)(S_2\bar{S}_4,\\ &S_2S_3)(S_2S_4,\ S_1S_4)(S_2S_4;\\ &S_2S_3 \equiv \bar{S}_1\bar{S}_4 \equiv S_1\bar{S}_3 \equiv \bar{S}_2S_4;\\ &\qquad S_1S_3 \equiv \bar{S}_2\bar{S}_4 \equiv S_2\bar{S}_3 \equiv \bar{S}_1S_4. \qquad (9)\end{aligned}$$

It therefore seems likely that S_1, S_2, S_3, S_4, $\bar{S}_3$ and $\bar{S}_4$ will generate a triplet in almost all if not all cases and will generate a quadruplet in most. Indeed, by relabelling S_2 as $\bar{S}_2$ in the examples (8) and (8′)

which follow Ths. 8 and 9 the degenerate relation $\widehat{S_1S_1} \sim \widehat{S_2S_2}$ from (8) becomes $\widehat{S_1S_1} \equiv \widehat{S_2S_2}$ associated with the *quintuplets* obtained from (8′): whilst if the sets S_1, S_2, S_3, $\bar{S}_3$, S_4 and $\bar{S}_4$ are taken as defined in (8′) the three degenerate relations $\widehat{S_2S_4} \sim \widehat{S_1S_3}$ etc. (i.e. $\widehat{S_1S_3} \equiv \widehat{\bar{S}_2\bar{S}_4}$ etc.) are contained in (9). It may indeed be possible to prove that $S_1, S_2, \ldots, \bar{S}_4$ together generate a quintuplet in all cases but the proof will require much heavier machinery than that developed so far.

An interesting homometric pair

We show above that one necessary condition that S_1 or S_2 and S_3 or S_4 or $\bar{S}_3$ or $\bar{S}_4$ do not generate a homometric triplet is that, with S_1) (S_2, $\widehat{S_1S_1} \equiv \widehat{S_2S_2}$. We showed also that a solution of the two relations is contained in (8) with S_2 relabelled as $\bar{S}_2$. We now show that a more general solution of the pair of relations S_1) (S_2, $\widehat{S_1S_1} \equiv \widehat{S_2S_2}$, than that contained in

$$\Pi_4 = \begin{cases} S_1 = (0,\, a,\, \tfrac{1}{4},\, \tfrac{1}{2}+a;\ 1, 1, 1, 1) \\ S_2 = (0,\, a,\, \tfrac{1}{2}+a,\, \tfrac{3}{4};\ 1, 1, 1, 1) \end{cases}$$

exists. We shall restrict ourselves to points of equal weight arranged on a linear lattice. We consider sets of $n+2r$ points.

THEOREM 10: There exist solutions of

$$S_1 \,)\!-\!(\, S_2,\ \widehat{S_1S_1} \equiv \widehat{S_2S_2}\,,$$

for S_1 and S_2 each containing $n+2r (n \geq 2)$ points of equal weight.

The transforms of S_1 and S_2 are R_1 and R_2. We shall suppose them of the form

$$R_1 = R_1^{(1)} + R_1^{(2)}$$
$$R_2 = R_2^{(1)} + R_2^{(2)}$$

where

$$R_1^{(1)} = R_2^{(1)} \text{ for all } h\,,$$
$$R_1^{(2)} \neq R_2^{(2)} \text{ for some } h\,.$$

Thus, S_1) –(S_2 is not excluded. Because of the properties of the δ-functions representing S_1 and S_2, corresponding to $R_1^{(1)}$ is $S_1^{(1)}$, and corresponding to $R_1^{(2)}$ is $S_1^{(2)}$, etc.

Because of the arbitrary choice of origins of $\widehat{S_1S_1}$ and $\widehat{S_2S_2}$

$$\widehat{S_1S_1} \equiv \widehat{S_2S_2} \rightarrow R_1^2 = R_2^2 \exp 2\pi i h\alpha$$

but because the origin of S_1 or S_2 is arbitrary we can choose it so that

$$R_1^{(1)} = R_2^{(1)} \text{ for all } h\,,$$

where in this context $R_1^{(1)} = R_2^{(1)}$ is a more stringent condition than $R_1^{(1)} \equiv R_2^{(1)}$ and permits no relative shift of origin of $S_1^{(1)}$ and $S_2^{(1)}$.

We now choose specifically

$$R_1^{(1)} = R_2^{(1)} = \sum_{i=1}^{n} \zeta_i^h\,, \tag{10}$$

where the ζ_i are the n roots of $\zeta_i^n = 1$. Then $R_1^{(1)} = R_2^{(1)} = 0$, $h \not\equiv 0 \pmod n$ and $R_1^{(1)} = R_2^{(1)} = n$, $h \equiv 0 \pmod n$. Here the relation $\equiv$ is one of congruence in the sense defined by H.W. 49. We shall always follow a congruence relation with the modulus of that congruence so that there will be no possibility of confusion with the identity relation defined earlier. We shall use $a \not\equiv b \pmod u$ to deny congruence (mod u) between a and b.

If $\widehat{S_1S_1} \equiv \widehat{S_2S_2}$, then, writing $R_2^{(2)} = R_2'^{(2)} \exp 2\pi i h\beta$, we have

$$(R_1^{(2)})^2 \equiv (R_2'^{(2)})^2 \exp 4\pi i h\beta,\ h \not\equiv 0 \pmod n \tag{11}$$

$$(n+R_1^{(2)})^2 = (n+R_2'^{(2)} \exp 2\pi i h\beta)^2,\ h \equiv 0 \pmod n \tag{11′}$$

in which the parameter β is no longer quite arbitrary but fixes the relative origins of $S_1^{(2)}$ and $S_2^{(2)}$. We now choose

$$R_1^{(2)} = R_2'^{(2)} = R,\ h \not\equiv 0 \pmod n \tag{12}$$

so that (10) and (12) together mean†

$$R_1^2 = R_2^2 \exp -\{4\pi i h\beta\},\ h \not\equiv 0 \pmod n\,. \tag{12′}$$

At the same time we have satisfied

$$R_1\bar{R}_1 = R_2\bar{R}_2,\ h \not\equiv 0 \pmod n\,.$$

If

$$R_1\bar{R}_1 = R_2\bar{R}_2,\ h \equiv 0 \pmod n\,,$$

we must have either $h\beta \equiv 0 \pmod 1$, $h \equiv 0 \pmod n$; or $R = 0$, $h \equiv 0 \pmod n$. The first possibility reappears later in a discussion of the second possibility. We therefore choose $R = 0$, $h \equiv 0 \pmod n$ and then (11′) is satisfied also. Furthermore, (11′) is of the form

$$R_1^2 = R_2^2 \exp -\{4\pi i h\beta\},\ h \equiv 0 \pmod n$$

providing

$$2h\beta \equiv 0 \pmod 1,\ h \equiv 0 \pmod n \tag{12″}$$

so that

$$\beta = m/2n:\ m = 0, 1, \ldots, 2n-1\,. \tag{13}$$

We have now satisfied $\widehat{S_1S_1} \equiv \widehat{S_2S_2}$ and $R_1\bar{R}_1 = R_2\bar{R}_2$, all h. If $h\beta \equiv 0 \pmod 1$, $h \equiv 0 \pmod n$ we have $R_1^{(2)} = R_2^{(2)}$ for $h \equiv 0 \pmod n$ whether or not $R = 0$; and $R_1 = (n+R) = R_2 \exp -\{2\pi i h\beta\}$ for $h \equiv 0 \pmod n$. But already $R_1 = R_2 \exp -\{2\pi i h\beta\}$, $h \not\equiv 0 \pmod n$ and therefore, if $h\beta \equiv 0 \pmod 1$, $S_1 \equiv S_2$. If S_1) –(S_2 we must therefore have m in (13) odd; and, since $R_1^{(1)}$ is invariant under multiplication by $\exp 2\pi i h/n$ only the case $m = 1$ is of interest.

† (12′) means that the apparent origin of S_2 is displaced by β (or $\beta + \frac{1}{2}$) relative to the origin of S_1; the chosen origin of S_2 is the same as that of S_1, and (12″) makes the two origins compatible.

We propose now to choose R in the form $R=R^*\exp 2\pi iha$, where a is real and >0. Then, for general a, we cannot have $S_1\sim S_2$ and we have solutions of $\widehat{S_1S_1}\equiv\widehat{S_2S_2}$, S_1)–(S_2, providing only that we can find R^* such that

$$\begin{aligned} R^* &\neq 0, \text{ for some } h\not\equiv 0 \pmod n \\ R^* &= 0,\ h\equiv 0 \pmod n\,. \end{aligned} \tag{14}$$

A solution for R^* obeying (14) for all h except $h\equiv 0 \pmod{ns}$ is

$$R^*=\left(\sum_{t=1}^{s}\omega_t^h\right)\exp 2\pi ihb,\quad 0<b<1,$$

where the ω_t are such that the ω_t^n form a complete set of roots of $x^s=1$. In this case

$$R^*=0,\ \ h\equiv 0 \pmod n$$

but

$$R^*=s,\ \ h\equiv 0 \pmod{ns};$$

and if (11′) is to be satisfied

$$h\beta\equiv 0 \pmod 1,\ \ h\equiv 0 \pmod{ns}$$

or

$$s/2\equiv 0 \pmod 1\,.$$

Thus, s is even, $s=2r$: and the ω_t are of the form

$$\omega_t=\exp 2\pi iq_t/ns=\exp \pi iq_t/nr\,,$$

where

$$q_t\equiv 0,\,1,\,\ldots,\,(s-1) \pmod s$$

and constitute a complete set of residues (mod s).

A solution of $\widehat{S_1S_1}\equiv\widehat{S_2S_2}$, S_1)–(S_2, is therefore

$$\begin{aligned} R_1 &= \sum_{i=1}^{n}\zeta_i^h+\left(\sum_{t=1}^{2r}\omega_t^h\right)\exp 2\pi iha \\ R_2 &= \sum_{i=1}^{n}\zeta_i^h+\left(\sum_{t=1}^{2r}\omega_t^h\right)\exp 2\pi ih(a+1/2n); \end{aligned} \tag{15}$$

where $\zeta_i^n=1$, $\omega_t^{2nr}=1$; S_1 and S_2 contain $n+2r$ points.

We can illustrate Th. 10 by choosing particular examples of (15).

(i) $n=2,\ r=1$: $S_1=0,\ a,\ \tfrac14+a,\ \tfrac12$;
$S_2=0,\ \tfrac14+a,\ \tfrac12,\ \tfrac12+a.$

Since $S_1\sim(0,\ a,\ \tfrac12+a,\ \tfrac34)$, and $S_2\sim(0,\ a,\ \tfrac14,\ \tfrac12+a)$, this pair is the pair Π_4.

(ii) When $n\geq 4$, the q_t can take on at least two distinct sets of values, e.g. $n=5$, $r=1$;

(*a*) $q_t=0,\ 1$

$$\left.\begin{aligned} S_1&=0,\ a,\ 1/10+a,\ 1/5,\ 2/5,\ 3/5,\ 4/5 \\ S_2&=0,\ a,\ 1/5,\ 2/5,\ 3/5,\ 4/5,\ 9/10+a \end{aligned}\right\}=\Pi_7^{(1)}$$

(*b*) $q_t=0,\ 3$

$$\left.\begin{aligned} S_1&=0,\ a,\ 1/5,\ 3/10+a,\ 2/5,\ 3/5,\ 4/5 \\ S_2&=0,\ a,\ 1/5,\ 2/5,\ 3/5,\ 7/10+a,\ 4/5 \end{aligned}\right\}=\Pi_7^{(2)}$$

It is evident that for $q_t=0,\ 5$, $S_1\equiv S_2$; and that $q_t=0,\ n-u$ is identical with $q_t=0,\ u$. When n is even there are $\tfrac12 n$ distinct homometric pairs with $r=1$; when n is odd there are $\tfrac12(n-1)$ homometric pairs with $r=1$.

(iii) $n=3$, $r=2$: one example is
$S_1=0,\ a,\ 1/12+a,\ 1/6+a,\ 1/4+a,\ 1/3,\ 2/3$;
$S_2=0,\ a,\ 1/12+a,\ 1/3,\ 2/3,\ 5/6+a,\ 11/12+a$.

But (15) is not the only solution illustrating Th. 10. The only restriction on R^* was

$$R^*=0,\ h\equiv 0 \pmod n\,,$$

and

$$R^*=\sum_s R_s^*=\sum_s\left(\sum_{t=1}^{s}\omega_{t,s}^h\right)\exp 2\pi ihb_s$$

is a possible solution providing the $(\omega_{t,s})^n$ are the s distinct s *th*-roots of unity. The simplest case is $s=2r$ for each kind s specified by b_s: an example is

(iv) $n=3,\ r=1$; $b_1=0,\ b_2=b-a$;
$0<a<1/6,\ \ 1/3<b<1/2$
$S_1=0,\ a,\ 1/6+a,\ 1/3,\ b,\ 1/6+b,\ 2/3$;
$S_2=0,\ a,\ b-1/6,\ 1/3,\ b,\ 2/3,\ 5/6+a$;

but there can be as many parameters b_s as we wish. The condition on R^* can also be satisfied by choosing different weights z_s for the members of different subsets specified by s: z_s must be the same for all members of the same subset s; z_s may be irrational.

We may also have $s=2r_s$ for each subset s, where the r_s are distinct. An example is

(v) $n=3,\ r_1=1,\ r_2=2$; $b_1=0,\ b_2=b-a$;
$0<a<1/6,\ 1/3<b<5/12$
$S_1=0,\ a,\ 1/6+a,\ 1/3,\ b,\ 1/12+b,\ 1/6+b,$
$1/4+b,\ 2/3$;
$S_2=0,\ a,\ b-1/6,\ b-1/12,\ 1/3,\ b,\ 1/12+b,$
$2/3,\ 5/6+a$.

The families of h.s. obeying S_1)–(S_2, $\widehat{S_1S_1}\equiv\widehat{S_2S_2}$, are in many respects the simplest possible h.s. Patterson (1944) gave the simple generalization of Π_4.

$$\Pi_{n+2}^{(1)}=\begin{cases} S_1=0,\ a,\ 1/2n+a,\ 1/n,\ 2/n,\ \ldots,\ (n-1)/n; \\ S_2=0,\ a,\ 1/n,\ 2/n,\ \ldots,\ \ldots,\ (n-1)/n, \\ (2n-1)/2n+a\,. \end{cases}$$

In example (ii) and Th. 10 we demonstrated the existence of closely related pairs

$$\Pi_{n+2}^{(i)},\ i=1,\,2,\,\ldots,\,\tfrac12 n^*,$$

where $n^*=n$ for n even and $n^*=n-1$ for n odd. We shall show also in a later paper that Π_4 is itself the only pair of h.s. of four points containing a variable parameter. It will become clear too that the $\Pi_{n+2}^{(i)}$ are, to some extent, unusual in that they exist for all $N=(n+2)$. In a later paper we shall show that the

$\Pi^{(i)}_{n;2}$ have an invariance property which takes a simpler form than that associated with any other families of h.s. we have so far discovered. It would be interesting to know if any solutions of $\widehat{S_1S_1} \equiv \widehat{S_2S_2}$, S_1) (S_2, exist which are not trivial generalizations of (15).

Some homometric multiplets

Whilst the condition $\widehat{S_1S_1} \equiv \widehat{S_2S_2}$ on the relation of S_1) (S_2 has proved useful in demonstrating the structure of certain simple h.s., it is a restrictive condition. If the condition is removed we can demonstrate the existence of homometric r-tuplets related to (15) and which seem to be the simplest possible homometric r-tuplets.

THEOREM 11: There exist at least $\frac{1}{2}n^*$ sets of homometric r-tuplets of $n+r$ points of equal weight.

As in Th. 10 we choose $R_1 = R_1^{(1)} + R_1^{(2)}$: $R_2 = R_2^{(1)} + R_2^{(2)}$: with $R_1^{(1)}$ and $R_2^{(1)}$ given by (10), and $R_1^{(2)} \neq R_2^{(2)}$ for some h. If

$$R_1^{(2)} = R: \; R_2^{(2)} = R \exp 2\pi i h\beta; \; h \not\equiv 0 \pmod n$$

then

$$R_1\bar{R}_1 = R_2\bar{R}_2, \; h \not\equiv 0 \pmod n .$$

And if

$$R_1\bar{R}_1 = R_2\bar{R}_2, \; h \equiv 0 \pmod n ,$$

a possible solution is $R=0$, $h \equiv 0 \pmod n$,

If we choose $R = R^* \exp 2\pi i h a$ with

$$R^* = \left(\sum_{t=1}^{r} \omega_t^h\right) \exp 2\pi i h b, \; 0 < b < 1:$$

where the ω_t^n form a complete set of roots of $x^s = 1$, then

$$R^* = 0, \; h \equiv 0 \pmod n; \; R^* = r, \; h \equiv 0 \pmod{nr} .$$

The condition on β is now only that

$$h\beta \equiv 0 \pmod 1, \; h \equiv 0 \pmod{nr}$$

so that

$$\beta = m/nr; \; m = 0, 1, \ldots, nr-1 .$$

Since $R_1^{(1)} = R_2^{(1)}$ is invariant under multiplication by $\exp 2\pi i h/n$, only $r-1$ of these values of m, for which $m = 1, 2, \ldots, r-1$, are distinct.

The expression for the ω_t, namely

$$\omega_t = \exp 2\pi i q_t/nr ,$$

applies, with $q_t \equiv 0, 1, \ldots, (r-1) \pmod r$, a complete set of residues (mod r).

The solution analogous to (15) is

$$R_1 = \sum_{i=1}^{n} \zeta_i^h + \left(\sum_{t=1}^{r} \omega_t^h\right) \exp 2\pi i h a$$

$$R_2 = \sum_{i=1}^{n} \zeta_i^h + \left(\sum_{t=1}^{r} \omega_t^h\right) \exp 2\pi i h (a + m/nr)$$

in which m can adopt the values $1, 2, \ldots, r-1$. The set of sets for which $m = 0, 1, 2, \ldots, (r-1)$ constitute a homometric r-tuplet of $n+r$ points. The statement in Th. 11 that there are at least $\frac{1}{2}n^*$ homometric r-tuplets is best left to the examples below.

(vi) $n=2$, $r=3$:

$S_1 = 0, a, 1/6+a, 1/3+a, 1/2$;
$S_2 = 0, a, 1/6+a, 1/2, 5/6+a$;
$S_3 = 0, a, 1/2, 2/3+a, 5/6+a$.

We shall show in a later paper that this is the only homometric triplet of five equal points: and that there are no homometric r-tuplets for $r>2$ for sets of four equal points or r-tuplets for $r>3$ for five equal points. Indeed we shall show that there are no homometric r-tuplets of N equal points for $N < r+2$.

(vii) $n=3$, $r=3$:

$S_1 = 0, a, 1/9+a, 2/9+a, 1/3, 2/3$;
$S_2 = 0, a, 1/9+a, 1/3, 2/3, 8/9+a$;
$S_3 = 0, a, 1/3, 2/3, 7/9+a, 8/9+a$;

or

$S_1 = 0, a, 1/9+a, 1/3, 5/9+a, 2/3$;
$S_2 = 0, a, 1/3, 4/9+a, 2/3, 8/9+a$;
$S_3 = 0, 1/3, 1/3+a, 2/3, 7/9+a, 8/9+a$;

or

$S_1 = 0, a, 2/9+a, 1/3, 4/9+a, 2/3$;
$S_2 = 0, 1/9+a, 1/3, 1/3+a, 2/3, 8/9+a$;
$S_3 = 0, a, 2/9+a, 1/3, 2/3, 7/9+a$.

(viii) $n=3$, $r=4$:

We give one member of each of six distinct homometric quadruplets. The other members of one quadruplet are obtained by shifting $S_2^{(2)}$ by $1/nr = 1/12$ relative to $S_1^{(2)}$

$S_1 = 0, a, 1/12+a, 1/6+a, 1/4+a, 1/3, 2/3$;
or $S_1 = 0, a, 1/12+a, 1/6+a, 1/3, 7/12+a, 2/3$;
or $S_1 = 0, a, 1/12+a, 1/4+a, 1/3, 1/2+a, 2/3$;
or $S_1 = 0, a, 1/12+a, 1/4+a, 1/3, 2/3, 5/6+a$;
or $S_1 = 0, a, 1/6+a, 1/4+a, 1/3, 2/3, 3/4+a$;
or $S_1 = 0, a, 1/6+a, 1/3, 5/12+a, 7/12+a, 2/3$.

There is also a degenerate quadruplet which reduces to the pair

$S_1 = 0, a, 1/12+a, 1/3, 1/2+a, 7/12+a, 2/3$;
$S_2 = 0, a, 1/3, 5/12+a, 1/2+a, 2/3, 11/12+a$.

It is evident that for general a there are at least $\frac{1}{2}n^*$ multiplets. For large n, homometric multiplets can become very abundant. Indeed, much of the difficulty of the theory of h.s. resides in the enormous abundance of h.s. for $N >$ about 6. Theorems 3, 4, 6, 7, 8 and 9 together are a prolific source of h.s. That they are insufficient in themselves to generate all possible h.s. from a few subsets of very few points rests on the following theorem:

Theorem 12: If $S \equiv \widehat{S_1 S_2}$ is a set of N points for which $(z_0, z_1, \ldots, z_{N-1}) = 1$ then, if the $z_j^{(1)}$ are the weights of N_1 points in S_1 and the $z_k^{(2)}$ are the weights of N_2 points in S_2,

$$\sum_{i=0}^{N-1} z_i \text{ is a factor of } \left(\sum_{j=0}^{N_1-1} z_j^{(1)}\right) \times \left(\sum_{k=0}^{N_2-1} z_k^{(2)}\right) .$$

For

$$w \times \sum_{i=0}^{N-1} z_i = \left(\sum_{j=0}^{N_1-1} z_j^{(1)}\right) \times \left(\sum_{k=0}^{N_2-1} z_k^{(2)}\right) ,$$

where w is a positive integer; and we assume without loss of generality that both

$$(z_0^{(1)}, z_1^{(1)}, \ldots, z_{N_1-1}^{(1)}) = 1$$
$$(z_0^{(2)}, z_1^{(2)}, \ldots, z_{N_2-1}^{(2)}) = 1 .$$

From Th. 12 it follows that if

$$\sum_{i=0}^{N-1} z_i \text{ is a prime, } p, \text{ then } \sum_{i=0}^{N_1-1} z_i^{(1)}$$

at least has a factor p.

We may think of h.s. as having factor sets (in general) from which they can be generated by Ths. 3, 4, 6, 7, 8 and 9. We have not shown of course that these theorems are the sole source of h.s. from subsets. However, if $S \,)\text{-}(\, S'$ and S and S' contain a common 'factor', $S \equiv \widehat{S_1 S_3} \,)\text{-}(\, \widehat{S_1 S_4} \equiv S'$ and

$$\widehat{S_1 \bar{S}_1} \widehat{S_3 \bar{S}_3} \equiv \widehat{S_1 \bar{S}_1} \widehat{S_4 \bar{S}_4} \rightarrow S_3 \,)\text{-}(\, S_4 \text{ or } S_3 \sim S_4$$

(since $S_3 \not\equiv S_4$) providing $R_1 \neq 0$. But if $\widehat{S_1 S_2} \,)\text{-}(\, \widehat{S_3 S_4}$ we cannot at the moment say anything about the relationship between S_1, S_2, S_3 and S_4.

We may think of h.s. with no factor sets as 'prime sets' but there is no guarantee that the decomposition of h.s. into prime subsets is unique*: we already have many cases for which $\widehat{S_1 S_2} \equiv \widehat{S_3 S_4}$. According to Th. 3 not all factor sets are h.s. and not all 'prime' sets will be h.s. According to Th. 12 there is at least one 'prime' set associated with each prime p but there are almost certainly more 'prime' sets than primes p for there is certainly more than one h.s. for which $\Sigma z_i = p$ for all $p > 3$.

One might ask for all prime sets sufficient to generate all h.s. with $\sum_{i=0}^{N-1} z_i \leq Z$. If in such prime sets $\sum_{j=0}^{N_1-1} z_j = Z_1$ it is then reasonable to demand $Z_1 \leq Z$ for otherwise it would be necessary to explore a much larger range of h.s. in order to find a smaller one. Even when Z is not a prime not all h.s. with $\sum_{i=0}^{N-1} z_i = Z$ can be obtained from prime sets with $Z_1 < Z$, for consider $N = 4$ and $z_i = 1$ for $i = 0, \ldots, 3$. According to Th. 12 either $Z_1 = 4w$ or $Z_1 = 2w'$ and $Z_2 = 2w''$. If now $Z_1, Z_2 < 4$ both w' and w'' are unity, but we show later that neither of the two pairs of h.s. for which $N = 4$ and $Z = 4$ can be generated from two subsets of two points of equal weight. Accordingly the h.s. with $N = 4$, $Z = 4$ can be generated only by subsets for which $Z_1 \geq 4$: it seems probable that the h.s. with $N = 4$, $Z = 4$ are in fact prime sets.

Whilst Ths. 3–9 are a prolific source of h.s. they are in some respects too powerful: it is not obvious, despite possible arguments like those of Ths. 10 and 11, which sets to choose for S_1, S_2, S_3 or S_4 in order to obtain h.s. with previously specified characteristics as to number of points, relative weights of points, etc. Nor do these theorems give any indication whether they have generated all possible h.s. with given characteristics. Thus it seems proper to adopt for later work a point of view rather different from that of the present paper.

* The failure of the so called 'Fundamental Theorem' is common to a large number of number 'fields' in Number Theory (H.W. 211).

Summary

The theorems of this paper are not really suitable for summary; but as the symbolism of the paper may appear a little formidable at first sight it seems worthwhile to state in simple terms and very roughly both the contents of the paper and the ideas behind it.

Hosemann & Bagchi (1954) have already shown that two homometric sets of points can be built up from two pairs of subsets in which one set is common to each pair and one set of one pair is the enantiomorph of another in the other. However, sets so built from subsets are not always homometric: they may be enantiomorphic or even identical. Conditions on the subsets are given such that all pairs of sets generated from the subsets by Hosemann's & Bagchi's method are genuinely homometric, and generalizations of their theorem are given which enable homometric sets to be generated from subsets which are themselves homometric rather than identical or enantiomorphic.

In order to determine *all* homometric sets of given numbers of points of specificied weights (or simply of given numbers of points) it is necessary to define what constitutes a *single distinguishable* homometric pair. Patterson (1944) has already shown that pairs of sets can be homometric over a continuous range of values of certain co-ordinate parameters, and it seems reasonable to call all pairs differing only in the choice of the values of these parameters the same homometric pair. It is shown also (Lemma 1) that if two sets are homometric they remain homometric after being subjected to the same non-singular affine deformation; and we therefore call all pairs related by non-singular affine deformations the same homometric pair. From the last it is necessary to abstract two sets which are homometric to each other but can be obtained from each other by a non-singular affine deformation: it is clearly necessary to treat sets so related as distinct h.s.

The first part of this paper is therefore concerned with the definition of a homometric set (h.s). The second is concerned with the proof of theorems analogous to that of Hosemann & Bagchi (1954). Just as in Hosemann's & Bagchi's original formulation of their theorem it is difficult to eliminate the possibility of generating the same set or its enantiomorph from different pairs of subsets. It is shown, however, that if the eight possible h.s. which can be generated from two pairs of subsets and their enantiomorphs do not contain a homometric triplet certain very restrictive conditions must exist on the subsets. An investigation of one of these restrictive conditions leads to the discovery of some interesting generalizations of the family of h.s. given for a general number of points by Patterson (1944). These generalizations of Patterson's pair of sets are extended further and include families of multiplets providing the sets contain five or more points. It is difficult to avoid the conclusion that h.s. are very abundant when the number of points in the sets is large and it is surprising that so few have been reported in practice.

As an indication for further work it is pointed out (Theorem 12) that not all h.s. of a large number of points can be generated from subsets containing a smaller total weight of points. Such sets may be thought of as having no factor sets and are analogous to prime numbers in Number Theory. It is a major task in the theory of h.s. to calculate these 'prime' sets: but unfortunately this task is likely to prove as difficult as a central problem of Number Theory—the calculation of prime numbers.

The literature on h.s. is still small, and at the suggestion of the referee I add a comment on several other papers devoted to h.s. The results obtained by Patterson (1944) largely supersede Patterson (1939*a*, *b*). Patterson (1944) laid the foundations of a method of direct attack on the determination of h.s. for given N which has been extended by Garrido (1951). Since this method is the one we adopt in later papers of this series, comment on Garrido's paper (G) can more properly be made in them. However, we may remark that G's 'necessary and sufficient conditions' are by no means rigorously necessary. It is not necessary that two sets be isovectorial in G's sense for them to be homometric†: they may also have identical co-ordinates as Hosemann & Bagchi (1954) Fig. 8 show.

The existence of isovectorial companions of any particular point set is always accompanied by the failure of standard methods (e.g. Clastre & Gay, 1950*a*, *b*) for solving the Patterson function as Garrido (1951) shows. This is one reason why isovectorial sets are not a serious problem to crystallographers when N is small. One may also remark that sets of the type of HB's Fig. 8 can be eliminated when the weights of the points are *a priori* known. But h.s. with even the same co-ordinates *and the same weights* exist; e.g. consider

$$\left.\begin{aligned} S_1 &= (0,\ 1/6,\ 1/3,\ 1/2,\ 2/3,\ 5/6;\ \ 8,\ 6,\ 4,\ 2,\ 7,\ 9) \\ S_2 &= (0,\ 1/6,\ 1/3,\ 1/2,\ 2/3,\ 5/6;\ \ 8,\ 4,\ 2,\ 6,\ 7,\ 9) \end{aligned}\right\}. \qquad (16)$$

The sets of (16) have very special co-ordinates and it is certain that rearrangement of the z's become more difficult for more general sets of co-ordinates. Nevertheless, there remains the possibility that particular but not so obviously specialized sets of co-ordinates exist which permit rearrangement of the z's. It is certainly true that the condition $S_1 \,)\!-\!(\, S_2$ always restricts S_1 and S_2; but in the author's opinion our knowledge of this restriction is at present insufficient for us to conclude with Garrido that the existence of h.s. necessarily 'exige des conditions très speciales qui seront remplies seulement dans des cas particuliers'.

Earlier work on h.s. (Menzer, 1928; Pauling & Shappell, 1930; Patterson, 1939*a*) suggested that h.s. are necessarily confined to special positions in highly symmetrical sets, and later work (Patterson, 1944) still left the suspicion that specific readily identifiable positions were necessary (e.g. 3/4, 1/4, 1/5 or 1/2—or $1/N$—in one dimension). But even this last condition is unnecessary: consider the 7 point periodic h.s. of equal weight

$$\begin{aligned} S_1 = {} & 0,\ a,\ 5a+4d,\ 1/4+5a+5d,\ 1/4+6a+5d, \\ & 1/2+6a+6d,\ 3/4+3a+3d; \end{aligned}$$

$$\begin{aligned} S_2 = {} & 0,\ a,\ 1/4+a+d,\ 1/4+2a+d,\ 1/4+6a+5d, \\ & 1/2+6a+6d,\ 3/4+3a+3d; \end{aligned}$$

and try (say) $a=\sqrt{2}/100$, $d=\sqrt{3}/100$.

For these reasons an attack on h.s. by consideration of special points and symmetries (Patterson, 1939*a*: Menzer, 1949), of great interest in itself, is likely to be too restricted. Symmetry is a restrictive condition on h.s.; e.g. the sets Π_4 of (8) are h.s. in $\mathfrak{p}m$ if, and only if, $a=1/8$; and we show later that these h.s. are the only h.s. of 4 points of equal weight in $\mathfrak{p}m$. If S is a h.s. with $N=PQ$, the condition that S contains P sets of Q *equivalent* points introduces at most $P(Q-1)$ relations between each of the N weights and $N-1$ co-ordinates. But sets with different symmetries can be homometric (Garrido, 1951; Hosemann & Bagchi, 1954) and it is probable that the requirement of P sets of Q equivalent points reduces the total number of parameters by less than $2P(Q-1)$.†

There can certainly be more h.s. with P sets of $Q(>1)$ equivalent points than with P points, for e.g. there are no h.s. of 2 points in $\mathfrak{p}1$ but there is one in

† i.e. the 'non-existence de structures isovectorielles' is not *sufficient* for the non-existence of h.s.

† The evidence is still inadequate. We suggest later that h.s. with no symmetry contain at most $N-3$ co-ordinate parameters and (when $N>5$) $N-2$ weight parameters: in T_h^7 one and only one pair of h.s. (and these with only one co-ordinate parameter) exists for $N=24$. The set Π_4 in $\mathfrak{p}1$ has one co-ordinate parameter and in general three weight parameters: in $\mathfrak{p}m$ with $a=\frac{1}{8}$ there are no co-ordinate and two weight parameters.

pm with 2 sets of 2 equivalent points. Thus when P is the number of sets of equivalent points, increasing P to $P+1$ probably increases the number of h.s. more rapidly than does the increase of N to $N+1$ in sets of no symmetry; and it is even possible that the number of h.s. for given N is asymptotically independent of symmetry.

Nevertheless, high symmetry imposes a severe restriction on h.s. with small P as the existence of apparently only one pair of h.s. for $N=24$ in T_h^7-Ia3 shows (Pauling & Shappell, 1930; Menzer, 1949; Garrido, 1951): as a second example we may add here that there are *no* h.s. for $N=8$ in $P2_1/c$ (Bullough, 1957). The fact that h.s. were first discovered in highly symmetrical sets is evidence not that h.s. are associated with high symmetry but that h.s. become abundant when N is large.

Menzer's (1949) conclusion that the introduction of atoms of different weight in systems of high symmetry reduces the number of h.s. below the number for one set of equivalent points is misleading for it relies on the ability to distinguish between peak shapes as well as peak weights. In general the condition $z_i^{(1)}=z_i^{(2)}=z$ for all $i=1, \ldots, N$ members of two *point* sets restricts h.s., and homometric pairs with this property are a subclass of the more general class of homometric pairs without it.

From the evidence at present available the author cannot agree with Menzer (1949) and Garrido (1951) that h.s. are necessarily rare although homometric alternatives are fairly easy to detect when N is small. It is by no means obvious that this will continue to be so when $N \simeq 30$ (say): the number of h.s. is probably much smaller than the number of possible sets; but it offers small consolation to crystallographers that the number of h.s. is probably 'enumerable' (in the technical sense, i.e. it has the cardinal number of the integers; because h.s. exist for a continuous range of coordinate parameters, the number of *these* sets is not enumerable) whilst the number of possible sets has the number of the continuum. If vector point sets are given with a small error in the vector co-ordinates it seems probable that for large enough N there will always exist a pair of h.s. with a vector set within the error of that of the given set. For this reason a real upper limit probably exists on the usefulness of the Patterson function (or of X-ray data unsupported by other evidence)—although this limit is probably beyond the point where overlap of finite peak widths already restricts the use of that function. In this series of papers we investigate h.s. as a problem of interest in its own right; but a reliable estimate of the importance of h.s. to crystallographers can only be obtained from greater knowledge of the properties of h.s.

I am indebted to the University of Leeds for a Fellowship during the tenure of which the bulk of this work was done. I am also indebted to the British Rayon Research Association for facilities to complete this paper.

References

BIRKHOFF, G. & MACLANE, S. (1953). *A Survey of Modern Algebra*. Revised ed., p. 253. New York: MacMillan.
BULLOUGH, R. K. (1957). Thesis. University of Leeds.
CLASTRE, J. & GAY, R. (1950*a*). *C. R. Acad. Sci., Paris*, **230**, 1976.
CLASTRE, J. & GAY, R. (1950*b*). *J. Phys. Radium*, **11**, 75.
GARRIDO, J. (1951). *Bull. Soc. Franç. Min. Crist.* **74**, 397.
HARDY, G. H. & WRIGHT, E. M. (1954). *An Introduction to the Theory of Numbers*, 3rd ed. Oxford: Clarendon Press.
HOSEMANN, R. & BAGCHI, S. N. (1954). *Acta Cryst.* **7**. 237.
MENZER, G. (1928). *Z. Kristallogr.* **69**, 312.
MENZER, G. (1949). *Z. Naturforsch.* **4a**, 11.
PATTERSON, A. L. (1939*a*). *Nature, Lond.* **143**, 939.
PATTERSON, A. L. (1939*b*). *Phys. Rev.* **55**, 682.
PATTERSON, A. L. (1944). *Phys. Rev.* **65**, 195.
PAULING, L. & SHAPPELL, M. D. (1930). *Z. Kristallogr.* **75**, 128.