Jordan schemes: relaxing associativity, keeping symmetry

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Association schemes

Association schemes were invented by Bose and his school as carriers of partially balanced incomplete-block designs, in cases where balanced designs are not available. They can be defined in several ways: I use the matrix definition.

An association scheme is defined by a set $\{A_0, A_1, \ldots, A_r\}$ of zero-one matrices of order n satisfying

- the sum of the matrices is the all-1 matrix J;
- $A_0 = I$, the identity matrix;
- each A_i is symmetric;
- $A_iA_j = \sum_{k=0}^{r} p_{ij}^k A_k$ for all i, j; that is, the linear span of the matrices is closed under multiplication.

The matrices are called the basis matrices of the scheme.

Note that another way of thinking of an association scheme is as a partition of the set of unordered pairs from $N = \{1, \ldots, n\}$. We say that i and j are p-th associates if $(A_p)_{ij} = 1$. (This holds for a unique p.)

Partially balanced designs

An incomplete block design is said to be partially balanced with respect to the association scheme $\mathcal{A}$ if the concurrence of two points i and j (the number of blocks containing both) depends only on the value of p for which i and j are p-th associates.

Since the concurrence of i and j is symmetric, it is natural to use symmetric matrices in this context.

In the days before computers, partially balanced designs gave rise to information matrices which were easier to invert: one need deal with matrices of order $r+1$ rather than n.

This is because we can work within the Bose–Mesner algebra of the scheme, the commutative associative algebra generated by $\{A_0, \ldots, A_r\}$, which is isomorphic to the algebra of (smaller) matrices generated by $\{P_0, \ldots, P_r\}$ (where $(P_j)_{ik} = p_{ij}^k$).

Meet and join

The set of all partitions of a given set Ω is a partially ordered set. (The partition P is below the partition Q if each part of P is contained in a part of Q.)

This partially ordered set is actually a lattice: it has operations of meet (greatest lower bound) and join (least upper bound).

The meet $P \wedge Q$ of partitions P and Q is the partition whose parts are all non-empty intersections of a part of P with a part of Q.

The join is a little more complicated. The part of $P \vee Q$ containing x consists of all points that can be reached from x by moving within a part of P, then within a part of Q, then within a part of P, and so on.

For example, if $P = \{\{1,2,3\},\{4,5\},\{6,7\}\}$, and $Q = \{\{1,4\},\{2,3\},\{5\},\{6\},\{7\}\}$, then $P \vee Q$ has parts $\{1,2,3,4,5\}$ and $\{6,7\}$.

For association schemes?

An association scheme is a rather special partition of N^2, where $N = \{1, \ldots, n\}$.

Theorem

The join of association schemes is an association scheme.

Proof.

The Bose–Mesner algebra of the join is the intersection of the Bose–Mesner algebras of the two association schemes. □

However, the meet of association schemes is not in general an association scheme. (Consider, for example, two association schemes on five points where the "first associate" relation is a pentagon, but the pentagons in the two cases are $(1, 2, 3, 4, 5)$ and $(1, 2, 3, 5, 4)$.)

Some history

As I said, the theory of association schemes was developed by R. C. Bose and his students and colleagues, beginning in the 1930s. The Bose–Mesner algebra first appeared in the 1950s. In the 1960s, two developments occurred in different parts of the world, in different areas of mathematics, but which produced the same mathematical objects. Donald Higman in the USA defined coherent configurations, and Boris Weisfeiler in the USSR defined cellular algebras. The term "coherent configurations" has now become standard for these, since "cellular algebra" has meanwhile acquired a different meaning. For more information on the history, I refer you to the slides of talks at a recent conference in Pilsen:
`https://www.iti.zcu.cz/wl2018/slides.html`

Coherent configurations

Coherent configurations are like association schemes, but relax the conditions in two ways:

- ☞ the basis matrices are not required to be symmetric, and are not required to commute (but it is required that the set of basis matrices is closed under transposition);
- ☞ the identity is required to be a sum of basis matrices rather than a single matrix.

As in an association scheme, the basis matrices span an algebra.
Also like an association scheme, a coherent configuration can also be regarded as a partition of $\{1, \ldots, n\}^2$.
Higman was a group theorist; if a group G acts on the set N, then the partition of N^2 into orbits of G is a coherent configuration. Many interesting examples arise in this way.
I will say something about Weisfeiler's approach later.

Meet and join

Theorem

Coherent configurations, ordered by the usual ordering of partitions of N^2, form a lattice; that is, two c.c.s have a meet and a join.

The proof for join is just as for association schemes, since the intersection of matrix algebras is again a matrix algebra.

The proof for meet is different. We first observe that there is a unique minimal coherent configuration on a set, which is below every other coherent configuration in the partial order: its parts are just all the subsets of N^2 of cardinality 1. Now, given two coherent configurations P and Q, the set of coherent configurations below both P and Q is non-empty, and so we can take the join of all these configurations; this is clearly the greatest lower bound of P and Q.

This argument fails for association schemes since there may be no association scheme below P and Q. Note also that the meet of c.c.s is not necessarily their meet in the partition lattice.

Weisfeiler–Leman

More generally, the same argument shows that, given any partition P of N^2, there is a unique greatest coherent configuration below P.

Weisfeiler and Leman gave an algorithm to find this configuration. Regard P as an edge-coloured directed graph on the vertex set N (by associating a colour with each part of P.)

One step in the algorithm consists in forming the multiset of edge-colours on all paths of length 2 between i and j, for all i and j. List the multisets that occur, and create a new edge-coloured digraph by giving (i,j) the k-th colour if the multiset associated with (i,j) is the kth in the list.

Repeat until the process stabilises; the resulting partition will be the required coherent configuration.

Weisfeiler and Leman were motivated by the graph isomorphism problem; and their method lies close to the heart of Babai's recent breakthrough (finding a quasi-polynomial algorithm for the graph isomorphism problem).

Where are the symmetric matrices?

Can we keep the algebraic structure (and closure under meet) associated with coherent configurations while restricting ourselves to symmetric matrices?

The product of symmetric matrices is symmetric if and only if they commute. So using ordinary multiplication this takes us back to association schemes.

An alternative which has been considered by several people is to replace ordinary multiplication by the Jordan product (named after the physicist Pascual Jordan), given by

$$A * B = \frac{1}{2}(AB + BA).$$

It is easily verified that, if A and B are symmetric, then so is $A * B$. So the set of real symmetric matrices, equipped with addition and Jordan product, is a (non-associative) algebra.

Jordan algebras

The Jordan product satisfies the identities

$$\begin{aligned} A * B &= B * A \\ (A * B) * (A * A) &= A * (B * (A * A)). \end{aligned}$$

A bilinear product satisfying these identities defines a Jordan algebra.

As well as their applications in physics, there is an extensive mathematical theory of Jordan algebras, which parallels that for associative algebras. For example, the analogue of Wedderburn's theorem, classifying the simple algebras, is the Jordan–von Neumann–Wigner theorem; apart from infinite families, there is an exceptional Jordan algebra of degree 27, related to the exceptional Lie algebra of type E_6.

Jordan schemes

The analogue for Jordan product of an association scheme is a set $\mathcal{A} = \{A_1, \ldots, A_r\}$ of symmetric zero-one matrices of order n (the basis matrices) satisfying

- ☞ the sum of the matrices is the all-1 matrix J;
- ☞ the identity matrix is a sum of basis matrices;
- ☞ each A_i is symmetric;
- ☞ $A_i * A_j = \sum_{k=0}^{r} q_{ij}^k A_k$ for all i, j; that is, the linear span of the matrices is closed under Jordan product.

I will call such an object a Jordan scheme.

As with association schemes, a Jordan scheme can be regarded as a partition of the set of unordered pairs of elements of N^2, where $N = \{1, \ldots, n\}$.

Properties

Basic formal properties of Jordan schemes are similar to those of coherent configurations. A Jordan scheme has a "Bose–Mesner algebra" which is a Jordan algebra.
What we have gained is the lattice structure:

Theorem

Jordan schemes, ordered by the usual ordering of partitions of N^2, form a lattice; that is, two Jordan schemes have a meet and a join.

The proof is as before. The BM algebra of the join of two schemes is the intersection of the BM algebras of the two schemes (and the intersection of Jordan algebras is a Jordan algebra). There is a minimal Jordan scheme, the partition of the set of unordered pairs into singleton sets, which is below every Jordan scheme; so we can define the meet of two Jordan schemes to be the join of all the Jordan schemes below both.

A construction and a problem

Here is a general construction for Jordan schemes.
Take any coherent configuration, and symmetrise it; that is, if A is a basis matrix satisfying $A \neq A^\top$, then replace A and $A^\top$ by the single matrix $A + A^\top$.

Problem

True or false? Every Jordan scheme arises in this way.

Initially I hoped that this would be false; that is, there would be interesting examples of Jordan schemes not arising in this way. But some experimentation (to be described) failed to find any examples.

Problem

Can a theory of Jordan schemes be developed, so as to be of some use to statisticians?

Again, I would hope so!

Some more history

The idea of Jordan schemes was introduced into statistics by B. V. Shah in 1959.

He cites as motivation the triple rectangular lattices introduced by Harshbarger in 1946, which are not partially balanced with respect to any association scheme (although their duals are).

Justus Seely in 1971 discussed Jordan algebras of real symmetric matrices, under the name quadratic subspaces.

James D. Malley set out the theory in his 1986 book. These authors were primarily interested in estimation of variance components.

Various authors returned to the question, including me in 2003 and 2006, and there is an account Chapter 12 of Bailey's *Association Schemes* book.

But the problems on the last slide remain unresolved.

Symmetric Weisfeiler–Leman

A small modification of the Weisfeiler–Leman algorithm finds Jordan schemes, indeed, finds the coarsest Jordan scheme below a given partition.

Recall the operation of WL: at each pass, we create the multiset of colour sequences of paths of length 2 between pairs of vertices; list these multisets, and replace the colour of (i, j) by a new colour k if the multiset for (i, j) is the k-th in the list.

We can symmetrise this algorithm by listing the colour sequences of paths from i to j and from j to i. Then, as in the usual WL algorithm, repeat this step until the procedure stabilises.

Now a small variant of our earlier problem is the following:

Problem

Is it true that the output of the symmetric WL algorithm is always the same as what is obtained by symmetrising the coherent configuration output by the usual WL algorithm?

The concurrence graph and the Laplacian

I finish with a related approach due to Mikhail Kagan.

Given a block design with n points (treatments), the concurrence matrix of the design is the matrix whose (i, j) entry is the number of blocks containing both i and j (counted with appropriate multiplicity if the design is not binary). We insist that $i \neq j$, that is, we do not put replication numbers on the diagonal.

The concurrence matrix can be thought of as the adjacency matrix of a graph (possibly with multiple edges): the number of edges between vertices i and j is the (i, j) entry of the matrix.

Now we define the Laplacian matrix of the graph to be $L = D - A$, where A is the adjacency matrix as above, and D is the diagonal matrix whose ith diagonal entry is the number of blocks containing i. Thus L is a positive semi-definite symmetric matrix with all row and column sums zero.

If the design has constant block size k, the information matrix of the design is L/k.

Resistances and resistance distance

Now suppose that we regard the graph as an electrical network, with each edge replaced with a 1-ohm resistor. If we connect a 1-volt battery between two terminals, then current will flow in the network (assuming it is connected); the effective resistance between the two terminals is the inverse of the current that flows.

The effective resistance between two terminals can be computed using Kirchhoff's voltage and current laws and Ohm's Law. It has two important properties:

- ☞ Apart from scaling, the effective resistance between i and j is equal to the variance of the estimator of the differences between treatments i and j in the origial design. Thus the average resistance between all pairs of terminals is the value of the A-optimality criterion for the design.
- ☞ Effective distance is a metric: that is, it satisfies the triangle inequality. This metric is called resistance distance.

Some questions

Mikhail Kagan and Misha Klin have proposed resistance distance as a replacement for symmetric Weisfeiler–Leman.

Suppose that we start with a simple graph, and compute the resistance distances between all pairs of vertices.

We obtain a partition of the set of unordered pairs of vertices, two pairs lying in the same class if their distances are equal.

But note that this cannot distinguish one point from another, since a point always has distance 0 from itself. So maybe the questions below only make sense if the Jordan scheme is homogeneous (the identity is a basis matrix).

Problem

- ☞ *Is the partition we obtain from resistance distances a Jordan scheme?*
- ☞ *If so, is it the largest Jordan scheme lying below the partition of pairs into edges and nonedges of the graph (the output of the symmetrised Weisfeiler–Leman algorithm)?*

…for your attention.
A list of references follows.

References

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