Combinatorics of optimal designs

R. A. Bailey and Peter J. Cameron

Queen Mary
University of London

p.j.cameron@qmul.ac.uk

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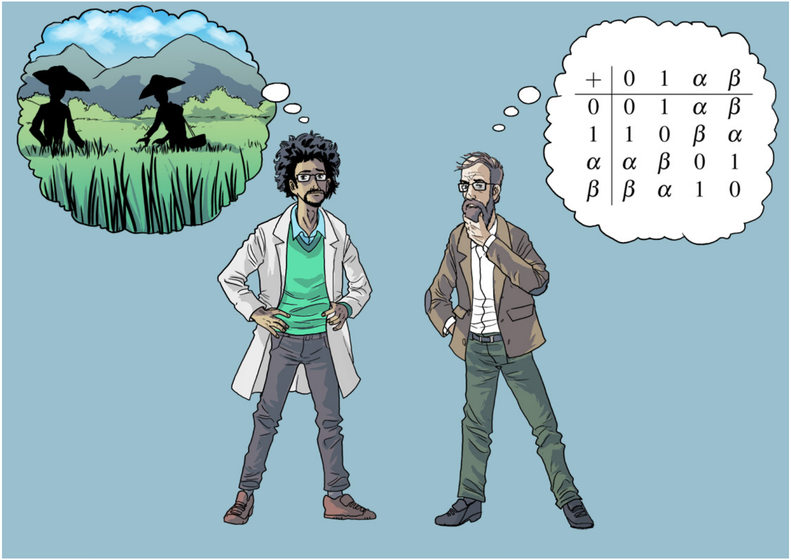
Mathematicians and statisticians

There is a very famous joke about Bose's work in Giridh. Professor Mahalanobis wanted Bose to visit the paddy fields and advise him on sampling problems for the estimation of yield of paddy. Bose did not very much like the idea, and he used to spend most of the time at home working on combinatorial problems using Galois fields. The workers of the ISI used to make a joke about this. Whenever Professor Mahalanobis asked about Bose, his secretary would say that Bose is working in fields, which kept the Professor happy.

Bose memorial session, in *Sankhyā* **54** (1992) (special issue devoted to the memory of Raj Chandra Bose), i–viii.

Mathematicians and statisticians



First topic

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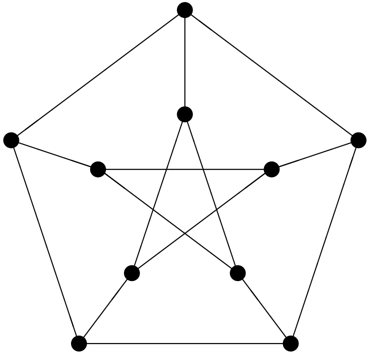
What graph-theoretic properties make it a "good" block design, in the sense that the information obtained from an experiment is as accurate as possible given the resources?

Which graph is best?



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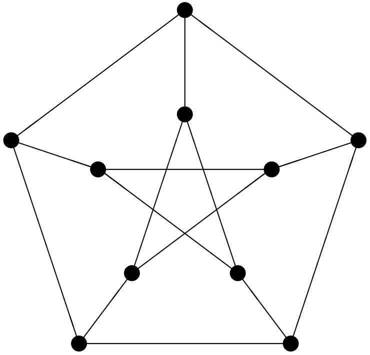

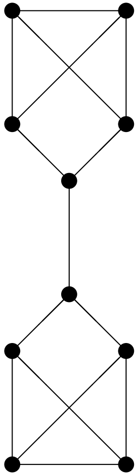

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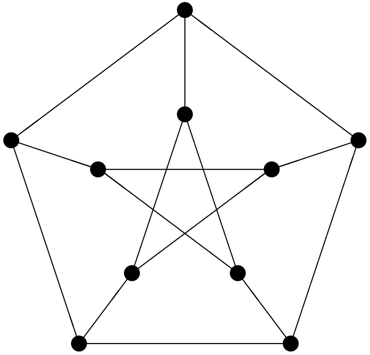

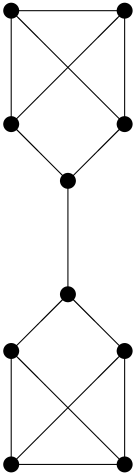

Of course the question is not well defined. But which would you choose for a network, if you were concerned about connectivity, reliability, etc.?

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- How many spanning trees does it have? The more spanning trees, the better connected. The first graph has 2000 spanning trees, the second has 576.
- Electrical resistance. Imagine that the graph is an electrical network with each edge being a 1-ohm resistor. Now calculate the resistance between each pair of terminals, and sum over all pairs; the lower the total, the better connected. In the first graph, the sum is 33; in the second, it is 206/3.

Which graph is best connected?

- Isoperimetric number. This is defined to be

$$i(G) = \min \left\{ \frac{|\partial S|}{|S|} : S \subseteq V(G),\ 0 < |S| \leq v/2 \right\},$$

where $v = |V(G)|$ and for a set S of vertices, ∂S is the set of edges from S to its complement. Large isoperimetric number means that there are many edges out of any set of vertices. The isoperimetric number for the first graph is 1 (there are just five edges between the inner and outer pentagons), that of the second graph is $1/5$ (there is just one edge between the top and bottom components).

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This is a real symmetric matrix; its eigenvalues are the Laplacian eigenvalues of G. Note that its row sums are zero.

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- The number of spanning trees of G is the product of the non-trivial Laplacian eigenvalues, divided by v: this is Kirchhoff's Matrix-Tree Theorem.

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Recently, Krivelevich and Sudakov have shown that, in a k-regular graph G on v vertices, if μ_1 is large enough in terms of v and k, then G is Hamiltonian. Pyber used this to show that all but finitely many strongly regular graphs are Hamiltonian.

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We model the result of each trial as giving a number for each of the two treatments in the trial, which is the sum of an effect due to a treatment, an effect due to the trial, and some random variation.

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Each treatment contrast estimator is a random variable, and the smaller its variance, the more accurate the estimate. Accurate estimates are important to reduce the risk that we rate one treatment better than another just because of random variation.

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There are other types of optimality too, but these will do for now! (For D-optimality, we need to assume the errors are independent normal.)

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So E-optimal graphs will tend to have large isoperimetric numbers.

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Perhaps we should regard it as a hypergraph of some kind?
It will turn out that optimality properties of such a block design are determined by a graph, the concurrence graph of the block design, no matter what the block size. So we do not need a new theory!

What is a block design?

We wish to do an experiment to test v different treatments. We have available bk experimental units, divided into b "blocks" of k; there are systematic but unknown differences between the blocks. We model the response of an experimental unit as the sum of a treatment effect, a block effect, and random variation, and we want to estimate treatment differences, or more generally, treatment contrasts.

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In fact there is a much more serious problem …

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An example, continued

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It is known that VB-designs are E-optimal as long as they don't have too much "badness" (multiple occurrences of treatments in blocks). See the paper for details.

The concurrence graph

The concurrence graph of a block design is defined as follows. The vertex set is the set of v treatments. There are no loops. For every occurrence of treatments i and j together in a block, we put an edge from i to j. (For example, if a block contains p occurrences of treatment i and q of treatment j, then it contributes pq edges from i to j.)

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We form the Laplacian matrix of this graph in the usual way: the (i,i) entry is the valency of vertex i; and for $i \neq j$, the (i,j) entry is the negative of the number of edges from i to j.

Estimation and variance

This topic is covered in detail in the paper. The upshot is that, in order to extract information about treatment differences from the experimental results, we require a matrix called the information matrix of the design, and we require its non-trivial eigenvalues to be “large”.

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So optimality criteria can be expressed in terms of the Laplacian eigenvalues …

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The interpretation of A- and D-optimality in terms of resistances and spanning trees is exactly as before.

Which graphs are concurrence graphs?

Let $w_1, \ldots, w_m$ be positive integers with sum k. Define a weighted clique with weights $w_1, \ldots, w_m$ in a graph to be a clique of m vertices, numbered $1, \ldots, m$, such that the number of edges joining i to j is $w_i w_j$.

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Our example corresponds to a partition of $2K_5$ into six triangles and one double edge (with weights 1 and 2).

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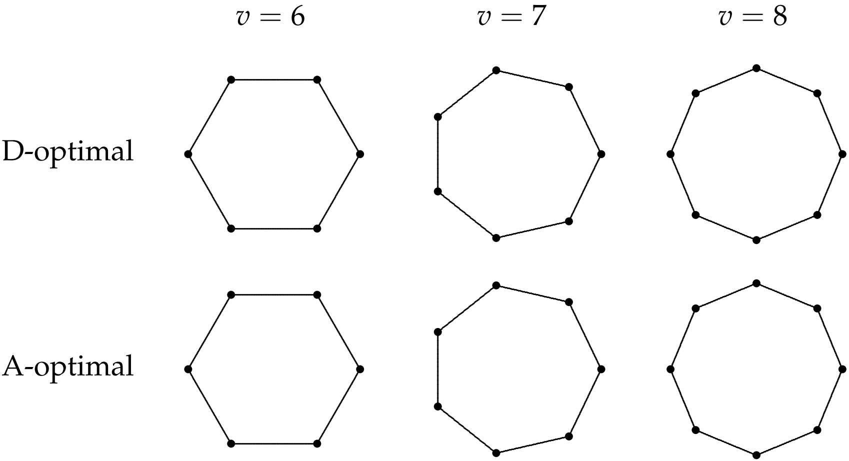
Now we look at the case where $k = 2$ and $b = v$ (so the design is a unicyclic graph). What is the "nicest" unicyclic graph?

Optimal designs when $b = v$, $k = 2$



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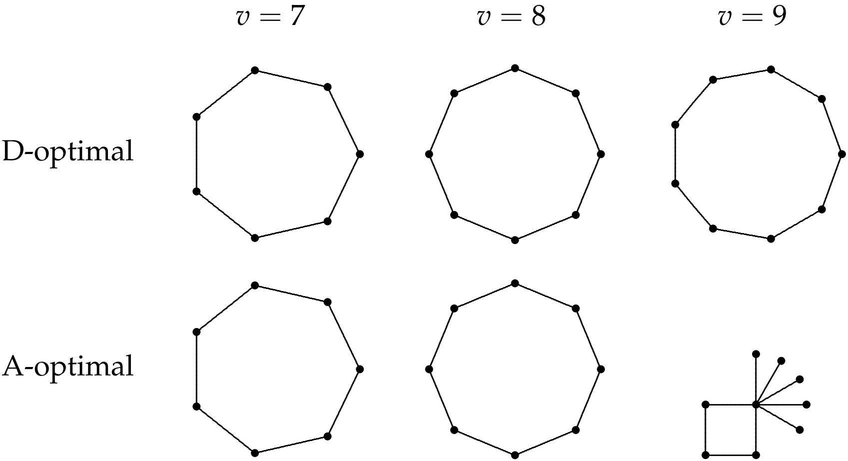

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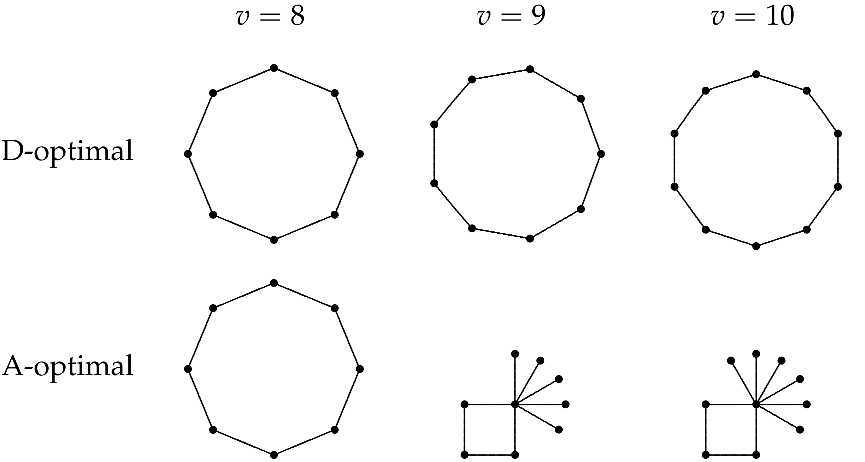

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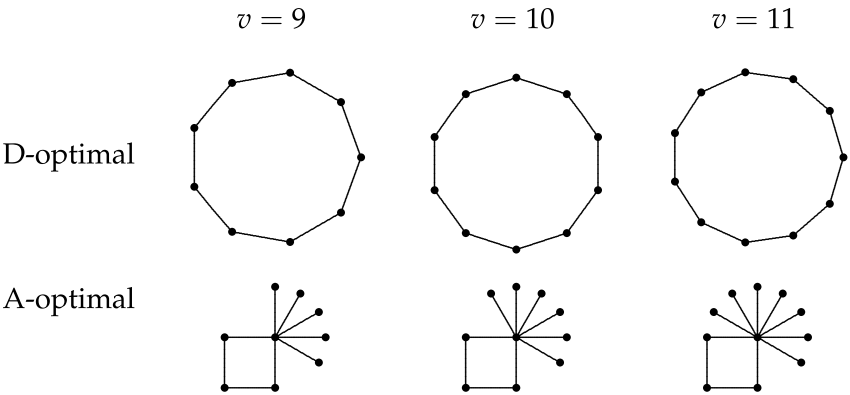

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You can find the proof in the paper.

Things to do (a short list)

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- Develop an existence theory for VB-designs similar to Wilson's existence theory for 2-designs. (The number of blocks is not determined by the parameters v, k, λ; the theory should also take account of possible numbers of blocks.)
- For designs with block size 2, is there a "threshold" for edge density below which the A- and E-optimal designs look very different? What about larger block size?
- Are "nice" designs such as generalized polygons optimal in any sense? (The example of ordinary polygons earlier gives motivation for this.)

… for your attention!