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

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Outline

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2. Triple arrays and sesqui-arrays.
3. How the new designs were discovered, part I.
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5. How the new designs were discovered, part II.
6. What happened next.
7. Semi-Latin squares.
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Chapter 1

Square lattice designs.

Resolvable block designs

Trials of new crop varieties typically have a large number of varieties.
Even at a well-run testing centre,
inhomogeneity among the plots (experimental units) makes it desirable to group the plots into homogeneous blocks,
usually too small to contain all the varieties.
For management reasons, it is often convenient if the blocks can themselves be grouped into replicates, in such a way that each variety occurs exactly once in each replicate. Such a block design is called resolvable.
(Some people call these *resolved* designs.
Williams (1977) called them *generalized lattice* designs.)

Square lattice designs

Yates (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.
Imagine the varieties listed in an abstract $n \times n$ square array.
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.

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.

Here is a Latin square of order 4.

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

Mutually orthogonal Latin squares

Definition
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.

Here are a pair of orthogonal Latin squares of order 4.

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

α	β	γ	δ
γ	δ	α	β
δ	γ	β	α
β	α	δ	γ

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

α	β	γ	δ
γ	δ	α	β
δ	γ	β	α
β	α	δ	γ

Replicate 1

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

Replicate 2

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

Replicate 3

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

Replicate 4

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

Using a third Latin square orthogonal to the previous two Latin squares gives a fifth replicate, if required.

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

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

Square lattice designs for n^2 varieties, arranged in r replicates, each replicate consisting of n blocks of size n.

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 $i - 2$.

Good property I: Last-minute changes or area damage

Adding or removing a replicate to/from a square lattice design gives another square lattice design, which can permit last-minute changes in the number of replicates used.

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.

Good property II: Nearly equal concurrences

The concurrence of two varieties is the number of blocks in which they both occur.

It is widely believed that good designs have all concurrences as equal as possible, and so this condition is often used in the search for good designs.

In square lattice designs, all concurrences are equal to 0 or 1.

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

Efficiency factors and optimality

Given an incomplete-block design for a set $\mathcal{T}$ of 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, and the scaled information matrix is $I - (rk)^{-1}\Lambda$.

The constant vectors are in the null space of the scaled information matrix.

The eigenvalues for the other eigenvectors are called canonical efficiency factors: the larger the better.

Let μ_A be the harmonic mean of the canonical efficiency factors.

The average variance of the estimate of a difference between two varieties in this design is

$$\frac{1}{\mu_A} \times \begin{array}{l}\text{the average variance in an experiment}\\ \text{with the same resources but no blocks}\end{array}$$

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.

Good property III: Optimality

Cheng and Bailey (1991) showed that, if $r \leq n+1$, square lattice designs are optimal among block designs of this size, even over non-resolvable designs.

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

We have a problem when $n = 6$

If $n \in \{2,3,4,5,7,8,9\}$ then there is a complete set of $n-1$ mutually orthogonal Latin squares of order n.

Using these gives a square lattice design for n^2 treatments in $n(n+1)$ blocks of size n, which is a balanced incomplete-block design.

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 (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.

- (A1) There is exactly one letter in each row–column intersection.
- (A2) No letter occurs more than once in any row or column.
- (A3) Each letter occurs k times, where $k > 1$ and $vk = rc$.
- (A4) The number of letters common to any row and column is k.
- (A5) The number of letters common to any two rows is the non-zero constant $c(k-1)/(r-1)$.
- (A6) The number of letters common to any two columns is the non-zero constant $r(k-1)/(c-1)$.

A triple array with $r = 4$, $c = 9$, $v = 12$ and $k = 3$

- (A4) The number of letters common to any row and column is $k = 3$.
- (A5) The number of letters common to any two rows is the non-zero constant $c(k-1)/(r-1) = 6$.
- (A6) The number of letters common to any two columns is the non-zero constant $r(k-1)/(c-1) = 1$.

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
G	E	A	H	I	B	D	C	F

Why triple arrays?

- (A4) The number of letters common to any row and column is $k = 3$.
- (A5) The number of letters common to any two rows is the non-zero constant $c(k-1)/(r-1) = 6$.
- (A6) The number of letters common to any two columns is the non-zero constant $r(k-1)/(c-1) = 1$.
- (A5) Rows are balanced with respect to letters.
- (A6) Columns are balanced with respect to letters.
- (A4) Rows and columns are orthogonal to each other after they have been adjusted for letters.

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.

(A1) There is exactly one letter in each row–column intersection.

(A2) No letter occurs more than once in any row or column.

(A3) Each letter occurs k times, where $k > 1$ and $vk = rc$.

(A4) The number of letters common to any row and column is k.

(A5) The number of letters common to any two rows is the non-zero constant $c(k-1)/(r-1)$.

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.

By weakening triple array to sesqui-array, TN and PJC hoped to give a construction for all n.

TN found a general construction, using a pair of mutually orthogonal Latin squares of order n. So this works for all positive integers n except for $n \in \{1,2,6\}$.

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

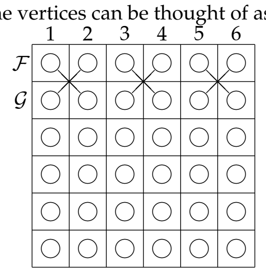
Later, RAB found a simpler version of TN's construction, that needs a Latin square of order n but not orthogonal Latin squares. So $n = 6$ is covered. If this had been known earlier, PJC would not have found the nice design for $n = 6$.

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



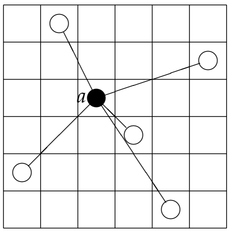
Rows are labelled by the one-factorizations (edge-colourings) of K_6.

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

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

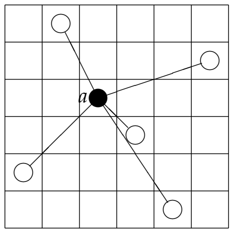
The Sylvester graph and its starfish

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.



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.

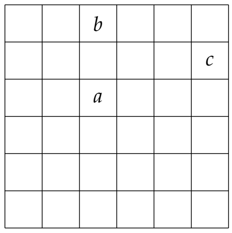
Pedantic naming



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



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

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

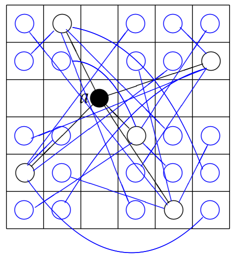
These are square lattice designs.

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
all columns of the grid
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



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

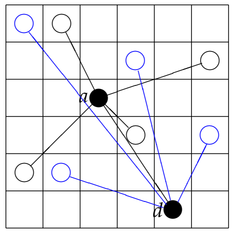
This implies that, if a is any vertex, the vertices at distance 2 from vertex a are precisely those vertices which are not in the starfish $S(a)$ or the row containing a or the column containing a.

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;
- vertices at distance 2 in Σ

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 $1 \leq m \leq 6$
R, $*^m$	all rows; galaxies of starfish from m columns
C, $*^m$	all columns; galaxies of starfish from m columns
R, C, $*^m$	all rows; all columns; galaxies of starfish from m columns,

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. Otherwise, we use computational algebra (GAP) to calculate them exactly.

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.

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

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

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

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.

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

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

The harmonic mean is $\mu_A = 0.8507$.

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.

$$\text{concurrence} = \begin{cases} 2 & \text{for vertices joined by an edge} \\ 1 & \text{otherwise} \end{cases}$$

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

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

These wonderful designs are a fortunate byproduct of a wrong turning in the search for sesqui-arrays.

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?

PJC: Not yet. I will just program GAP to do it for me.

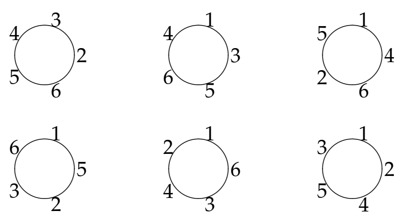
A bit later, PJC: Oh no! My construction does not work after all.
Each column has the correct set of letters,
but their arrangement in rows is wrong,
because each row has some letters occurring 5 times.

	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	$*$	

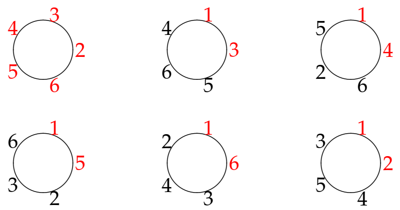
Forestry to the rescue

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.

RAB: Easy peasy. That is a neighbour-balanced design for 6 treatments in 6 circular blocks of size 5. I made one of those for experiments in forestry 25 years ago.



How does that work then?



	1	2	3	4	5	6
$*$	1	2	3	4	5	6
1	$*$	1	1	1	1	1
2	23	$*$	2	2	2	2
3	34	3	$*$	3	3	3
4	45	4	4	$*$	4	4
5	56	5	5	5	$*$	5
6	62	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
at the meeting on *Latest advances in the theory and applications of design and analysis of experiments*
in the Banff International Research Station in Canada.

They video all lectures, and make them available on the web.

Emlyn Williams learnt about this,
and watched the video of my lecture.

This motivated him to re-run that computer search from the 1970s with a more up-to-date version of his search program on a more up-to date computer.

Thus he found resolvable designs for 36 varieties in up to eight replicates of blocks of size six.

All concurrences are in $\{0,1,2\}$.

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.

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

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 ζ	A ϵ	B^* β	C γ^+	E δ	F α
F δ	E α	C^* γ	B β^+	D ϵ	A ζ
E β	B ζ	A^* α	D δ^+	F γ	C ϵ
B ϵ	F β	D^* δ	A α^+	C ζ	E γ
A γ	C δ	E^* ϵ	F ζ^+	B α	D β
C α	D γ	F^* ζ	E ϵ^+	A β	B δ

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

Trojan squares

Definition
If a semi-Latin square is made by superposing s mutually orthogonal $n \times n$ Latin squares then it is called a Trojan square.

A semi-Latin square does not have to be made by superposing Latin squares.

Theorem
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.

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

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

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.
In 2013, LHS gave a $(6 \times 6)/6$ semi-Latin square made superposing Latin squares,
so it gives $(6 \times 6)/s$ semi-Latin squares for $2 \leq s \leq 6$.
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

partially balanced $\qquad$ 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.

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.
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

Are any of the new designs the same?

Two block designs are isomorphic
if one can be converted into the other by
a permutation of varieties and a permutation of blocks.

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

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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.

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.