

# Optimal Designs for Diallel Experiments

R. A. Bailey



r.a.bailey@qmul.ac.uk

Sixth International Triennial Calcutta Symposium on Probability  
and Statistics  
December 2006

# Abstract

In a **half-diallel** experiment, the treatments are effectively the unordered pairs from a set of parental lines.

# Abstract

In a half-diallel experiment, the treatments are effectively the unordered pairs from a set of parental lines.

If the response can be modelled as the analogue of main effects (called **general combining ability** in the diallel case) then the experiment need not include all pairs.

In a half-diallel experiment, the treatments are effectively the unordered pairs from a set of parental lines.

If the response can be modelled as the analogue of main effects (called general combining ability in the diallel case) then the experiment need not include all pairs.

Then the experiment becomes formally equivalent to an **incomplete-block design** in which only block totals are measured.

In a half-diallel experiment, the treatments are effectively the unordered pairs from a set of parental lines.

If the response can be modelled as the analogue of main effects (called general combining ability in the diallel case) then the experiment need not include all pairs.

Then the experiment becomes formally equivalent to an incomplete-block design in which only block totals are measured.

Except in special cases, designs which are optimal for one situation may be very bad for the other one. Although Curnow noted this forty years ago, his results seem to have been ignored.

# Abstract

In a half-diallel experiment, the treatments are effectively the unordered pairs from a set of parental lines.

If the response can be modelled as the analogue of main effects (called general combining ability in the diallel case) then the experiment need not include all pairs.

Then the experiment becomes formally equivalent to an incomplete-block design in which only block totals are measured.

Except in special cases, designs which are optimal for one situation may be very bad for the other one. Although Curnow noted this forty years ago, his results seem to have been ignored.

I shall state a result which gives optimality in some special cases and use this as a heuristic guide to optimality more generally.

Treatments are unordered pairs from  $n$  parental lines,  
because  $\{i,j\}$  represents the cross between line  $i$  and line  $j$ .

Treatments are unordered pairs from  $n$  parental lines, because  $\{i,j\}$  represents the cross between line  $i$  and line  $j$ .

If we assume that the specific combining ability is zero, then the model is

$$\mathbf{E}(Y_{\{i,j\}}) = \alpha_i + \alpha_j$$

where  $\alpha_i$  is the **general combining ability** for parental type  $i$ .

A design for this model is formally equivalent to an incomplete-block design for  $n$  treatments in blocks of size 2 where we can analyse only the block totals.

A design for this model is formally equivalent to an incomplete-block design for  $n$  treatments in blocks of size 2 where we can analyse only the block totals.

Kempthorne and Curnow noticed this in 1961.

A design for this model is formally equivalent to an incomplete-block design for  $n$  treatments in blocks of size 2 where we can analyse only the block totals.

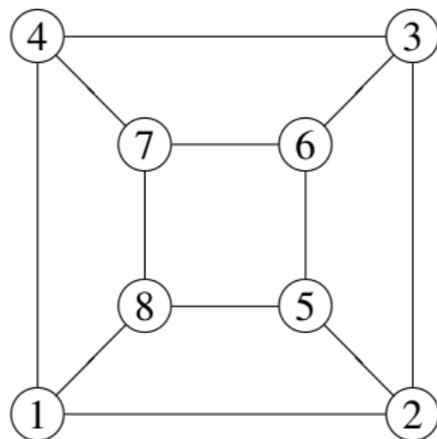
Kempthorne and Curnow noticed this in 1961.

If there are  $n$  parental lines and the replication is  $r$ , the design can be represented by a graph with  $n$  vertices and valency  $r$ : each edge represents a cross that is used in the experiment.

## Example of a design shown as a graph

The pairs are:

$\{1,2\}$ ,  $\{1,4\}$ ,  $\{1,8\}$ ,  $\{2,3\}$ ,  $\{2,5\}$ ,  $\{3,4\}$   $\{3,6\}$ ,  $\{4,7\}$ ,  $\{5,6\}$ ,  
 $\{5,8\}$ ,  $\{6,7\}$ ,  $\{7,8\}$ .



# Balance

An incomplete-block design is said to be **balanced** if every pair of distinct treatments occurs in the same number of blocks.

An incomplete-block design is said to be **balanced** if every pair of distinct treatments occurs in the same number of blocks.

When the blocks have size two, a design can be balanced only if all possible pairs occur as blocks, the same number of times.

An incomplete-block design is said to be **balanced** if every pair of distinct treatments occurs in the same number of blocks.

When the blocks have size two, a design can be balanced only if all possible pairs occur as blocks, the same number of times.

For the model with no specific combining ability we should be able to estimate the general combining abilities from far fewer blocks.

# Balance

An incomplete-block design is said to be **balanced** if every pair of distinct treatments occurs in the same number of blocks.

When the blocks have size two, a design can be balanced only if all possible pairs occur as blocks, the same number of times.

For the model with no specific combining ability we should be able to estimate the general combining abilities from far fewer blocks.

How should we choose which pairs to use?

# What makes an incomplete-block design good? (1)

Put  $\lambda_{ij} =$  number of blocks containing  $i$  and  $j$  if  $i \neq j$

$$\lambda_{ii} = r$$

$$\Lambda = [\lambda_{ij}].$$

# What makes an incomplete-block design good? (1)

Put  $\lambda_{ij}$  = number of blocks containing  $i$  and  $j$  if  $i \neq j$   
 $\lambda_{ii}$  =  $r$   
 $\Lambda$  =  $[\lambda_{ij}]$ .

The matrix  $I - \frac{1}{2r}\Lambda$  has eigenvalue 0 on the all-1 vector.

The other eigenvalues  $\epsilon_1, \epsilon_2, \dots, \epsilon_{n-1}$  are called the **canonical efficiency factors** in the within-blocks stratum.

# What makes an incomplete-block design good? (1)

Put  $\lambda_{ij}$  = number of blocks containing  $i$  and  $j$  if  $i \neq j$   
 $\lambda_{ii}$  =  $r$   
 $\Lambda$  =  $[\lambda_{ij}]$ .

The matrix  $I - \frac{1}{2r}\Lambda$  has eigenvalue 0 on the all-1 vector.

The other eigenvalues  $\varepsilon_1, \varepsilon_2, \dots, \varepsilon_{n-1}$  are called the **canonical efficiency factors** in the within-blocks stratum.

Put  $A$  = harmonic mean of  $\varepsilon_1, \varepsilon_2, \dots, \varepsilon_{n-1}$ .

Then the average pairwise variance is  $\frac{1}{rA}\sigma^2$ .

## What makes an incomplete-block design good? (2)

There are **canonical efficiency factors**

$$\begin{array}{ll} \varepsilon_1, \varepsilon_2, \dots, \varepsilon_{n-1} & \text{in the within-blocks stratum} \\ \varepsilon_1^*, \varepsilon_2^*, \dots, \varepsilon_{n-1}^* & \text{in the between-blocks stratum} \end{array}$$

where  $\varepsilon_i^* = 1 - \varepsilon_i$ .

## What makes an incomplete-block design good? (2)

There are **canonical efficiency factors**

$$\begin{array}{ll} \varepsilon_1, \varepsilon_2, \dots, \varepsilon_{n-1} & \text{in the within-blocks stratum} \\ \varepsilon_1^*, \varepsilon_2^*, \dots, \varepsilon_{n-1}^* & \text{in the between-blocks stratum} \end{array}$$

where  $\varepsilon_i^* = 1 - \varepsilon_i$ .

For the usual (within-blocks) analysis,  
an incomplete-block design is optimal if it maximizes

$$A = \text{harmonic mean of } \varepsilon_1, \varepsilon_2, \dots, \varepsilon_{n-1}$$

## What makes an incomplete-block design good? (2)

There are **canonical efficiency factors**

$$\begin{array}{ll} \varepsilon_1, \varepsilon_2, \dots, \varepsilon_{n-1} & \text{in the within-blocks stratum} \\ \varepsilon_1^*, \varepsilon_2^*, \dots, \varepsilon_{n-1}^* & \text{in the between-blocks stratum} \end{array}$$

where  $\varepsilon_i^* = 1 - \varepsilon_i$ .

For the usual (within-blocks) analysis,  
an incomplete-block design is optimal if it maximizes

$$A = \text{harmonic mean of } \varepsilon_1, \varepsilon_2, \dots, \varepsilon_{n-1}$$

For our analysis (using only block totals), an incomplete-block design  
is optimal if it maximizes

$$A^* = \text{harmonic mean of } \varepsilon_1^*, \varepsilon_2^*, \dots, \varepsilon_{n-1}^*.$$

# Good and bad news

## Easy Theorem

$$\begin{array}{ccc} \text{balance} & & \\ \updownarrow & & \\ \epsilon_1 = \dots = \epsilon_{n-1} & \iff & \epsilon_1^* = \dots = \epsilon_{n-1}^* \\ \updownarrow & & \updownarrow \\ A \text{ is maximal} & & A^* \text{ is maximal} \end{array}$$

# Good and bad news

## Easy Theorem

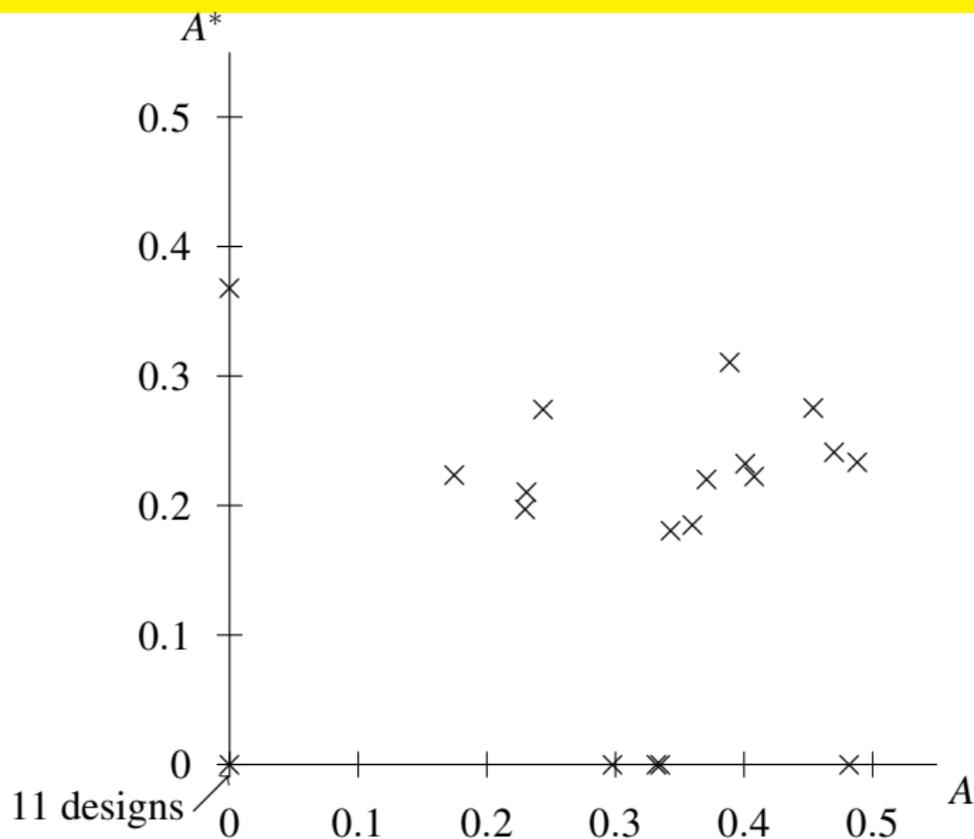
$$\begin{array}{ccc} \text{balance} & & \\ \updownarrow & & \\ \varepsilon_1 = \cdots = \varepsilon_{n-1} & \iff & \varepsilon_1^* = \cdots = \varepsilon_{n-1}^* \\ \updownarrow & & \updownarrow \\ A \text{ is maximal} & & A^* \text{ is maximal} \end{array}$$

## Warning!

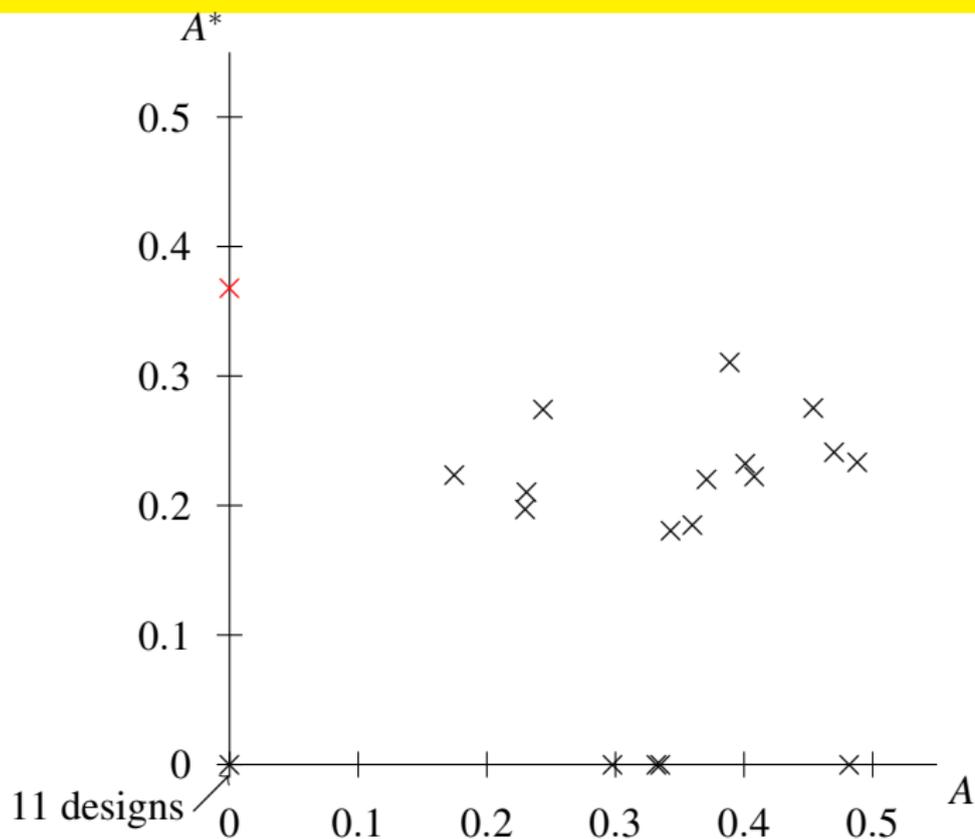
If there is no balanced incomplete block design (for the given numbers of blocks, treatments and block size), then a design which is optimal for the usual analysis may not be optimal for the analysis of block totals.

Curnow noticed this in 1963 when he examined some small designs.

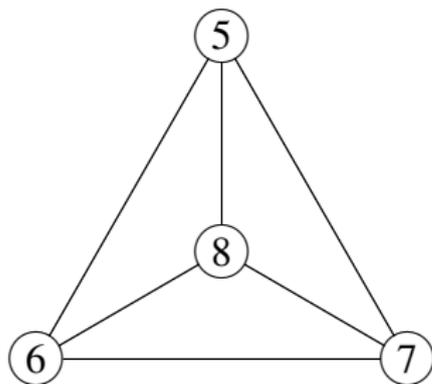
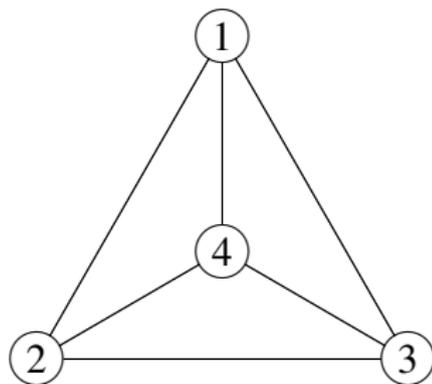
# All designs with $n = 8$ and $r = 3$



# All designs with $n = 8$ and $r = 3$

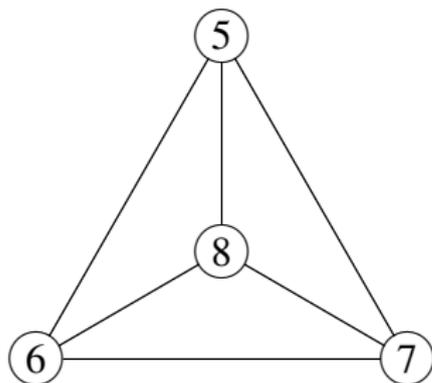
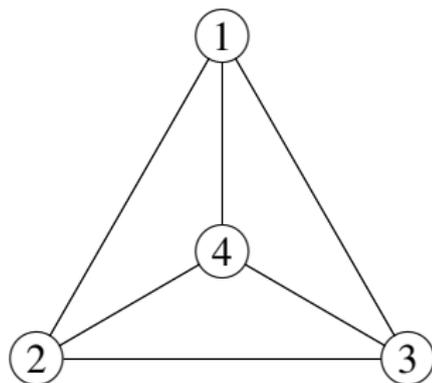


# One extreme



The design is disconnected.

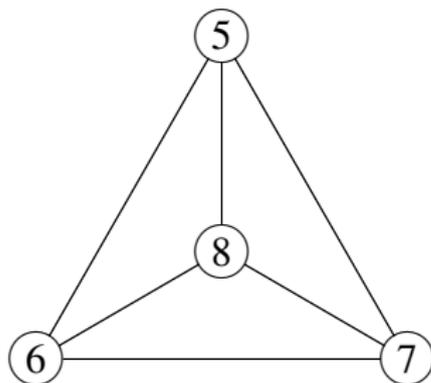
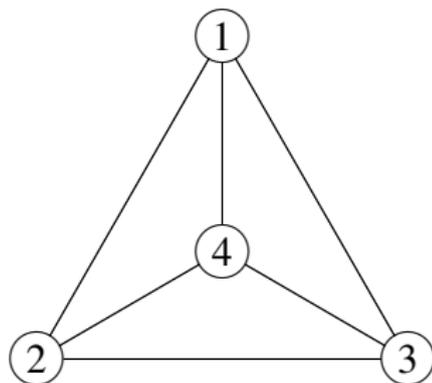
# One extreme



The design is disconnected.

The difference between the two components is not estimable within blocks.

## One extreme

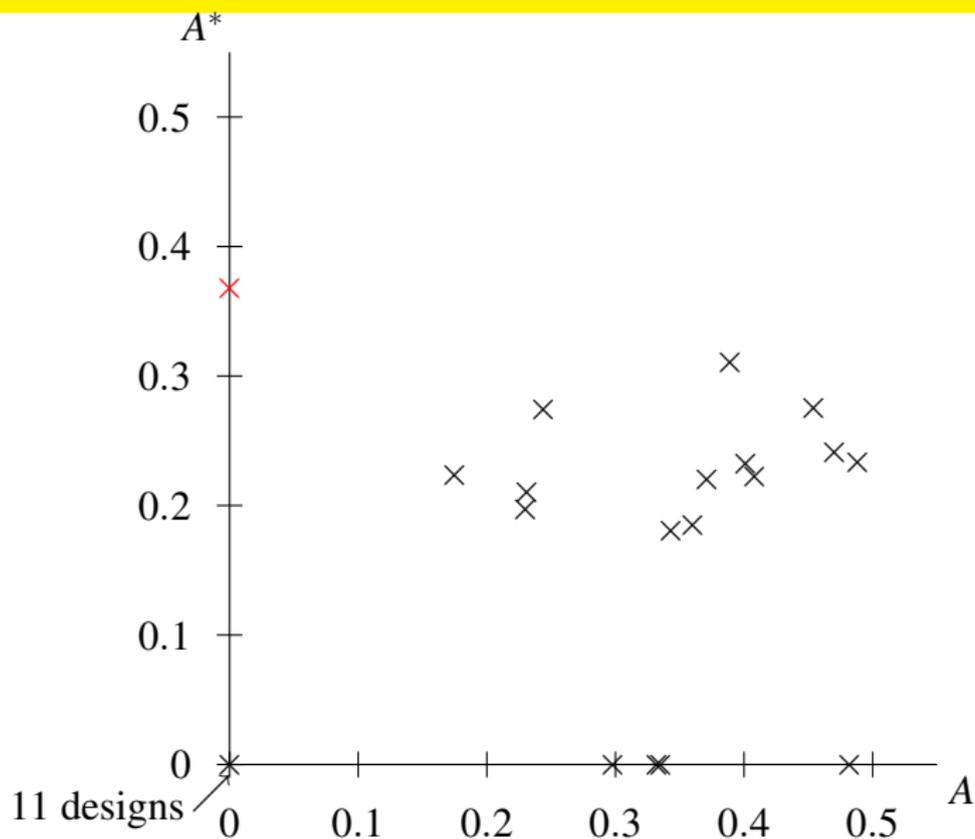


The design is disconnected.

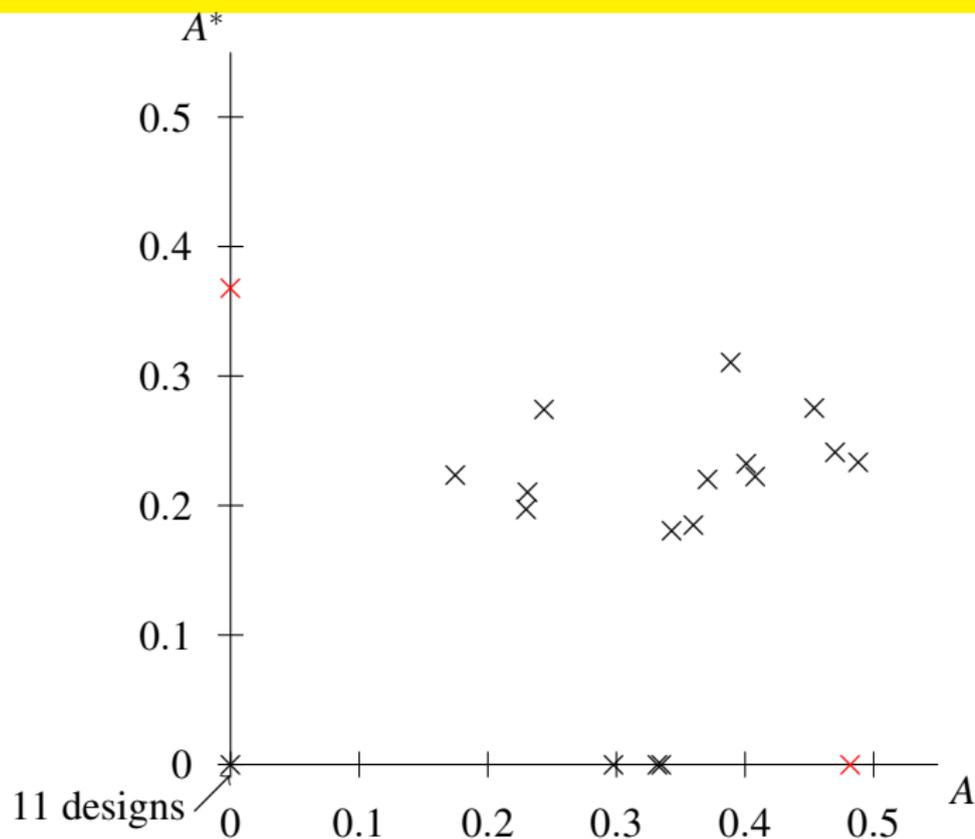
The difference between the two components is not estimable within blocks.

But this design is optimal for the analysis using block totals.

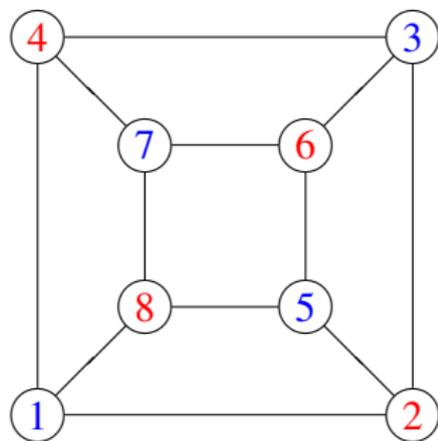
# All designs with $n = 8$ and $r = 3$



# All designs with $n = 8$ and $r = 3$

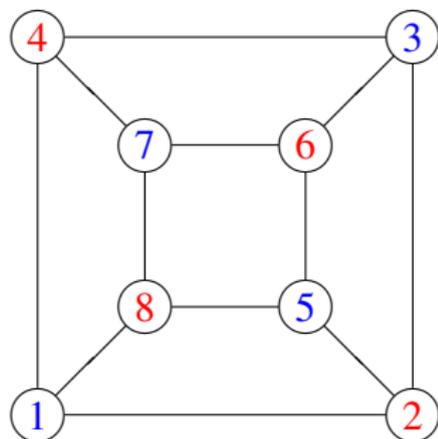


## Almost the other extreme



The design is bipartite because every edge joins an **even** treatment to an **odd** treatment.

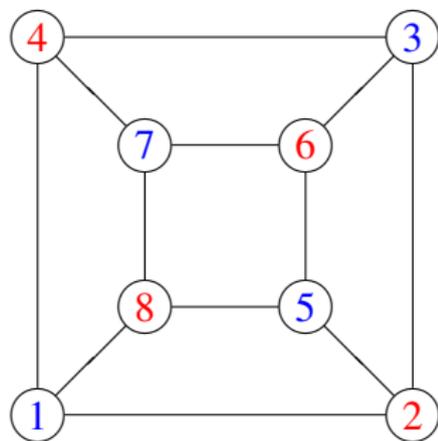
## Almost the other extreme



The design is bipartite because every edge joins an **even** treatment to an **odd** treatment.

The difference between even and odd is not estimable from the block totals.

## Almost the other extreme



The design is bipartite because every edge joins an **even** treatment to an **odd** treatment.

The difference between even and odd is not estimable from the block totals.

But this design is 2nd best for the usual within-blocks analysis.

# Theorem for incomplete-block designs with the usual analysis

In 1991, Cheng and Bailey proved that, for the usual analysis:  
if

- ▶  $\epsilon_1, \dots, \epsilon_{n-1}$  take only two values, one of which is 1, and
- ▶ the design is partially balanced with two associate classes, and concurrences differing by 1,

then  $A$  is maximal.

# Theorem for incomplete-block designs with the usual analysis

In 1991, Cheng and Bailey proved that, for the usual analysis:  
if

- ▶  $\varepsilon_1, \dots, \varepsilon_{n-1}$  take only two values, one of which is 1, and
- ▶ the design is partially balanced with two associate classes, and concurrences differing by 1,

then  $A$  is maximal.

(Note that  $\varepsilon_i = 1$  implies that  $\varepsilon_i^* = 0$  and so the corresponding contrast is not estimable from the block totals.)

# Theorem for incomplete-block designs with the usual analysis

In 1991, Cheng and Bailey proved that, for the usual analysis:  
if

- ▶  $\varepsilon_1, \dots, \varepsilon_{n-1}$  take only two values, one of which is 1, and
- ▶ the design is partially balanced with two associate classes, and concurrences differing by 1,

then  $A$  is maximal.

(Note that  $\varepsilon_i = 1$  implies that  $\varepsilon_i^* = 0$  and so the corresponding contrast is not estimable from the block totals.)

(The design is also E-optimal and D-optimal: in fact, all symmetric convex functions of the eigenvalues are maximized.)

# Theorem for incomplete-block designs with the analysis using only block totals

The **same proof** shows that, for the analysis using block totals,  
if the design is a disjoint union of complete graphs of the same size  
then  $A^*$  is maximal.

# Theorem for incomplete-block designs with the analysis using only block totals

The same proof shows that, for the analysis using block totals,  
if the design is a disjoint union of complete graphs of the same size  
then  $A^*$  is maximal.

(Some  $\epsilon^* = 1 \Rightarrow$  the design is disconnected;  
the only disconnected association scheme with two associate classes  
is the disjoint union of complete graphs of the same size.)

# Theorem for incomplete-block designs with the analysis using only block totals

The same proof shows that, for the analysis using block totals, if the design is a disjoint union of complete graphs of the same size then  $A^*$  is maximal.

(Some  $\varepsilon^* = 1 \Rightarrow$  the design is disconnected; the only disconnected association scheme with two associate classes is the disjoint union of complete graphs of the same size.)

(Note that the contrasts between the components are not estimable within-blocks.)

# Theorem for incomplete-block designs with the analysis using only block totals

The same proof shows that, for the analysis using block totals,  
if the design is a disjoint union of complete graphs of the same size  
then  $A^*$  is maximal.

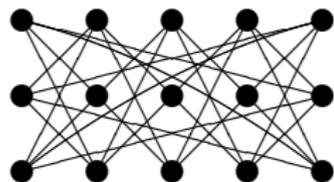
(Some  $\varepsilon^* = 1 \Rightarrow$  the design is disconnected;  
the only disconnected association scheme with two associate classes  
is the disjoint union of complete graphs of the same size.)

(Note that the contrasts between the components are not estimable  
within-blocks.)

( $E^*$ ,  $D^*$  etc are also maximal.)

Mukerjee proved a similar result for  $E$ -optimality in 1997.

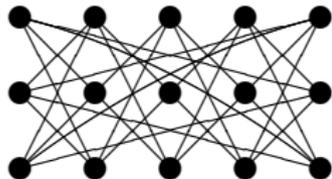
# Example with $n = 15$ and $r = 4$



best design for usual analysis

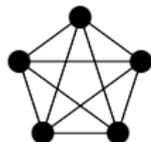
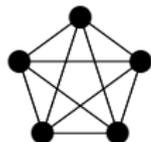
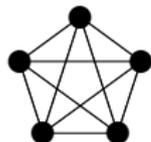
NO

# Example with $n = 15$ and $r = 4$



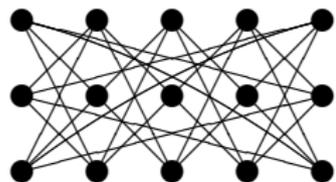
best design for usual analysis

NO



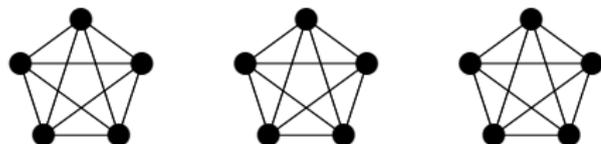
YES

# Example with $n = 15$ and $r = 4$



best design for usual analysis

NO



YES



NO

# Heuristic

For  $n$  parental lines, each involved in  $r$  crosses, let  $q$  be the smallest number such that

- ▶  $r + 1$  divides  $n - q$

Then the optimal design should be of the following form:

- ▶  $\frac{n - q}{r + 1}$  copies of the complete graph on  $r + 1$  vertices;

# Heuristic

For  $n$  parental lines, each involved in  $r$  crosses, let  $q$  be the smallest number such that

- ▶  $r + 1$  divides  $n - q$
- ▶ if  $r$  is odd then  $q$  is even

Then the optimal design should be of the following form:

- ▶  $\frac{n - q}{r + 1}$  copies of the complete graph on  $r + 1$  vertices;
- ▶ a connected graph with  $q$  vertices and valency  $r$ ,

# Heuristic

For  $n$  parental lines, each involved in  $r$  crosses, let  $q$  be the smallest number such that

- ▶  $r + 1$  divides  $n - q$
- ▶ if  $r$  is odd then  $q$  is even
- ▶  $q = 0$  or  $q > r + 1$ .

Then the optimal design should be of the following form:

- ▶  $\frac{n - q}{r + 1}$  copies of the complete graph on  $r + 1$  vertices;
- ▶ a connected graph with  $q$  vertices and valency  $r$ , with no pair repeated.

# Heuristic

For  $n$  parental lines, each involved in  $r$  crosses, let  $q$  be the smallest number such that

- ▶  $r + 1$  divides  $n - q$
- ▶ if  $r$  is odd then  $q$  is even
- ▶  $q = 0$  or  $q > r + 1$ .

Then the optimal design should be of the following form:

- ▶  $\frac{n - q}{r + 1}$  copies of the complete graph on  $r + 1$  vertices;
- ▶ a connected graph with  $q$  vertices and valency  $r$ , with no pair repeated.

## Exception

For  $r = 2$  and  $n = 3m + 10$ , use  $m$  triangles and 2 pentagons.

## Example for $n = 15$ and $r = 6$

The best design for the usual analysis is a triangular partially balanced design.

When used for an analysis by block totals, the pairwise variances are

$$\begin{array}{r} 0.4762 \quad 45 \text{ times} \\ 0.3810 \quad 60 \text{ times} \\ \hline 0.4218 \quad \text{average} \end{array}$$

and  $A^* = 0.3952$ .

## Example for $n = 15$ and $r = 6$

The best design for the usual analysis is a triangular partially balanced design.

When used for an analysis by block totals, the pairwise variances are

0.4762	45 times
0.3810	60 times
<hr/>	
0.4218	average

and  $A^* = 0.3952$ .

The heuristic choice consists of one complete graph on 7 treatments and a graph on 8 points which has all edges except for diagonal pairs.

When used for an analysis by block totals, the pairwise variances are

0.4167	24 times
0.4000	21 times
0.3709	56 times
0.3333	4 times
<hr/>	
0.3857	average

and  $A^* = 0.4321$ .

# Tomatoes in glasshouses





## Possible extensions

In experiments on tomatoes in glasshouses, several plants are grown close together. Each is tied to a vertical string. When the stalk reaches the top of the stake, it is tied around a horizontal rail. So several plants are tied around the same rail, and their fruit is all mixed up.

## Possible extensions

In experiments on tomatoes in glasshouses, several plants are grown close together. Each is tied to a vertical string. When the stalk reaches the top of the stake, it is tied around a horizontal rail. So several plants are tied around the same rail, and their fruit is all mixed up.

I have always said that the plants which are mixed up like this should all be of the same variety. But perhaps we could have  $k$  different varieties: then we would measure a response whose expectation is

$$\alpha_1 + \alpha_2 + \cdots + \alpha_k.$$

## Possible extensions

In experiments on tomatoes in glasshouses, several plants are grown close together. Each is tied to a vertical string. When the stalk reaches the top of the stake, it is tied around a horizontal rail. So several plants are tied around the same rail, and their fruit is all mixed up.

I have always said that the plants which are mixed up like this should all be of the same variety. But perhaps we could have  $k$  different varieties: then we would measure a response whose expectation is

$$\alpha_1 + \alpha_2 + \cdots + \alpha_k.$$

Then the problem of designing such experiments is formally equivalent to designing experiments in incomplete blocks of size  $k$ .

## Possible extensions

In experiments on tomatoes in glasshouses, several plants are grown close together. Each is tied to a vertical string. When the stalk reaches the top of the stake, it is tied around a horizontal rail. So several plants are tied around the same rail, and their fruit is all mixed up.

I have always said that the plants which are mixed up like this should all be of the same variety. But perhaps we could have  $k$  different varieties: then we would measure a response whose expectation is

$$\alpha_1 + \alpha_2 + \cdots + \alpha_k.$$

Then the problem of designing such experiments is formally equivalent to designing experiments in incomplete blocks of size  $k$ .

However, the efficiency criteria are different for the two situations. If a balanced design exists it is optimal for both situations; otherwise, it can happen that the design that is most efficient for one situation is worst for the other. Thus conventional lists of optimal block designs must be treated with care.

- ▶ O. Kempthorne and R. N. Curnow: The partial diallel cross. *Biometrics* **17** 1961, 229–250.
- ▶ R. N. Curnow: Sampling the diallel cross. *Biometrics* **19** 1963, 287–307.
- ▶ C.-S. Cheng and R. A. Bailey: Optimality of some two-associate-class partially balanced incomplete-block designs. *Annals of Statistics* **19** 1991, 1667–1671.
- ▶ R. Mukerjee: Optimal partial diallel crosses. *Biometrika* **84** 1997, 939–948.
- ▶ A. Das, A. M. Dean and S. Gupta: On optimality of some partial diallel cross designs. *Sankyā, Series B* **60** 1998, 511–524.