Finding good designs for experiments

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5. Computer search?

The set-up: treatments and experimental units

I have v treatments that I want to compare.
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How should I choose a design?

Case 1

The experimental units are all alike.

Estimation and variance

We measure the response Y on each unit.

If that unit has treatment i then we assume that

$$Y = \tau_i + \text{random noise}.$$

We want to estimate all the simple differences $\tau_i - \tau_j$.

Put $V_{ij} =$ variance of the best linear unbiased estimator for $\tau_i - \tau_j$.

We want all the V_{ij} to be small.

The design is A-optimal if it minimizes $\sum_{i=1}^{v} \sum_{j=i+1}^{v} V_{ij}$.

How do we calculate variance?

The replication r_i of treatment i is its number of occurrences.
So one constraint is

$$\sum_{i=1}^{v} r_i = N.$$

Theorem

Assume that all the noise is independent, with variance σ^2. Then

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Theorem

$\bar{V}$ is minimized when the replications are as equal as possible, in the sense that no pair differ by more than 1.

Proof.

I set this to my undergraduates. □

Case 2

The experimental units are divided into b blocks of k units each.

Model when there are blocks

We measure the response Y on each unit in each block.

If that unit has treatment i and block m, then we assume that

$$Y = \tau_i + \beta_m + \text{random noise}.$$

To get rid of the β parameters, we look at $(I - P)Y$,
where P is the $N \times N$ matrix of orthogonal projection onto the space spanned by the characteristic vectors of the blocks.

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Let X be the $N \times v$ incidence matrix of treatments in experimental units.
The information matrix is $X^\top(I - P)X$.

Design $\to$ graph

If $i \neq j$, the concurrence λ_{ij} of treatments i and j is the number of occurrences of the pair $\{i, j\}$ in blocks, counted according to multiplicity.

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The concurrence graph G of the design has the treatments as vertices.
There are no loops.
If $i \neq j$ then there are λ_{ij} edges between i and j.
So the valency d_i of vertex i is

$$d_i = \sum_{j \neq i} \lambda_{ij}.$$

Graph $\to$ matrix

The Laplacian matrix L of this graph has

(i,i)-entry equal to $d_i = \sum_{j \neq i} \lambda_{ij}$

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The information matrix is precisely $k^{-1}L$.

Estimation and variance when there are blocks

Theorem

Assume that all the noise is independent, with variance σ^2. Then the variance of the best linear unbiased estimator of the simple difference $\tau_i - \tau_j$ is

$$V_{ij} = \left(L^-_{ii} + L^-_{jj} - 2L^-_{ij}\right) k\sigma^2,$$

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Put $\bar{V} =$ average value of the V_{ij}. Then

$$\bar{V} = \frac{2k\sigma^2 \operatorname{Tr}(L^-)}{v-1} = 2k\sigma^2 \times \frac{1}{\text{harmonic mean of } \theta_1, \ldots, \theta_{v-1}},$$

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$$\begin{aligned} \text{A-optimal} \quad &\Longleftrightarrow \quad \text{minimize } \bar{V} \\ &\Longleftrightarrow \quad \text{maximize harmonic mean of } \theta_1, \ldots, \theta_{v-1}. \end{aligned}$$

First folklore for block designs

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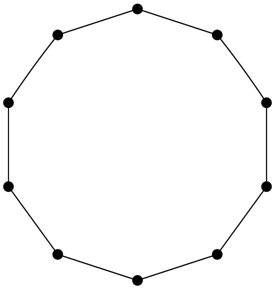
If v divides N and there are b blocks of size k where $b > 1$ then the set of equireplicate designs contains some A-optimal designs.

This was believed from the introduction of incomplete-block designs in the 1930s, so the search for good designs was restricted to equireplicate ones.

By the 1990s, it had been shown to be false in general.

Designs for $k = 2$ when $b = v$ (blocks shown as edges)

The only connected equireplicate design is the cycle.



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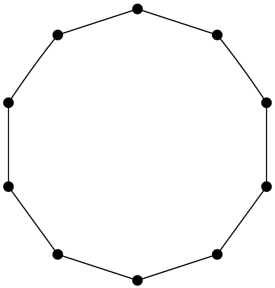

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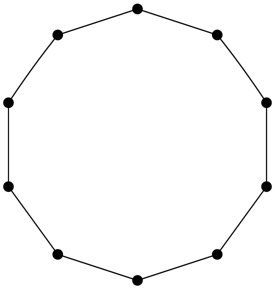

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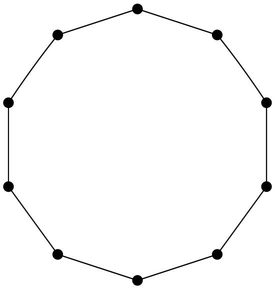

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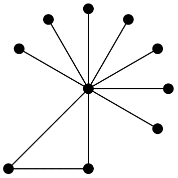

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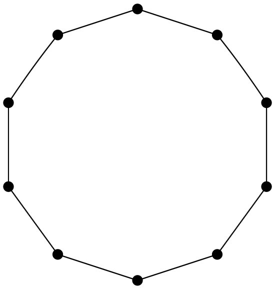

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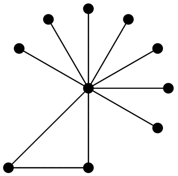

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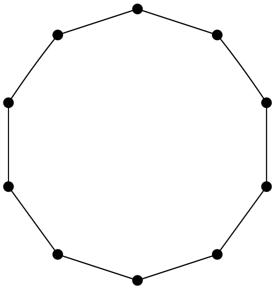

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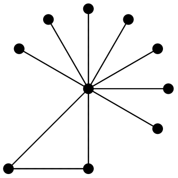

$V_{ij} \leq 4\sigma^2$ for all i, j.

A star attached to a triangle is A-optimal for all $v \geq 12$.

Reactions

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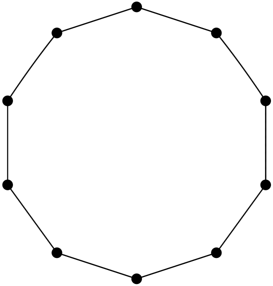
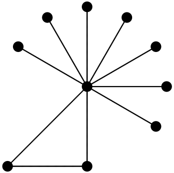
Biologist: the second design should be used, because we know that we should compare all treatments with the same thing.

Producer of one of the compared treatments: that's not fair! My treatment has replication only one, so the variances of its comparisons with other treatments will be too large.

What about symmetry and regularity?

Design		
Automorphisms	2×10	$2 \times 7!$
	regular	more symmetries

Some history

In 1980, Jones and Eccleston published a short paper in JRSSB on the results of a computer search for A-optimal designs with
$k = 2$ and $v = b \leq 10$
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Their work was ignored by most statisticians, because we were so sure that equireplicate designs are best that we assumed that there was an error in the computation.

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Definition

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This is nonsense: the theorem is comparing designs using the same number of experimental units.

A comparison

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If k divides v and there is a BIBD for v treatments in $b - (v/k)$ blocks of size k, then the best thing to do is to use that BIBD and make the extra blocks out of any partition of the treatments into sets of size k.

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Example

Suppose that $v=6$, $b=12$ and $k=3$.

Design	$\bar{V}/\sigma^2$
BIBD with 10 blocks	0.5
That BIBD with two more blocks	0.42
Develop $\{0,1,2\}$ and $\{0,1,3\}$ modulo 6	0.4196...

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Regular Graph Design

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			where $I + A_1 + \cdots + A_s = J$ and
			$A_i A_j$ is a linear combination of $I, A_1, \ldots, A_s$.

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Regular Graph Design

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In particular, this is true if the design is partially balanced with two associate classes, which means that the information matrix is in the Bose–Mesner algebra of a strongly regular graph.

Variance and concurrence

Folklore surrogate

If there are any regular graph designs, all optimal designs are RGDs.

Folklore surrogate

Variance V_{ij} is a decreasing function of λ_{ij}.

Neither is true in general. Counterexamples exist.

Theorem

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In particular, this is true if the design is partially balanced with two associate classes, which means that the information matrix is in the Bose–Mesner algebra of a strongly regular graph.

Theorem

If the design is partially balanced with two associate classes, and the concurrences differ by 1, and one of those eigenvalues is equal to r, then the block design is A-optimal.

What about distance in the concurrence graph G?

Recall: G has one vertex for each treatment
and λ_{ij} edges between vertices i and j.

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Variance increases with distance in the concurrence graph.

This is not true in general.

Electrical networks

We can consider the concurrence graph as an electrical network with a 1-ohm resistance in each edge. Connect a 1-volt battery between vertices i and j. Current flows in the network, according to these rules.

1. Ohm's Law:
   In every edge, voltage drop = current $\times$ resistance = current.
2. Kirchhoff's Voltage Law:
   The total voltage drop from one vertex to any other vertex is the same no matter which path we take from one to the other.
3. Kirchhoff's Current Law:
   At every vertex which is not connected to the battery, the total current coming in is equal to the total current going out.

Find the total current I from i to j, then use Ohm's Law to define the effective resistance R_{ij} between i and j as $1/I$.

Electrical networks: resistance distance

Theorem

The effective resistance R_{ij} between vertices i and j is

$$R_{ij} = \left(L^-_{ii} + L^-_{jj} - 2L^-_{ij} \right).$$

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So

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In other words, variance is proportional to resistance distance.
Effective resistances are easy to calculate without matrix inversion if the graph is sparse.

So how do we find good designs?

The numbers v, b and k are specified to us.
It is rather rare for these to fit one of the theorems that guarantees a design to be A-optimal.
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So how do we find a good design?

1. Computer search.
2. Use patterns.
3. Accident.

Computer search

Except for very small designs,
exhaustive search is not usually feasible.
Here is one common approach.

1. Start with a random design.
2. Search among “close” designs
   (for example, swap a pair of treatments between blocks).
3. If a neighbouring design is better, move to it,
   and repeat from Step 2.
4. If no neighbouring design is better, record this design.
5. Repeat from Step 1 many times.
   Then choose the best of the recorded designs.

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The purpose of the last step is to avoid being stuck in a local optimum.

How successful is computer search?

It usually finds fairly good designs.

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However, if the optimal design has a high degree of symmetry, then it is often sitting on the top of a mountain with very steep sides, and so this approach will not find it.

Use patterns

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and then see if I can use the patterns in that
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- if $v = 12$ use the faces of a regular dodecahedron;
- if $v = 21$ use the points of the projective plane over the finite field with 4 elements.

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If the optimal design is highly symmetric,
this method can find it when computer search does not.

It usually finds good designs, but will not find the optimal one if none of the optimal ones is highly symmetric.

An example: $v = 10$, $b = 30$, $k = 2$ $(A = 2\sigma^2/(r\bar{V}))$

Method	Patterns	Search
Design	Treatments are all pairs from $\{1,2,3,4,5\}$. Two pairs form a block if they overlap.	Treatments are the vertices of a 6-cycle and 4 more points. Blocks are the edges of the 6-cycle, and all duos with one from the 6 and one from the 4.
$\bar{V}/\sigma^2$	0.63333	0.62698
A	0.52632	0.53165
Auto-morphisms	$5! = 120$	$12 \times 4! = 288$
	regular	more symmetries

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A block design is A-optimal if it minimizes the sum of the variances of the estimators of differences between varieties.

Square lattice designs

Yates (Rothamsted Experimental Station: 1936, 1937) introduced square lattice designs for this purpose.
The number of varieties has the form n^2 for some integer n, and each replicate consists of n blocks of n plots.

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The rows of this array form the blocks of the first replicate, and the columns of this array form the blocks of the second replicate.

Let r be the number of replicates. If $r > 2$ then $r - 2$ mutually orthogonal Latin squares of order n are needed. For each of these Latin squares, each letter determines a block of size n.

Mutually orthogonal Latin squares

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A pair of Latin squares of order n are orthogonal to each other if, when they are superposed, each letter of one occurs exactly once with each letter of the other.

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C	D	A	B
D	C	B	A

α	β	γ	δ
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Definition

A collection of Latin squares of the same order is mutually orthogonal if every pair is orthogonal.

Square lattice designs for 16 varieties in 2–4 replicates

1	2	3	4
5	6	7	8
9	10	11	12
13	14	15	16

A	B	C	D
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Replicate 4

1	2	3	4
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12	11	10	9
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Using a third Latin square orthogonal to the previous two Latin squares gives a fifth replicate, if required.

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Square lattice designs are resolvable and A-optimal.
All pairwise variety concurrences are in $\{0, 1\}$.

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There is not even a pair of mutually orthogonal Latin squares of order 6, so square lattice designs for 36 treatments are available for 2 or 3 replicates only.

Patterson and Williams (University of Edinburgh: 1976)
used computer search to find a design for
36 treatments in 4 replicates of blocks of size 6
with all concurrences in $\{0, 1, 2\}$.
The average variance is very little more than the unachievable lower bound.

A new design problem: sesqui-arrays

A sesqui-array of order n is an allocation of $n(n+1)$ letters to the cells of rectangle with $n+1$ rows and n^2 columns, satisfying conditions (i) and (ii) below.

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Example with $n = 3$

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A	*K*	*I*	*B*	*J*	*G*	*C*	*L*	*H*
J	*A*	*L*	*D*	*B*	*F*	*K*	*E*	*C*
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Condition (i) Each letter occurs in all rows except one.

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Condition (i) Each letter occurs in all rows except one.

Condition (ii) Each row has n letters in common with each column.

Constructing sesqui-arrays

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This motivated PJC to find a sesqui-array for $n = 6$.

Later, RAB found a simpler version of TN's construction, that needs a Latin square of order n but not orthogonal Latin squares. So $n = 6$ is covered. If this had been known earlier, PJC would not have found the nice design for $n = 6$.

Naughty but nice

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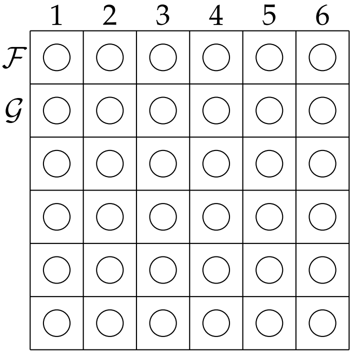
This can be used to construct the Sylvester graph,
which has 36 vertices, all with valency 5.

The Sylvester graph

The vertices can be thought of as the cells of a 6×6 grid.



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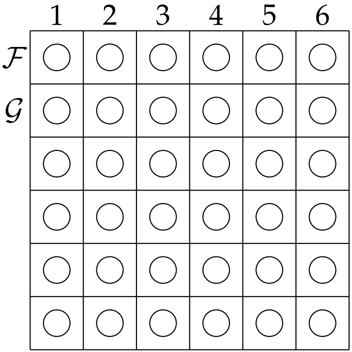

Rows are labelled by the one-factorizations (edge-colourings) of K_6.

$$\mathcal{F} = ||12|34|56||13|25|46||14|26|35||15|24|36||16|23|45||$$

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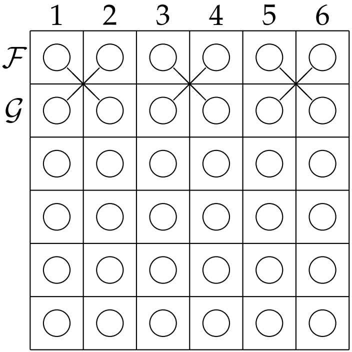

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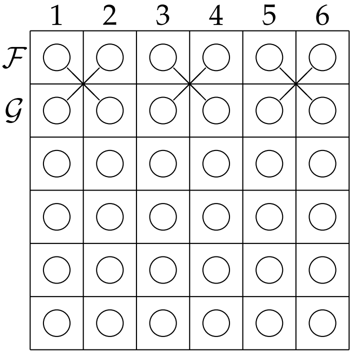

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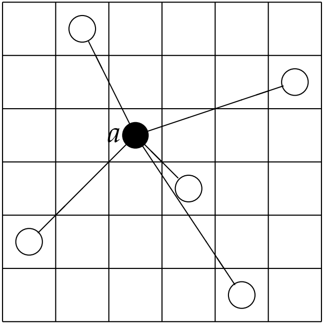
Automorphisms: S_6 on rows and on columns at the same time; the outer automorphism of S_6 swaps rows with columns.

The Sylvester graph and its starfish

At each vertex a, the *starfish* $S(a)$ defined by the 5 edges at a has 6 vertices, one in each row and one in each column.



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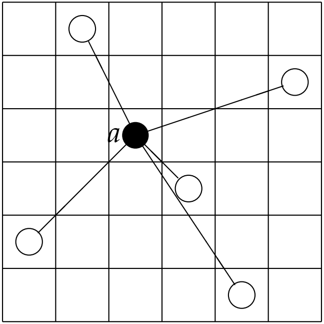

Use each starfish as a block of size 6.

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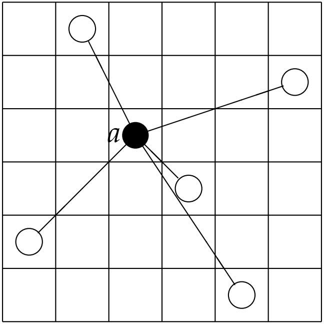

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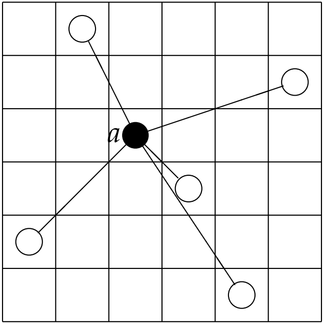
The *galaxy* of starfish with centres in a single column give a single replicate.

The Sylvester graph and its starfish

At each vertex a, the *starfish* $S(a)$ defined by the 5 edges at a has 6 vertices, one in each row and one in each column.



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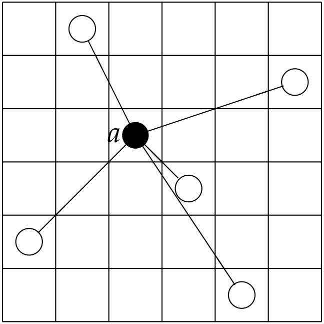

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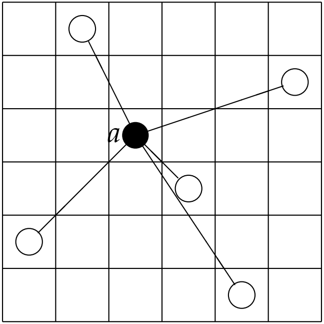

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Rows and columns give two further replicates, if needed.
All these designs have average variance very close to the unachievable lower bound.

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I gave a talk about these designs in August 2017
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These two designs have exactly the same value of $\bar{V}$,
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Our design has an automorphism group of order $2 \times 6! = 1440$
while Emlyn Williams' design has no automorphisms other than the identity.

But there is a permutation of the varieties taking one concurrence matrix to the other,
which explains why they have exactly the same value of $\bar{V}$.

Case 3

There are two or more systems of blocks.

An example of a two-phase experiment

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Now the design consists of one function allocating bean varieties to plots in the field, and another function allocating each plot to a run of the cooking machine.

Model when there are two systems of blocks

We measure the response Y on each sample.

If that sample is from a plot in block m with treatment i in Phase I and it is allocated to day n in Phase II, then we assume that

$$Y = \tau_i + \beta_m + \gamma_n + \text{random noise}.$$

To get rid of the β parameters and the γ parameters, we look at $(I - P_*)Y$, where P_* is the $N \times N$ matrix of orthogonal projection onto the space spanned by the characteristic vectors of the blocks in Phase I and the characteristic vectors of the days in Phase II.

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Let X be the $N \times v$ incidence matrix of treatments in experimental units.
The information matrix is $X^\top (I - P_*) X$.

Computer search

At a conference on variety-testing in Słupia Wielka, Poland, in June 2018, Nha Vo-Thanh (Universität Hohenheim) gave a talk explaining his work with Hans-Peter Piepho on several different methods of computer search to find a good design for this experiment.

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That evening, I got out some paper and a pen, and scribbled down some ideas, using my pattern approach. Very soon, I had a design with a smaller value of $\bar{V}$ than he had found.

Principle: Consider the smaller blocks first

The blocks in Phase II are smaller than those in Phase I,
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A	B	C	E	F	G	H	D	B	D	A	F	A	E	B
E	H	F	H	J	I	J	I	C	J	C	G	D	G	I
C	A	B	G	E	F	B	C	I	A	G	C	E	B	A
H	F	E	J	I	H	D	H	J	F	J	D	I	D	G

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E	H	F	H	J	I	J	I	C	J	C	G	D	G	I
C	A	B	G	E	F	B	C	I	A	G	C	E	B	A
H	F	E	J	I	H	D	H	J	F	J	D	I	D	G

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E	H	F	H	J	I	J	I	C	J	C	G	D	G	I
C	A	B	G	E	F	B	C	I	A	G	C	E	B	A
H	F	E	J	I	H	D	H	J	F	J	D	I	D	G

The non-intuitive step

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E	H	F	H	J	I	J	I	C	J	C	G	D	G	I
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A	*B*	*C*	*E*	*F*	*G*	*H*	*D*	*B*	*D*	*A*	*F*	*A*	*E*	*B*
E	*H*	*F*	*H*	*J*	*I*	*J*	*I*	*C*	*J*	*C*	*G*	*D*	*G*	*I*
C	*A*	*B*	*G*	*E*	*F*	*B*	*C*	*I*	*A*	*G*	*C*	*E*	*B*	*A*
H	*F*	*E*	*J*	*I*	*H*	*D*	*H*	*J*	*F*	*J*	*D*	*I*	*D*	*G*

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A	B	C	E	F	G	H	D	B	D	A	F	A	E	B
E	H	F	H	J	I	J	I	C	J	C	G	D	G	I
C	A	B	G	E	F	B	C	I	A	G	C	E	B	A
H	F	E	J	I	H	D	H	J	F	J	D	I	D	G

Use each row as a field block in Phase I.
The treatment information lost to field blocks is the same as the information lost to rectangles, which is part of the information already lost to days, so no further information is lost in Phase I.

A surprising theorem

Theorem

In a nested row-column design,
if the rows within each rectangle have exactly the same treatments
then the loss of information on treatment differences is the same
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then the loss of information on treatment differences is the same
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In this example, the best design for Phase I alone cannot be arranged as a nested row-column design with this property.

Comparison of designs

Design	computer search	patterns
A	0.80896	0.83333

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Two possibilities come to mind immediately.

12	13	14		12	13	14
34	24	23		23	34	24
14	12	13	and	14	12	13
23	34	24		34	24	23

How do those guys talk to each other?

Theorems

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↓

Folklore

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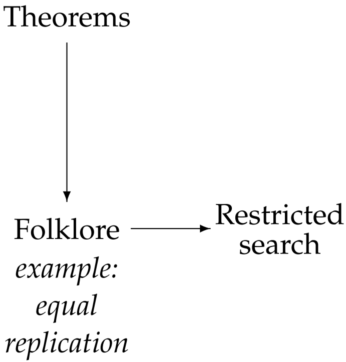
Theorems

↓

Folklore

example:
equal
replication

How do those guys talk to each other?



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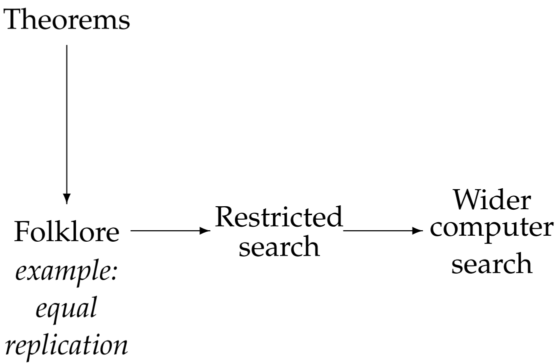

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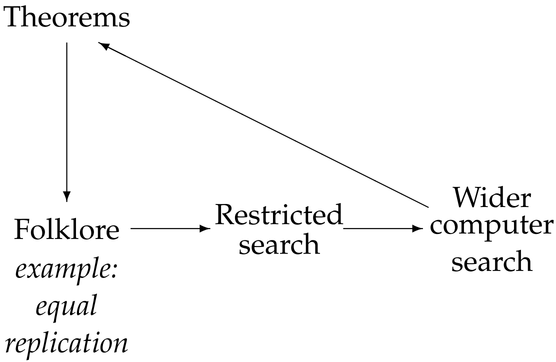

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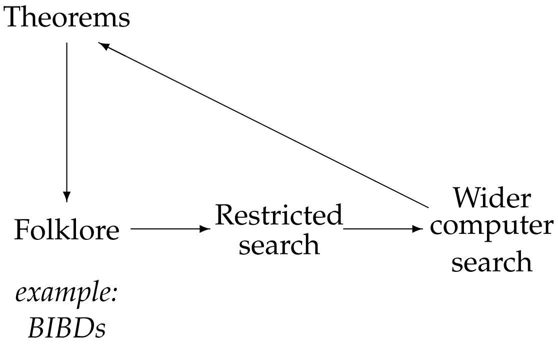

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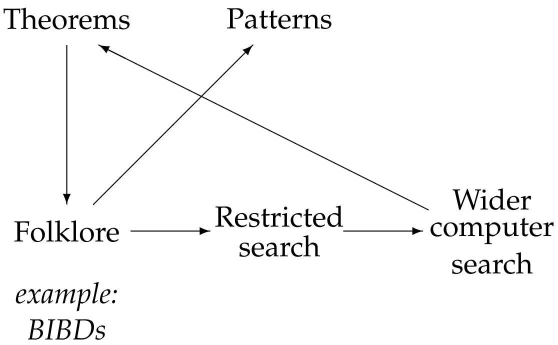

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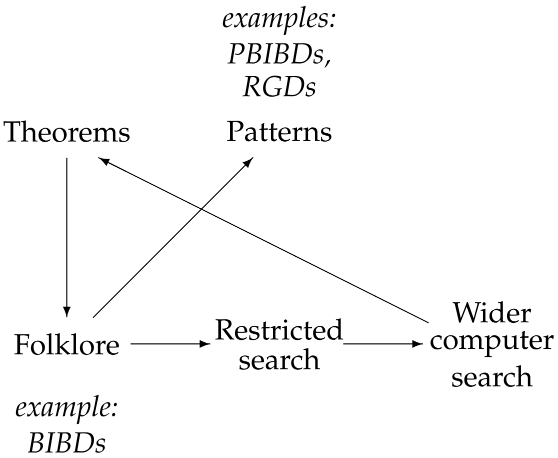

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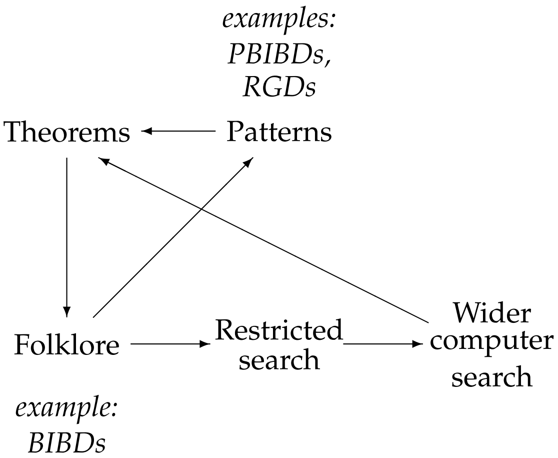

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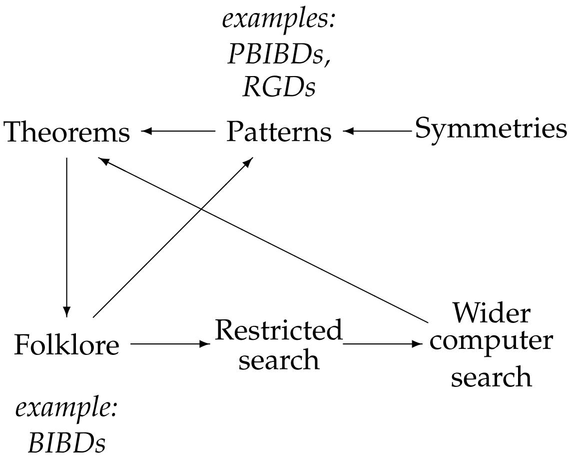

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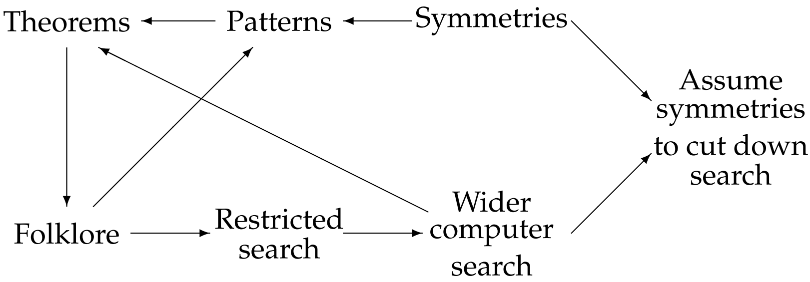

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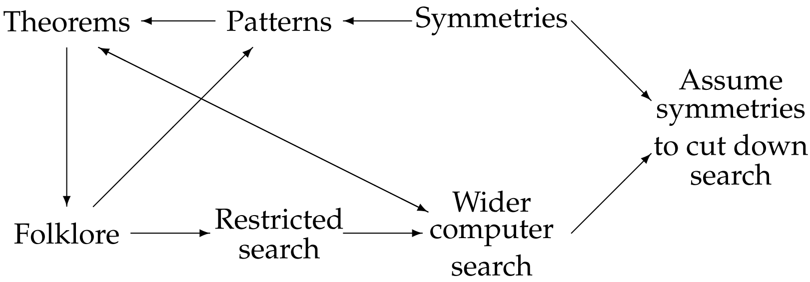

After I showed my design to NVT and HPP, they adapted their search method to incorporate that theorem

Conclusion

So—good luck with your search for good designs!

Which method will you use?