Treasure hunt: mistakes and wrong turnings in the search for good designs

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Joint work with Peter Cameron (University of St Andrews)
and Tomas Nilson (Mid-Sweden University)

Outline

1. Square lattice designs.
2. Triple arrays and sesqui-arrays.
3. How the new designs were discovered, part I.
4. Resolvable designs for 36 treatments in blocks of size 6.
5. How the new designs were discovered, part II.
6. What happened next.
7. Semi-Latin squares.
8. Comparison of designs.

Chapter 1

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(Some people call these *resolved* designs.
Williams (1977) called them *generalized lattice* designs.)

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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.

What is a Latin square?

Definition

Let n be a positive integer.
A Latin square of order n is an $n \times n$ array of cells in which n symbols are placed, one per cell, in such a way that each symbol occurs once in each row and once in each column.

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Here is a Latin square of order 4.

A	B	C	D
B	A	D	C
C	D	A	B
D	C	B	A

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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

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Replicate 1

1	5	9	13
2	6	10	14
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Replicate 2

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All pairwise variety concurrences are in $\{0, 1\}$.

Square lattice designs for n^2 varieties in rn blocks of n

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Construction

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

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If the replicates are large natural areas that might be damaged (for example, nearby crows eat all the crop, or heavy rain starts before the last replicate is harvested) then the loss of that replicate leaves another square lattice design.

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If $r = n + 1$ then all concurrences are equal to 1 and so the design is balanced.

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So $\mu_A \leq 1$, and a design maximizing μ_A, for given values of r and k and number of varieties, is A-optimal.

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Thus the aforementioned addition or removal of a replicate does not result in a poor design.

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Patterson and Williams (1976) used computer search to find a design for 36 treatments in 4 replicates of blocks of size 6.
All pairwise treatment concurrences are in $\{0, 1, 2\}$.
The value of its A-criterion μ_A is 0.836, which compares well with the unachievable upper bound of 0.840.

Chapter 2

Triple arrays and sesqui-arrays.

Triple arrays

Triple arrays were introduced independently by Preece (1966) and Agrawal (1966), and later named by McSorley, Phillips, Wallis and Yucas (2005).

They are row–column designs with r rows, c columns and v letters, satisfying the following conditions.

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Sterling and Wormald (1976) gave this triple array.

D	*H*	*F*	*L*	*E*	*K*	*I*	*G*	*J*
A	*K*	*I*	*B*	*J*	*G*	*C*	*L*	*H*
J	*A*	*L*	*D*	*B*	*F*	*K*	*E*	*C*
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If letters are blocks, rows are levels of treatment factor $T1$, columns are levels of treatment factor $T2$, and there is no interaction between $T1$ and $T2$, then this is a good design.

My coauthors

Tomas Nilson (left)
and
Peter Cameron (right)
at LinStat 2018
at Będlewo, Poland
in August 2018

Sesqui-arrays are a weakening of triple arrays

Cameron and Nilson introduced the weaker concept of sesqui-array by dropping the condition on pairs of columns. They are row–column designs with r rows, c columns and v letters, satisfying the following conditions.

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Chapter 3

How the new designs were discovered, part I.

The story: Part I

Consider designs with $n+1$ rows, n^2 columns and $n(n+1)$ letters. Triple arrays have been constructed for $n \in \{3,4,5\}$ by Agrawal (1966) and Sterling and Wormald (1976); for $n \in \{7,8,11,13\}$ by McSorley, Phillips, Wallis and Yucas (2005). There are values of n, such as $n=6$, for which a BIBD for n^2 treatments in $n(n+1)$ blocks of size n does not exist.

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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 $n = 6$.

Chapter 4

Resolvable designs for 36 treatments in blocks of size 6.

The Sylvester graph

The Sylvester graph Σ is a graph on 36 vertices with valency 5.

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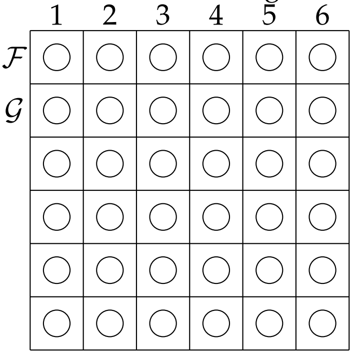

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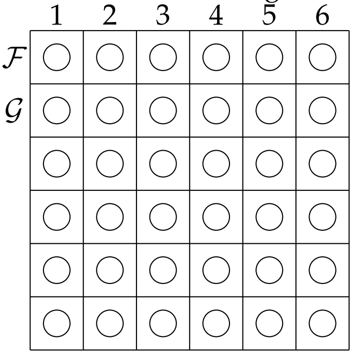

Rows are labelled by the one-factorizations (edge-colourings) of K_6.

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

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

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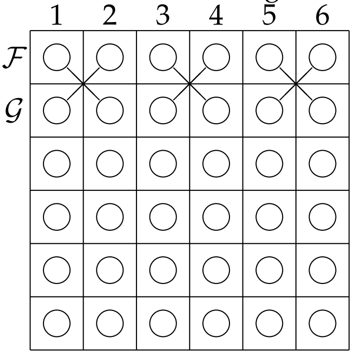

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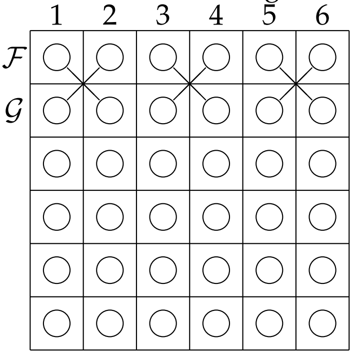

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Automorphisms: S_6 on rows and on columns at the same time; the outer automorphism of S_6 swaps rows with columns.

The Sylvester graph and its starfish

The Sylvester graph Σ has a transitive group of automorphisms (permutations of the vertices which take edges to edges), so it looks the same from each vertex.

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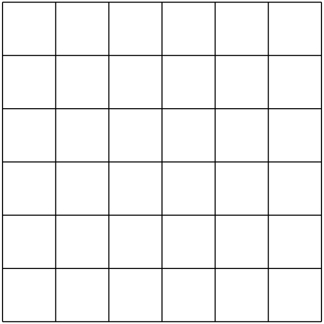

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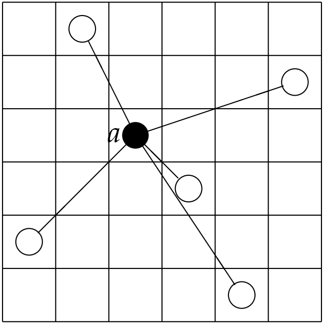
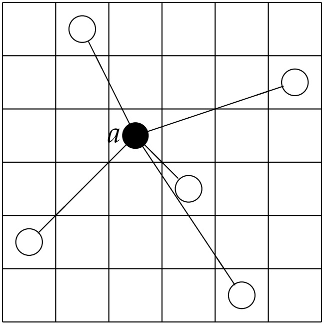


At each vertex a, the *starfish* $S(a)$ defined by the 5 edges at a has 6 vertices, one in each row and one in each column.

Pedantic naming



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I called this set of six vertices the spider centred at a.

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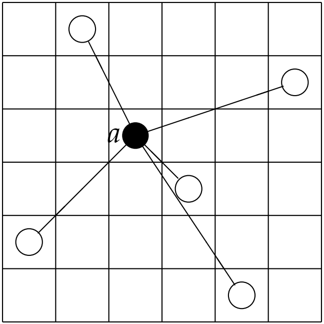
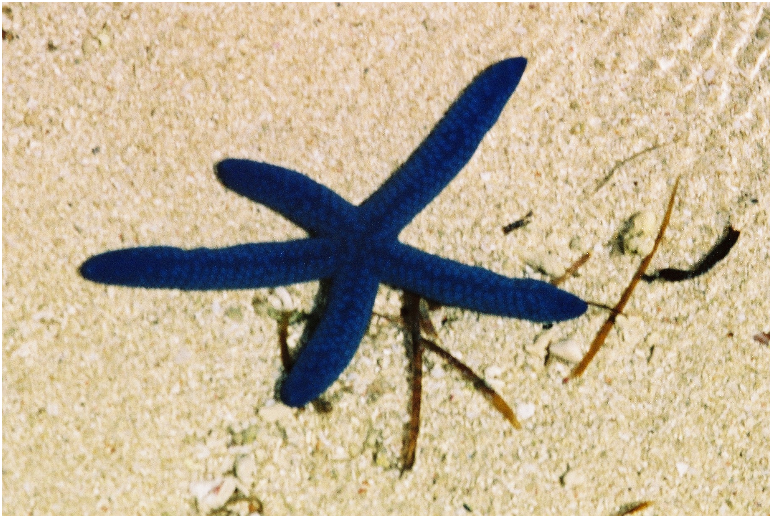


When I started to explain these ideas,
I called this set of six vertices the spider centred at a.
Peter Cameron pointed out that spiders usually have more than five legs, whereas some starfish have five.

A real starfish



Starfish whose centres are in the same column

		b			
					c
		a			

If there is an edge from a to c and an edge from b to c
then the starfish $S(c)$ has two vertices in the third column.

Starfish whose centres are in the same column

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This cannot happen,
so the starfish $S(a)$ and $S(b)$ have no vertices in common.

Starfish whose centres are in the same column

		b			
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If there is an edge from a to c and an edge from b to c
then the starfish $S(c)$ has two vertices in the third column.
This cannot happen,
so the starfish $S(a)$ and $S(b)$ have no vertices in common.

So, for any one column,
the 6 starfish centred on vertices in that column do not overlap,
and so they give a single replicate of 6 blocks of size 6.

The galaxy of starfish centered on column 3

D	A	B^*	C	E	F
F	E	C^*	B	D	A
E	B	A^*	D	F	C
B	F	D^*	A	C	E
A	C	E^*	F	B	D
C	D	F^*	E	A	B

The galaxy of starfish centered on column 3

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E	B	A^*	D	F	C
B	F	D^*	A	C	E
A	C	E^*	F	B	D
C	D	F^*	E	A	B

This is a Latin square.

Constructing resolved designs with r replicates

For $r = 2$ or $r = 3$:

Replicate 1	the blocks are the rows of the grid
Replicate 2	the blocks are the columns of the grid
Replicate 3	the blocks are the starfish of one particular column

Constructing resolved designs with r replicates

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For $r = 4$, $r = 5$, $r = 6$, $r = 7$ or $r = 8$ we can construct very efficient resolved designs using some of

all rows of the grid
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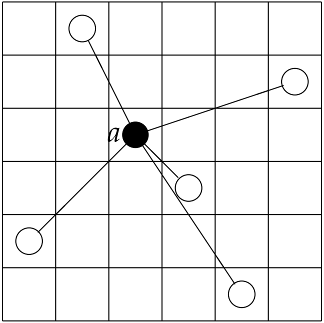
all starfish of some columns.

Note that, if there is an edge from a to c in the graph, then varieties a and c both occur in both starfish $S(a)$ and $S(c)$. So if we use the galaxies of starfish of two or more columns then some treatment concurrences will be bigger than 1.

More properties of the Sylvester graph



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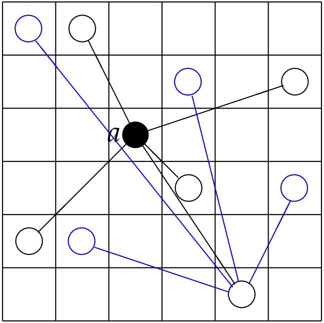

Vertices at distance 2 from a are all in rows and columns different from a.
The Sylvester graph has no triangles

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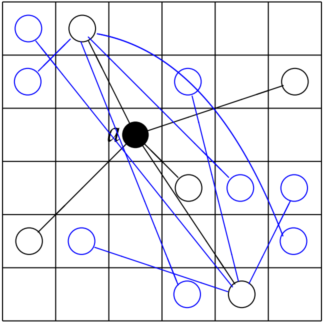

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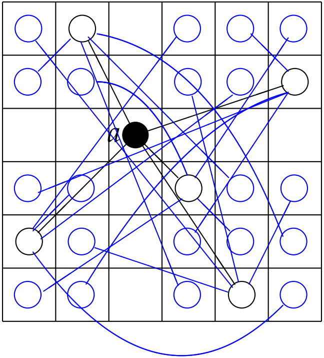


Vertices at distance 2 from a are all in rows and columns different from a.
The Sylvester graph has no triangles or quadrilaterals.

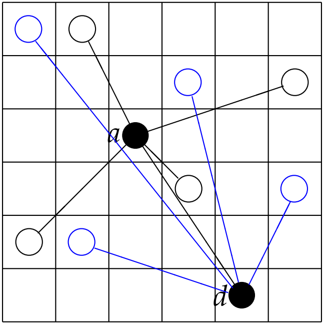
This implies that, if a is any vertex, the vertices at distance 2 from vertex a are precisely those vertices which are not in the starfish $S(a)$ or the row containing a or the column containing a.

Consquence I: concurrences

The Sylvester graph has no triangles or quadrilaterals.

Consequence

If we make each starfish into a block, then the only way that distinct treatments a and d can occur together in more than one block is for vertices a and d to be joined by an edge so that they both occur in the starfish $S(a)$ and $S(d)$.



Consquence II: association scheme

If a is any vertex, the vertices at distance 2 from vertex a are precisely those vertices which are not in the starfish $S(a)$ or the row containing a or the column containing a.

Consequence

The four binary relations:

- different vertices in the same row;
- different vertices in the same column;
- vertices joined by an edge in the Sylvester graph Σ;
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form an association scheme.

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form an association scheme.
So, for any incomplete-block design which is partially balanced with respect to this association scheme, the information matrix has five eigenspaces, which we know (in fact, they have dimensions 1, 5, 5, 9 and 16), so it is straightforward to calculate the eigenvalues and hence the canonical efficiency factors.

Our designs

$*^m$ galaxies of starfish from m columns, where $1 \leq m \leq 6$

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If $m = 6$ then the design is partially balanced
with respect to the association scheme just described
and so we can easily calculate the canonical efficiency factors.

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Otherwise, we use computational algebra (GAP) to calculate
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The large group of automorphisms tell us that

- the design R, $*^m$ has the same canonical efficiency factors as the design C, $*^m$;
- if we use the galaxies of starfish from m columns it does not matter which subset of m columns we use.

Constructing a PB resolved design with 6 replicates

For each column, make a replicate whose blocks are the 6 starfish whose centres are in that column.

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$$\text{concurrence} = \begin{cases} 2 & \text{for vertices joined by an edge} \\ 1 & \text{for vertices at distance 2} \\ 0 & \text{for vertices in the same row or column.} \end{cases}$$

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canonical efficiency factor	1	$\frac{8}{9}$	$\frac{3}{4}$
multiplicity	10	9	16

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The harmonic mean is $\mu_A = 0.8442$.

The unachievable upper bound given by the non-existent square lattice design is $\mu_A = 0.8537$.

Constructing a PB resolved design with 7 replicates

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canonical efficiency factor	1	$\frac{19}{21}$	$\frac{6}{7}$	$\frac{11}{14}$
multiplicity	5	9	5	16

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canonical efficiency factor	1	$\frac{19}{21}$	$\frac{6}{7}$	$\frac{11}{14}$
multiplicity	5	9	5	16

The harmonic mean is $\mu_A = 0.8507$.

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multiplicity	5	9	5	16

The harmonic mean is $\mu_A = 0.8507$.

The unachievable upper bound given by the non-existent square lattice design is $A = 0.8571$.

Constructing a PB resolved design with 8 replicates

For each column, make a replicate whose blocks are the 6 starfish whose centres are in that column.
For the 7-th replicate, the blocks are the columns.
For the 8-th replicate, the blocks are the rows.

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canonical efficiency factor	$\frac{11}{12}$	$\frac{7}{8}$	$\frac{13}{16}$
multiplicity	9	10	16

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canonical efficiency factor	$\frac{11}{12}$	$\frac{7}{8}$	$\frac{13}{16}$
multiplicity	9	10	16

The harmonic mean is $\mu_A = 0.8549$.

Constructing a PB resolved design with 8 replicates

For each column, make a replicate whose blocks are the 6 starfish whose centres are in that column.
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$$\text{concurrence} = \begin{cases} 2 & \text{for vertices joined by an edge} \\ 1 & \text{otherwise} \end{cases}$$

canonical efficiency factor	$\frac{11}{12}$	$\frac{7}{8}$	$\frac{13}{16}$
multiplicity	9	10	16

The harmonic mean is $\mu_A = 0.8549$.

The non-existent design consisting of a balanced design in 7 replicates with one more replicate adjoined would have $A = 0.8547$.

Values of μ_A for our designs

r	R, C, $*^{r-2}$	C, $*^{r-1}$	$*^r$	HDP/ERW 1976	square lattice
3	0.8235				0.8235
4	0.8380	0.8341	0.8285	0.836	0.8400
5	0.8453	0.8422	0.8383		0.8485
6	0.8498	0.8473	0.8442		0.8537
7	0.8528	0.8507			0.8571
8	0.8549				0.8547

Values of μ_A for our designs

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3	0.8235				0.8235
4	0.8380	0.8341	0.8285	0.836	0.8400
5	0.8453	0.8422	0.8383		0.8485
6	0.8498	0.8473	0.8442		0.8537
7	0.8528	0.8507			0.8571
8	0.8549				0.8547

Highlighted entries correspond to partially balanced designs.
Blue entries correspond to designs which do not exist.

Chapter 5

How the new designs were discovered, part II.

Back to the sesqui-arrays

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Back to the sesqui-arrays

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How do we take the one with 7 replicates and turn its dual into a 7×36 sesqui-array with 42 letters?

The story: Part II

RAB: I am typing up some of these new designs. Is your sesqui-array for $n = 6$ written out explicitly?

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A bit later, PJC: Oh no! My construction does not work after all.
Each column has the correct set of letters,
but their arrangement in rows is wrong,
because each row has some letters occurring 5 times.

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Each column has the correct set of letters,
but their arrangement in rows is wrong,
because each row has some letters occurring 5 times.

	1	2	3	4	5	6	← six sets of six columns
$*$	1	2	3	4	5	6	← six sets of six letters
1	$*$	1	1	1	1	1	
2	2	$*$	2	2	2	2	
3	3	3	$*$	3	3	3	
4	4	4	4	$*$	4	4	
5	5	5	5	5	$*$	5	
6	6	6	6	6	6	$*$	

Forestry to the rescue

Later, PJC: The only hope of putting this right is to permute the letters in each column. I need 6 permutations. Each fixes the first row and one other. The rest of each permutation gives a circle on the other 5 rows, and I want these circles to have every row following each other row exactly once.

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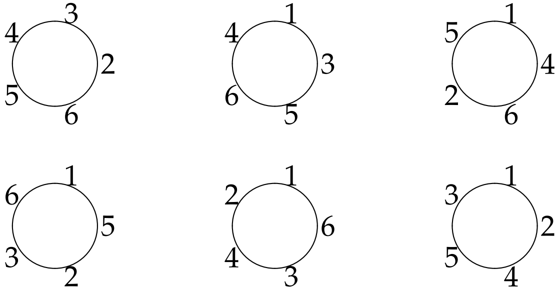
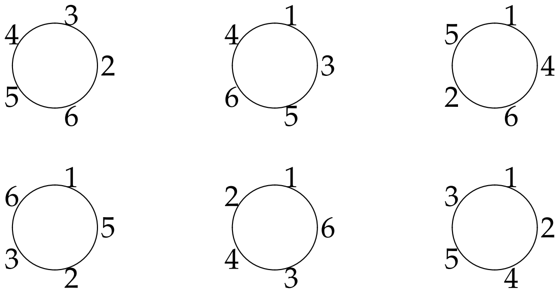


How does that work then?



	1	2	3	4	5	6
*	1	2	3	4	5	6
1	*	1	1	1	1	1
2	2	*	2	2	2	2
3	3	3	*	3	3	3
4	4	4	4	*	4	4
5	5	5	5	5	*	5
6	6	6	6	6	6	*

← sets of six columns

← sets of six letters

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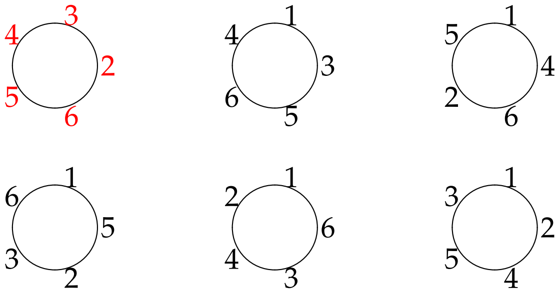

	1	2	3	4	5	6	← sets of six columns
*	1	2	3	4	5	6	← sets of six letters
1	*	1	1	1	1	1	
2	3	*	2	2	2	2	
3	4	3	*	3	3	3	
4	5	4	4	*	4	4	
5	6	5	5	5	*	5	
6	2	6	6	6	6	*	

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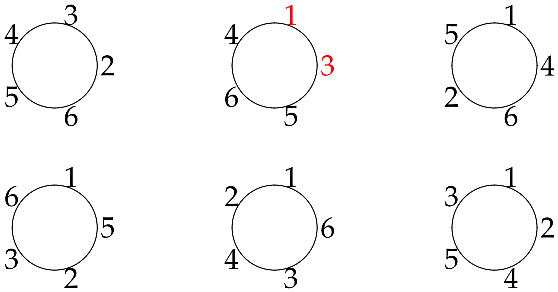

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1	*	1	1	1	1	1	
2	3	*	2	2	2	2	
3	4	3	*	3	3	3	
4	5	4	4	*	4	4	
5	6	5	5	5	*	5	
6	2	6	6	6	6	*	

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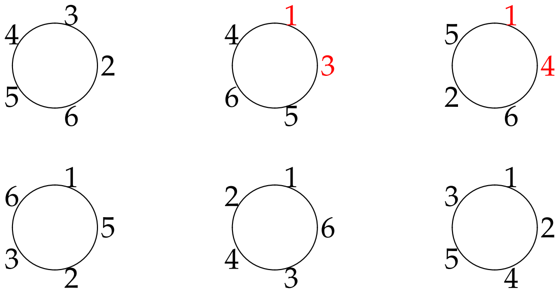

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1	*	1	1	1	1	1
2	3	*	2	2	2	2
3	4	3	*	3	3	3
4	5	4	4	*	4	4
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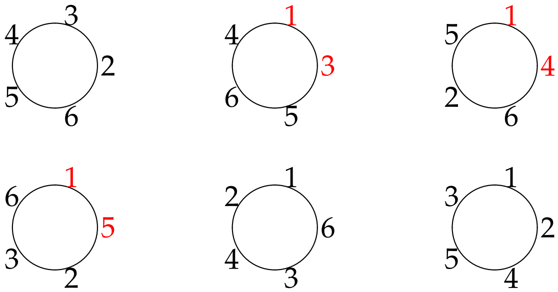

	1	2	3	4	5	6
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1	*	1	1	1	1	1
2	3	*	2	2	2	2
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4	5	4	4	*	4	4
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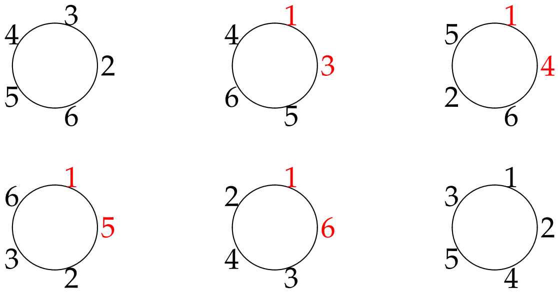

	1	2	3	4	5	6
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1	*	1	1	1	1	1
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3	4	3	*	3	3	3
4	5	4	4	*	4	4
5	6	5	5	5	*	5
6	2	6	6	6	6	*

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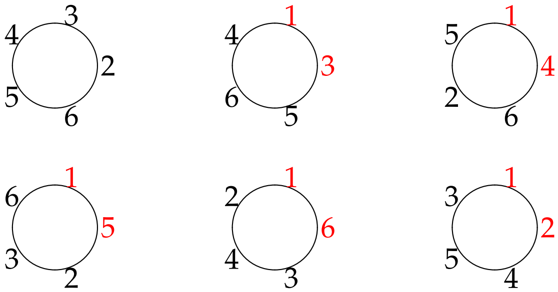

	1	2	3	4	5	6
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1	*	1	1	1	1	1
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3	4	3	*	3	3	3
4	5	4	4	*	4	4
5	6	5	5	5	*	5
6	2	6	6	6	6	*

← sets of six columns

← sets of six letters

Chapter 6

What happened next.

Personal communication from Emlyn Williams

I gave a talk about these designs in August 2017
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He emailed me these results in September 2017.

Another connection

I gave another talk about these designs in February 2018 in a seminar in St Andrews.

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I gave another talk about these designs in February 2018 in a seminar in St Andrews.

As I was preparing the talk (the day before),
I realised a connection with some other designs that I have studied, called semi-Latin squares.

Chapter 7

Semi-Latin squares.

What is a semi-Latin square?

Definition

A $(n \times n)/s$ semi-Latin square is an arrangement of ns letters in n^2 blocks of size s
which are laid out in a $n \times n$ square in such a way that each letter occurs once in each row and once in each column.

A $(6 \times 6)/2$ semi-Latin square

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

A $(6 \times 6)/2$ semi-Latin square

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

This one is not made from two Latin squares.

A $(6 \times 6)/2$ semi-Latin square

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

This one is not made from two Latin squares.

Automorphisms:
A_5 on rows, columns and letters at the same time;
reflection in the main diagonal, with
$(A\,L)(B\,J)(D\,G)(C\,K)(E\,H)(F\,I)$.

The semi-Latin square made from the galaxies of starfish centered on columns 3 and 4

$D \quad \zeta$	$A \quad \epsilon$	$B^* \quad \beta$	$C \quad \gamma^+$	$E \quad \delta$	$F \quad \alpha$
$F \quad \delta$	$E \quad \alpha$	$C^* \quad \gamma$	$B \quad \beta^+$	$D \quad \epsilon$	$A \quad \zeta$
$E \quad \beta$	$B \quad \zeta$	$A^* \quad \alpha$	$D \quad \delta^+$	$F \quad \gamma$	$C \quad \epsilon$
$B \quad \epsilon$	$F \quad \beta$	$D^* \quad \delta$	$A \quad \alpha^+$	$C \quad \zeta$	$E \quad \gamma$
$A \quad \gamma$	$C \quad \delta$	$E^* \quad \epsilon$	$F \quad \zeta^+$	$B \quad \alpha$	$D \quad \beta$
$C \quad \alpha$	$D \quad \gamma$	$F^* \quad \zeta$	$E \quad \epsilon^+$	$A \quad \beta$	$B \quad \delta$

*centre of Latin starfish $\qquad$ $^+$centre of Greek starfish

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If a Trojan square exists, then it is optimal among semi-Latin squares of that size.

What are the optimal ones when $n = 6$?

From semi-Latin square to block design

Suppose that we have a $(n \times n)/s$ semi-Latin square.

Construction

1. Write the varieties in an $n \times n$ square array.
2. Each of the ns letters gives a block of n varieties.

From semi-Latin square to block design

Suppose that we have a $(n \times n)/s$ semi-Latin square.

Construction

1. Write the varieties in an $n \times n$ square array.
2. Each of the ns letters gives a block of n varieties.

If the semi-Latin square is made by superposing s Latin squares then the block design is resolvable.

Good leads to good

Theorem

If the block design has A-criterion μ_A and the semi-Latin square has A-criterion λ_A then

$$\frac{35}{\mu_A} = 6(6-s) + \frac{6s-1}{\lambda_A}.$$

Good leads to good

Theorem

If the block design has A-criterion μ_A and the semi-Latin square has A-criterion λ_A then

$$\frac{35}{\mu_A} = 6(6-s) + \frac{6s-1}{\lambda_A}.$$

So maximizing μ_A is the same as maximizing λ_A (among semi-Latin squares which are superpositions of Latin squares, if we insist on resolvable designs).

What is known about good semi-Latin squares with $n = 6$?

Good designs have been found by RAB, Gordon Royle and Leonard Soicher, partly by computer search. Independently, Brickell (1984) found some in communications theory.

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The table shows values of λ_A.

not superposed Latin squares

s	$*^s$	Brickell RAB 1990	RAB/GR 1997	Brickell LHS web	LHS 2013	Trojan square
2	0.4889	0.5127	0.5133		0.5116	0.5238
3	0.6730			0.6922	0.6745	0.6939
4	0.7604				0.7614	0.7753
5	0.8111				0.8111	0.8227
6	0.8442				0.8442	0.8537

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partially balanced — do not exist

Semi-Latin square to block design: again

Just as with the designs made from the Sylvester graph, if we make a block design from a semi-Latin square then we have the option of including another replicate whose blocks are the rows and another replicate whose blocks are the columns.

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Just as with the designs made from the Sylvester graph, if we make a block design from a semi-Latin square then we have the option of including another replicate whose blocks are the rows and another replicate whose blocks are the columns.

As before, these two special replicates give us better designs than just using a semi-Latin square with 12 more letters.

Chapter 8

Comparison of designs.

Comparing the values of μ_A for the new designs

For $r = 2$ and $r = 3$ the designs in all three of the new series are square lattice designs.

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For $4 \leq r \leq 7$ the designs in all three series have efficiency factors μ_A not far below the unachievable upper bound.
For $r = 8$, they all do better than a balanced square lattice design with one replicate duplicated.

r	RAB/PJC R, C, $*^{r-2}$	LHS +R, C	ERW	square lattice
4	0.8380	0.8393	0.8393	0.8400
5	0.8453	0.8456	0.8464	0.8485
6	0.8498	0.8501	0.8510	0.8537
7	0.8528	0.8528	0.8542	0.8571
8	0.8549	0.8549	0.8549	0.8547

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If two designs are isomorphic
then their efficiency factors are the same,
but the converse may not be true.

Are any of these designs the same?

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It is possible that the LHS and ERW designs for $r = 4$ are isomorphic, and that the RAB/PJC and LHS designs for $r = 7$ are isomorphic.

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It is possible that the LHS and ERW designs for $r = 4$ are isomorphic, and that the RAB/PJC and LHS designs for $r = 7$ are isomorphic. Otherwise, for $4 \leq r \leq 7$, the efficiency factors of the three new designs differ slightly, so no pair of the new designs are isomorphic.

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For $r = 8$, all three new designs have the same efficiency factor. Their concurrence matrices are the same up to permutation of the treatments. Their automorphism groups have order 1440, 144 and 1 respectively, so no pair are isomorphic.