How group theory and statistics met in association schemes

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Abstract I

This talk has two beginnings, both in the 1930s.

I. Schur considered the orbits, of a transitive permutation group, on ordered pairs of points. The partition into orbits is very natural, and properties of the partition are helpful in understanding the groups. This is one fore-runner of coherent configurations.

R. C. Bose and his collaborators and students generalized earlier work of F. Yates by introducing partially balanced incomplete-block designs for parameters where no balanced incomplete-block design exists. The condition of partial balance ensures that the relevant matrices can be easily inverted by hand, which was important for data analysis in the pre-computer age. This condition relies on the existence of a (symmetric) association scheme.

Abstract II

In the 1950s, D. Mesner worked on association schemes as a PhD student, later combining with Bose to present what is now called the Bose–Mesner algebra.
He also devised a new type of association scheme, which he called negative Latin square type. He found one on 100 points.

In the 1960s Bose made the topic interesting to pure mathematicians by naming strongly regular graphs.
These proved fruitful in the search for sporadic simple groups, with the result that D. G. Higman and C. C. Sims rediscovered Mesner's association scheme on 100 points in 1968.

Meanwhile, other collaborators of Bose's, including C. R. Nair and J. N. Srivastava, were generalizing association schemes in different ways that now fit within the framework of coherent configurations.

Abstract III

I will conclude by mentioning the series of lectures on coherent configurations that D. G. Higman gave to research students in group theory at Oxford (including me).

It is a shame that some of the people that I mention died before all the connections were understood and acknowledged.

Schur rings

Given a finite group G, its corresponding group ring $\mathbb{Z}G$ consists of all formal sums $\sum_{g\in G} n_g g$ with coefficients n_g in $\mathbb{Z}$.
Addition and multiplication in this ring are done in the obvious way.

Suppose that G is partitioned into subsets $\Delta_0, \Delta_1, \ldots, \Delta_s$.
Put $\chi_i = \sum_{g\in\Delta_i} g$ for $i = 0, \ldots, s$. If

(i) Δ_0 consists just of the identity element of G,
(ii) if Δ_i is one of the subsets then so is $\{g^{-1} : g \in \Delta_i\}$,
(iii) $\chi_i\chi_j$ is a linear combination of $\chi_0, \ldots, \chi_s$ for all i and j,

then the subring of $\mathbb{Z}G$ generated by $\{\chi_0, \ldots, \chi_s\}$ is called a Schur ring.

Schur (1933) used this idea to prove various results about permutation groups.

Permutation groups

Wielandt's influential book *Finite Permutation Groups* was published in 1964, based on a German version of 1959.
Chapter IV explains Schur rings.

Chapter III explains how to obtain information about a permutation group G on a set Ω by examining the partition of $\Omega\times\Omega$ into orbits of G: sets of the form $\{(\alpha^g, \beta^g) : g \in G\}$.
If G is transitive then $\{(\alpha, \alpha) : \alpha \in \Omega\}$ is one such orbit.
If G has rank r then it has r orbits on $\Omega\times\Omega$.

Suppose that $|\Omega| = n$ and Γ_i is one of these orbits.
Its adjacency matrix A_i is the $n\times n$ matrix with rows and columns indexed by Ω and entries

$$A_i(\alpha, \beta) = \begin{cases} 1 & \text{if } (\alpha, \beta) \in \Gamma_i \\ 0 & \text{otherwise.} \end{cases}$$

Chapter V investigates these matrices.

Properties of the adjacency matrices

Let $A_0, \ldots, A_{r-1}$ be the adjacency matrices for the orbits of G on $\Omega \times \Omega$. These satisfy the following conditions.

(i) $A_0 = I$ if G is transitive on Ω;
if G has s orbits on Ω then
I is a sum of s adjacency matrices.

(ii) $\sum_i A_i = J$ (all-1 matrix).

(iii) If A_i is an adjacency matrix then so is its transpose $A_i^\top$.

(iv) If A_i and A_j are adjacency matrices then their product is an integer-linear-combination of adjacency matrices.

(The collection $\mathcal{A}$ of $n \times n$ matrices (over some field) which commute with the permutation matrix P_g for every g in G is closed under addition, scalar multiplication and matrix multiplication, so it forms an algebra, the centralizer algebra of G.)
G is called generously transitive (Neumann, 1975) if $A_0 = I$ and every A_i is symmetric.

Charles Sims and Donald Higman

These two group theorists independently continued the technique of considering the orbits of G on $\Omega \times \Omega$ to find out more about G.

If A_i is symmetric then the corresponding orbit is self-paired.
Its pairs (α, β) can be considered as the edges of an undirected graph Γ on which G acts as a group of automorphisms.
Sims (1967, 1968) used this idea to forge an interplay between graph theory and group theory.

On the other hand, Higman thought about the whole partition of $\Omega \times \Omega$, starting with groups of rank 3 in 1964, then concentrating on the matrices in 1967.

Pause

I will leave the group theory there for the moment, and start the story again in experimental design.

Experimental design

Suppose that I want to do an experiment to compare 8 varieties of wheat. My field has room for 56 plots, so I can grow each variety on 7 plots.

There may be differences between different parts of the field. Some plots may be close to the edge of a forest; some may be close to a stream. Some may be at the top of the hill; some at the bottom. Some may be more fertile in dry years, but less so in wet years.

We partition the set of plots into blocks, in such a way that

- within each block, all plots are reasonably alike;
- all blocks contain the same number of plots.

If there are 7 blocks of 8 plots each, then I can grow each variety on one plot per block. This is called a complete-block design.

Incomplete blocks

I still have 8 varieties and 56 plots,
but now I have to group them into 14 blocks of size 4.
These blocks must be incomplete, because $4 < 8$.

1 2 4 8	3 5 6 7	2 3 5 8	1 4 6 7
3 4 6 8	1 2 5 7	4 5 7 8	1 2 3 6
1 5 6 8	2 3 4 7	2 6 7 8	1 3 4 5
	1 3 7 8	2 4 5 6	

Every pair of distinct varieties occur together in the same number of blocks, so this block design is balanced.

Balanced incomplete-block designs were introduced by Yates (1936).

Concurrence matrix and information matrix

Given an incomplete-block design for a set $\mathcal{T}$ of v varieties in which all blocks have size k and all treatments occur r times, the $\mathcal{T} \times \mathcal{T}$ concurrence matrix Λ has (i,j)-entry equal to the number of blocks in which treatments i and j both occur (this number is the concurrence of i and j),
and the information matrix is $I - (rk)^{-1}\Lambda$.

In order to analyse the data from such an experiment,
and also in order to compare potential designs,
we need to invert the information matrix.

The constant vectors are in the null space of the information matrix, so we cannot actually invert it.

If M is the information matrix then we calculate

$$\left(M + v^{-1}J\right)^{-1} - v^{-1}J,$$

where J is the $v \times v$ matrix with every entry 1.
This can easily be done by hand if the design is balanced.

Suppose that balance is not possible?

Yates (1935, 1936, 1937) also considered various cases where balance cannot be achieved.

Suppose that I have 8 varieties but only 24 plots.

- If there are 3 blocks of size 8 then I can use a complete-block design.
- If there are 6 blocks of size 4 then I can use the 6 faces of a $2 \times 2 \times 2$ cube (concurrence is 2 for an edge, 1 for a face-diagonal, 0 for antipode).
- If there are 8 blocks of size 3 then I can develop $\{1, 2, 4\}$ modulo 8 (concurrence is 0 if the difference is ± 4, otherwise is 1).

Square lattice designs

If the number of varieties is m^2 and there are $g-2$ mutually orthogonal Latin squares of order m, then a design with gm blocks of size m can be made as follows.

1. Write the varieties in an $m \times m$ square array.
2. The first m blocks are given by the rows; the next m blocks are given by the columns.
3. If $g = 2$ then STOP.
4. Otherwise, write down $g-2$ mutually orthogonal Latin squares of order m.
5. For $i = 3$ to g, the next m blocks correspond to the letters in Latin square $i-2$.

If $g = m+1$ then the block design is balanced.

Partially balanced incomplete-block designs

Bose and Nair (1939) set up a general framework to include Yates's examples, defining them to be partially balanced incomplete-block designs.

If the distinct concurrences are $\lambda_1, \ldots, \lambda_s$, they defined a pair of distinct varieties to be *i*-th associates if they concur in λ_i blocks.

The $v \times v$ matrix A_i has (t, u)-entry equal to 1 if varieties t and u are i-th associates, and other entries equal to 0.
The $v \times v$ matrix A_0 is just I.

They insisted that each product $A_i A_j$ be a linear combination of $A_0, \ldots, A_s$ in order that the information matrix can be easily inverted by hand.

Definition of association scheme

Bose and Shimamoto (1952) relaxed the condition that different associate classes must have different concurrences. They also gave the first formal definition of an association scheme.

Definition
An association scheme of rank r on a finite set Ω is a partition of $\Omega \times \Omega$ into subsets $\Gamma_0, \ldots, \Gamma_{r-1}$ whose adjacency matrices $A_0, \ldots, A_{r-1}$ satisfy the following.

(i) $A_0 = I$.
(ii) $\sum_i A_i = J$ (obviously!).
(iii) $A_i^\top = A_i$ for $i = 0, 1, \ldots, r-1$.
(iv) There are integers p_{ij}^k such that if A_i and A_j are adjacency matrices then
$$A_i A_j = \sum_{k=0}^{r-1} p_{ij}^k A_k.$$

Association schemes of rank 3

Bose and Shimamoto classified association schemes of rank 3 as

group-divisible GD(m, n): the nm varieties are partitioned into n subsets of size m, and first associates are those in the same subset;

Latin square type $\mathrm{L}_g(m)$: the m^2 varieties have concurrence 0 or 1 as per a square lattice design;

triangular T_m: the $m(m-1)/2$ varieties are identified with unordered pairs from $\{1, \ldots, m\}$, which can overlap in either 0 or 1 element;

cyclic: the varieties are identified with $\mathbb{Z}_v$ where v is a prime congruent to 1 modulo 4, and the associate class of (i, j) depends on whether or not $i - j$ is a square;

miscellaneous: they hoped that there were not many more.

Dale Mesner

Dale Mesner was a PhD student at Michican State College (later renamed Michigan State University) from 1950 to 1956, supervised by Leo Katz.
His thesis was called "An investigation of certain combinatorial properties of partially balanced incomplete-block experimental designs and association schemes, with a detailed study of designs of Latin squares and related types".

One important part of this was the development of the algebra generated by the adjacency matrices of an association scheme. He did not know that R. C. Bose had assigned this topic to one of his own PhD students. When Bose heard about Mesner's work, he suggested collaboration, resulting in the important paper "On linear associative algebras corresponding to association schemes of partially balanced designs" in *Annals of Mathematical Statistics* **30** in 1959.

The Bose–Mesner algebra

The set $\mathcal{A}$ of real linear combinations of the adjacency matrices is called the Bose–Mesner algebra.
It consists of real symmetric matrices, is commutative, and has dimension r, where r is the rank of the association scheme.

So there are mutually orthogonal subspaces $W_0, \ldots, W_{r-1}$ of $\mathbb{R}^\Omega$ such that if $M \in \mathcal{A}$ then each eigenspace of M is either one of the W_i or the direct sum of two or more of $W_0, \ldots, W_{r-1}$.
We can always take W_0 to be the 1-dimensional space spanned by the all-1 vector.

Let Q_i be the matrix of orthogonal projection onto W_i.
These eigenprojectors are the minimal idempotents of $\mathcal{A}$.

So we have two natural bases for $\mathcal{A}$:
$\{A_0, \ldots, A_{r-1}\}$ is good for doing addition;
$\{Q_0, \ldots, Q_{r-1}\}$ is good for doing multiplication.

Character table and pseudo-inverses

Let λ_{ij} be the eigenvalue of A_i on W_j. Then

$$A_i = \sum_{j=0}^{r-1} \lambda_{ij} Q_j \qquad \text{for } i = 0, \ldots, r-1.$$

The $r \times r$ matrix with entries λ_{ij} is called the character table of the association scheme. Its columns are called the characters of the association scheme.

(The conventions are slightly different from those in group theory.)

If $M = \theta_1 Q_1 + \cdots + \theta_{r-1} Q_{r-1}$
(with θ_i non-zero for $1 \le i \le r-1$)
then the pseudo-inverse of M is $\theta_1^{-1} Q_1 + \cdots + \theta_{r-1}^{-1} Q_{r-1}$.

What else came out of Mesner's thesis?

He was at the University of North Carolina at Chapel Hill (where R. C. Bose worked) from 1964 to 1966.

While there, he wrote "Negative Latin square designs", which was published in 1964 as number 410 in the NC Mimeo series of the Institute of Statistics at UNC.
It was common to publish preprints in this way at UNC at the time.
The Bose–Mesner paper had been published as number 188 in 1958.

Mesner himself also published

- A note on parameters of PBIB association schemes, number 375, in 1963 (this became a paper in *Annals of Mathematical Statistics* in 1965)
- Sets of disjoint lines in $\mathrm{PG}(3, q)$, number 409, in 1964
- On the block structure of certain PBIB designs of partial geometry type, number 457, in 1966.

Negative Latin square type of association scheme

Dale M. Mesner published "A new family of partially balanced incomplete block designs with some Latin square design properties" in *Annals of Mathematical Statistics* **38** in April 1967.
It had been submitted in July 1964, then revised in August 1966.

A 2-class association scheme made from $g-2$ mutually orthogonal Latin squares of order m (where $2 \le g \le m$) has

vertices	valency	triangles per edge
$n = m^2$	$a_1 = g(m-1)$	$p_{11}^1 = g^2 - 3g + m$

Mesner's idea was to replace m and g by $-m$ and $-g$ to get an association scheme of negative Latin square type, $\mathrm{NL}_g(m)$.

vertices	valency	triangles per edge
$n = m^2$	$a_1 = g(m+1)$	$p_{11}^1 = g^2 + 3g - m$

Promise in the Introduction

vertices	valency	triangles per edge
$n = m^2$	$a_1 = g(m+1)$	$p_{11}^1 = g^2 + 3g - m$

> *A new method of construction in Section 4 will provide solutions for* $\mathrm{NL}_1(4)$, $\mathrm{NL}_2(8)$ *and* $\mathrm{NL}_2(9)$. *Methods to be presented in later papers give solutions for some of the foregoing as well as for* $\mathrm{NL}_3(9)$ *and* $\mathrm{NL}_2(10)$.

All of these had been done in his 1956 PhD thesis, and in that 1964 number 410 in the NC Mimeo Series.

The first lot were done in Section 3, not Section 4.

$\mathrm{NL}_2(10)$ has 100 vertices, valency 22 and no triangles.

Strongly regular graphs

In a 1963 paper in *Pacific Journal of Mathematics*, R. C. Bose coined the term strongly regular graph to denote the graph corresponding to one associate class of a two-class association scheme.

The time was ripe to capture the interest of pure combinatorialists and algebraists. Hoffman and Singleton had defined Moore graphs in 1960.

Finite simple groups

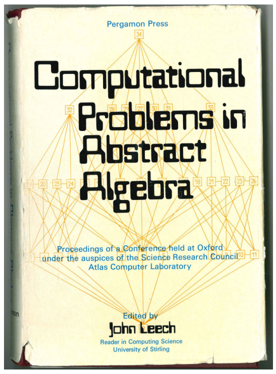
In the 1960s there was an explosion in the discovery of finite simple groups. Such a group is called sporadic if it does not belong to one of the well-known infinite families, such as the alternating groups.

Automorphism groups of highly symmetric combinatorial structures proved a fruitful source.

The non-trivial orbits (on ordered pairs of vertices) of any generously transitive permutation group of rank three are a complementary pair of strongly regular graphs.
D. G. Higman developed an extensive theory of such permutation groups.

1967 conference in Oxford

In 1967 a conference on "Computational Problems in Abstract Algebra" was held in Oxford. At this, Marshall Hall gave a lecture about how the Hall–Janko sporadic simple group had been constructed as (a subgroup of) the automorphism group of a strongly regular graph on 100 vertices with valency 36 and 14 triangles per edge.



Higman–Sims graph and Higman–Sims group

Don Higman and Charles Sims were at this conference, and were inspired by this talk. Sims (Bannai et al., 2009) said that they discussed ideas before, during and after the conference dinner, and by the early hours of the next morning had soon constructed a new sporadic simple group, now called the Higman–Sims group, as a subgroup of index 2 in the automorphism group of a strongly regular graph on 100 vertices with valency 22 and no triangles. They were able to construct this by starting with the Steiner system $\mathfrak{S}(3,6,22)$, so they did it with less effort than Mesner.

The vertices are ∞, the 22 points and the 77 blocks.

∞ is joined to the 22 points.

Each point is joined to ∞ and the 21 blocks containing it.

Each block is joined to the 6 points it contains and the 16 blocks disjoint from it.

If two blocks are disjoint then no block is disjoint from both.

New group; apparently new graph

Higman and Sims published their results in *Mathematische Zeitschrift* in 1968.

Many people now call this strongly regular graph the Higman–Sims graph.

Higman first referred to strongly regular graphs in a 1970 paper, submitted in July 1969.

However, in recent years, it seems that more online references are also crediting Dale Mesner with this graph.

Thanks to Edmund Roberston for showing me his article about this which will appear in Mactutor,
and to Colin Campbell for showing me his hard copy of the proceedings of that conference.

Who knew about this part of Mesner's work?

According to Jajcayová and Jajcay (2002),
J. J. Seidel at Eindhoven saw the thesis in 1968.

Goethals and Seidel (1970) mention negative-Latin-square graphs, referring to Mesner's 1967 paper but not apparently noticing his claim to have constructed $\mathrm{NL}_2(10)$.

Cameron, Goethals and Seidel (1978) include negative Latin square graphs in their classification of strongly regular graphs with strongly regular subconstituents.

Mesner visited Eindhoven in 1983–1984.
One outcome was a joint paper with A. E. Brouwer on strongly regular graphs in 1985.

The "bible" on *Distance-Regular Graphs* by Brouwer, Cohen and Neumaier, was published in 1989. It refers to Mesner's 1967 paper, but does not associate him with the Higman-Sims graph.

More details about what Dale Mesner did, and his later life

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Don Higman and coherent configurations

If you allow the group G not to be transitive on Ω, then I is a sum of two or more adjacency matrices, and some of the non-diagonal adjacency matrices are not symmetric.

Higman decided to extend the basic combinatorial ideas to such a set of matrices, irrespective of group actions. He called this a coherent configuration. If the diagonal is a single class, then it is a homogeneous coherent configuration.

Don Higman's lecture notes

I was a DPhil student in group theory at Oxford from 1969 to 1972. Don Higman visited for the academic year 1970–1971. He gave a series of lectures on his current thinking on coherent configurations. Peter Cameron and Susannah Howard took notes, which were approved by DGH before being typed up and published as "Combinatorial Considerations about Permutation Groups" in the Mathematical Institute series of lecture notes in 1971.

These notes were extraordinarily influential on that cohort of DPhil students.

Later, DGH developed them into two papers on coherent configurations (1975, 1976).

Did statisticians also go as far as coherent configurations?

In 1964, C. R. Nair generalized association schemes by dropping the requirement for symmetry.

He insisted that if A_i is an adjacency matrix then so is $A_i^\top$; and that the Bose–Mesner algebra is commutative.

Since concurrence matrices of incomplete-block designs are symmetric, this does not change the concept of a partially balanced incomplete-block design.

Multidimensional partial balance

In 1963, Bose and Srivastava started a different generalization, which Srivastava continued for many years. Suppose that I want to experiment on combinations of v varieties with n quantities of fertilizer. Let N_{12} be the $v \times n$ matrix whose (i, j)-entry is the number of plots which have variety i with amount j of fertilizer. Let N_{11} be the $v \times v$ diagonal matrix whose (i, i)-entry is the number of plots with variety i. Define N_{21} and N_{22} similarly.

The information matrix for varieties is a linear combination of N_{11} and $N_{12}N_{21}$. The information matrix for fertilizer quantities is a linear combination of N_{22} and $N_{21}N_{12}$.

If these matrices are in the algebra of a coherent configuration with diagonal classes $\{$varieties$\}$ and $\{$fertilizer quantities$\}$ then the information matrices can be (pseudo-)inverted easily.

Bose and Srivastava called these multidimensional partial balance schemes. They generalize to 3 or more diagonal classes.

Who knew what?

D. G. Higman died on 13 February 2006.
J. N. Srivastava died on 18 November 2010.
It seems that neither of them knew of each other's work.

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