match no.7 pp. 341 - 348 1979

BILATERAL CLASSES: A NEW CLASS CONCEPT OF GROUP THEORY

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Abstract

Bilateral classes constitute a new class concept of elementary group theory which includes the familiar notions of right and left cosets, double cosets and conjugacy classes as special cases. But moreover it provides a variety of other classification schemes which may be useful e.g. in the field of "constructive combinatorics", i.e. in identification and generation of discrete structures.

As an introduction, let us recall the mentioned group theoretical class concepts. For this purpose, let G be a group, A and B subgroups of G, and let g,a,b denote elements of G, A and B respectively. Then our objects are

1.	$Ag = \{ ag \mid a \in A \}$	right cosets
2.	$gB = \{ gb \mid b \in B \}$	left cosets
3.	$AgB = \{ agb \mid a \in A,\ b \in B \}$	double cosets
4	$C_A(g) = \{ aga^{-1} \mid a \in A \}$	conjugacy classes

Usually, the term conjugacy class refers to the case of A=G, but we may as well restrict the conjugating elements to any subgroup of G in order to obtain a classification by conjugation. The partitionings of the group G into the equivalence classes given above are due to the equivalence relations

1. $g' \sim g \iff \exists\, a \in A \quad : \quad g' = ag$

2. $g' \sim g \iff \exists\, b \in B \quad : \quad g' = gb$

3. $g' \sim g \iff \exists\, a \in A, b \in B \quad : \quad g' = agb$

4. $g' \sim g \iff \exists\, a \in A \quad : \quad g' = aga^{-1}$

In order to define the generalization to bilateral classes, let us introduce the external direct product $G \times G$ of G by itself, i.e. the cartesian product

$$G \times G = \left\{ (g,g') \mid g \in G,\ g' \in G \right\}$$

with group multiplication given by

$$(g_1, g_1')\,(g_2, g_2') = (g_1 g_2,\ g_1' g_2')$$

Now let P be any subgroup of $G \times G$. Then the relation

$$g' \sim g \iff \exists (a,b) \in P \quad : \quad g' = agb^{-1}$$

is an equivalence relation on G. Correspondingly G decomposes into equivalence classes

$$P(g) = \left\{ agb^{-1} \mid (a,b) \in P \right\}$$

which are called <u>bilateral</u> classes (with respect to P) [1].

By appropiate choices of P, the well-known classification schemes are immediately recovered.

1. $P = A \times E \quad : \quad P(g) = Ag$
2. $P = E \times B \quad : \quad P(g) = gB$
3. $P = A \times B \quad : \quad P(g) = AgB$
4. $P = (A \times A)_d \quad : \quad P(g) = C_A(g)$

In this table, E denotes the identity subgroup of G, and $(A \times A)_d$, the diagonal subgroup of A x A is given by the set of "diagonal elements" of A x A.

$$(A \times A)_d = \left\{ (a,a) \mid a \in A \right\}$$

Bilateral classes would lack practical implications if they only covered the known class concepts. They do, however, include a variety of new classification schemes. A survey of these is procided by a characterization of all subgroups of a direct product group G x G, as given by Goursat [2] in 1889.

Let A and B be subgroups of G, $\hat{A}$ and $\hat{B}$ normal subgroups of A and B respectively, such that the factor groups $A/\hat{A}$ and $B/\hat{B}$ are isomorphic. Given any isomorphism $\phi : A/\hat{A} \to B/\hat{B}$, we perform the coset decompositions

$$A = \dot{\bigcup_{i=1}^{p}} \hat{A} a_i \quad , \quad B = \dot{\bigcup_{i=1}^{p}} \hat{B} b_i$$

and we label the cosets according to the isomorphism ϕ , i.e. $\phi(\hat{A}a_i) = \hat{B}b_i$ for all $i = 1,2,\ldots p$

Then the union of cartesian products of matching cosets

$$P = \dot{\bigcup_{i=1}^{p}} \hat{A}a_i \times \hat{B}b_i$$

is a subgroup of G x G. In reverse, any subgroup of G x G is obtained by appropiate choice of A, $\hat{A}$, B, $\hat{B}$ and ϕ.

Correspondingly, bilateral classes have the structure

$$P(g) = \bigcup_{i=1}^{p} \hat{A}a_i g b_i^{-1} \hat{B}$$

i.e. they are unions (not necessarily disjoint, in contrast with the structure of P) of double cosets with respect to the normal subgroups $\hat{A}$ and $\hat{B}$.

Closed formulas for the order of bilateral classes and their number in a given decompostion of G are available. We only mention one which is quite convenient for the practical use. Let z denote the number of bilateral classes in the decompostion

$$G = \dot{\bigcup}_{j=1}^{z} P(g_j)$$

Then z is given by

$$z = \frac{|G|}{p\,|A|\,|B|} \sum_{\varrho} \sum_{i=1}^{p} \frac{|C_\varrho \cap \hat{A}a_i|\ |C_\varrho \cap \hat{B}b_i|}{|C_\varrho|}$$

In this formula, the first sum runs over all (ordinary) conjugacy classes of G, and the vertical bars denote the order of the set included. In the case of $G = S_n$, a symmetric group, membership of a permutation in one of the conjugacy classes can be read of its cycle structure. Therefore, the orders of the intersections $C_\varrho \cap \hat{A}a_i$, $C_\varrho \cap \hat{B}b_i$ can be determined by inspection if the cyclic notation is employed.

Bilateral classes occur in a natural fashion as "symmetry types" of bijective maps between finite sets. Let us consider 1-1-functions with domain D and range R, both of order n, and denote by S_D, S_R the symmetric groups of D and R, respectively. Then any subgroup P of $S_R \times S_D$ induces an equivalence relation on the set of all bijections from D to R:

$$\psi \sim \varphi \Leftrightarrow \exists (S_R, S_D) \ : \ \psi = S_R \varphi S_D^{-1}$$

More explicitely, this means

$$\psi(d) = S_R(\varphi(S_D^{-1}(d))) \qquad \text{for all } d \in D$$

Labelling the elements of D and those of R from 1 to n, we may identify the bijections φ, ψ as well as the permutations

S_R, S_D with permutations of the numbers 1 to n. Then equivalence classes of bijections under P are given by bilateral classes of the symmetric group S_n

$$P(\varphi) = \left\{ S_R \varphi S_D^{-1} \mid (S_R, S_D) \in P \right.$$

There is a natural interprtation for this scheme: the classification of bijections under symmetries of domain and range. Recalling the formulae

$$A = \dot{\bigcup_{i=1}^{p}} \hat{A}\, a_i \qquad B = \dot{\bigcup_{i=1}^{p}} \hat{B} b_i \quad ; \quad P = \dot{\bigcup_{i=1}^{p}} \hat{A}a_i \times \hat{B}b_i \ , \quad P(g) = \dot{\bigcup_{i=1}^{p}} \hat{A}a_i g b_i^{-1} \hat{B}$$

we consider A and B to represent symmetries of the range R and of the domain D, respectively. These symmetries are coupled into the group P, the group of generators of equivalent bijections There are in fact quite different types of such coupling of symmetries , depending on the choice of $\hat{A}$ and $\hat{B}$. Let us first consider the two extremal cases

(i) $\hat{A} = A$, $\hat{B} = B$

$$P = A \times B \quad ; \quad P(g) = AgB$$

(ii) $\hat{A} = \hat{B} = E$

$$P = \left\{ (a_i, b_i) \mid i=1, p \right\}, \quad P(g) = \left\{ a_i g b_i^{-1} \mid i=1,\ldots p \right\}$$

On comparison we recognize that in case (i) the symmetries of domain and range are completely independent in the sense that any two symmetry operations $a \in A$, $b \in B$ combine into a generator $(a,b) \in P$ of equivalent bijections. In case (ii), on the other hand, there is complete correlation between both these symmetries, i.e. any symmetry element of the range will generate equivalent bijections if and only if it is coupled to a unique symmetry element of the domain and vice versa. The group theoretical class concepts corresponding to the case of completely independent symmetries are the familiar double cosets or simple cosets, while comlete correlation leads to conjugacy classes or classes of similiar structure.

The general case is the one of various degrees of p a r t i al c o r r e l a t i o n , where the normal subgroups $\hat{A}$ and $\hat{B}$ represent the independent subsymmetries of range and domain, while the correlation is due to the pairing of cosets by the isomorphism of the factor groups $A/\hat{A}$ and $B/\hat{B}$.

A nontrivial example of bilateral classes occurs in the permutation group description of permutational isomers [3, 4] . For this purpose let us take

D = an assortment of $n = n_1+n_2+ \ldots +n_l$ ligands, n_1 of a first type, n_2 of a second one,..., and finally n_l of an l'th type

R = the set of n sites of a (spatially fixed) molecular skeleton

and consider for the symmetries of domain and range,

S_λ = $S_{n_1} \times S_{n_2} \times \ldots \times S_{n_l}$, the direct product of the symmetric groups of the subsets of ligands of the same type

G_P = the proper rotational symmetry group of the skeleton, as represented by permutations of the sites.

With the choice of $P = G_P \times S_\lambda$, i.e. of proper rotations from the skeleton symmetry group and permutations of identical ligands independently generating equivalent bijections, the double cosets $G_P \varphi S$ represent permutational isomers. This is quite evident if we visualize the bijections from D to R as distributions of the sets of ligands among the sites of the skeleton. Two such distributions represent the same permutational isomer if and only if they are mutually interconvertible by a proper rotation from the skeleton symmetry group and/or by a permutation of identical ligands.

Now let us assume an achiral skeleton and collet into the same class not only distributions belonging to the same permutational isomer but enantiomers as well. Then we have to consider different cases:

(i) <u>All ligands are achiral.</u>

This case strictly parallels the former one. Skeleton symmetry operations, proper as well as improper ones, and permutations of ligands of the same type still independently generate equivalent distributions. All we have to do is to pass over from G_p (p for proper) to G_i (i for improper), the permutation representation of the full skeleton symmetry group.

$$P = G_i \times S_\lambda \quad , \quad P(\varphi) = G_i \varphi S_\lambda$$

Since G_i can be split up according to $G_i = G_p \cup G_p\sigma$ into G_p and the coset $G_p\sigma$ of improper rotations, there is a corresponding decomposition

$$G_i \varphi S_\lambda = G_p \varphi S_\lambda \cup G_p \sigma S_\lambda$$

where these two double cosets represent enantiomers if they are disjoint, and an achiral isomer if they coincide.

(ii) <u>There are chiral ligands but the ligand assortment is racemic.</u>

An improper symmetry operation, besides permuting the ligands among the sites, effects an overall inversion of all chiral ligands. Therefore, the ligand assortment is changed - unless it is racemic -, and enantiomers are no longer permutational isomers. This case can be dealt with by a slightly generalized group theoretical formalism, but it is hardly worthwhile doing since there can be no achiral isomers unless the ligand assortment is racemic.

Now the symmetry of D is chosen to include the overall inversion of all chiral ligands, i.e. we pass from S_λ to $S_\lambda^* = S_\lambda \cup S_\lambda\tau$, where τ is a product of transpositions of enantiomeric ligands. Equivalent distributions are generated by proper rotations and permutations of identical ligands, while improper ones require the overall inversion, i.e. we have a partial coupling of the symmetries of domain and range according to

$$P = G_p \times S_\lambda \cup G_p\sigma \times S_\lambda\tau$$

Correspondingly, enantiomeric pairs and achiral isomers, respectively are represented by bilateral classes

$$P(\varphi) = G_p \varphi S_\lambda \cup G_p\sigma \varphi\tau S_\lambda$$

depending on whether both these double cosets are disjoint or coincident.

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