Templates for Design Key Construction

Ching-Shui Cheng

University of California, Berkeley

DAE 2012

Joint work with Pi-Wen Tsai

Design key

Patterson (1965, 1976), Bailey, (1977), Bailey, Gilchrist and Patterson (1977), Patterson and Bailey (1978)

- A useful unified device in the construction of factorial arrangements and the identification of confounding patterns
- Can be applied to symmetric and mixed-level designs.

For symmetric factorials where the number of factor levels is a prime or prime power, it is equivalent to the familiar method of using factorial effects (words) to partition the treatments into blocks, rows, columns, etc.

Split-plot designs

Block structure: (16 whole-plots)/(2 subplots)

Five two-level treatment factors

A, B: whole-plot treatment factors

S, T, U: subplot treatment factors.

More whole-plots than the # of whole-plot treatment combinations

Bingham, Schoen, and Sitter (2004)

First construct a design with 4 whole-plots each containing 8 subplots.

(1)	(a)	b	ab
stu	$astu$	$bstu$	$abstu$
st	ast	bst	$abst$
u	au	bu	abu
su	asu	bsu	$absu$
t	at	bt	abt
tu	atu	btu	$abtu$
s	as	bs	abs

Then use two interactions involving subplot treatment factors, say ST and SU, to divide each whole-plot into four quarters, each of which is considered as a whole-plot of size two. Then we have 16 whole-plots of size 2.

ST and SU are called independent splitting words (or splitting effects).

Then use two interactions involving subplot treatment factors, say ST and SU, to divide each whole-plot into four quarters, each of which is considered as a whole-plot of size two. Then we have 16 whole-plots of size 2.

ST and SU are called independent splitting words (or splitting effects).

When choosing the splitting words, one needs to check

- independence
- no main effects of subplot treatment factors get confounded with whole-plot contrasts.

unit contrasts and treatment contrasts

treatment contrasts representing factorial effects (main effects and interactions): 31 d.f.

unit contrasts and treatment contrasts

treatment contrasts representing factorial effects (main effects and interactions): 31 d.f.

unit contrasts: 31 d.f.

15 d.f. : whole-plot contrasts

16 d.f. : subplot contrasts

two strata

unit contrasts and treatment contrasts

treatment contrasts representing factorial effects (main effects and interactions): 31 d.f.

unit contrasts: 31 d.f.

15 d.f. : whole-plot contrasts

16 d.f. : subplot contrasts

two strata

Design key construction is done by choosing a unit alias for each treatment main effect

Represent the 32 units as combinations of five two-level unit factors

$\mathcal{W}_1, \mathcal{W}_2, \mathcal{W}_3, \mathcal{W}_4, \mathcal{S}$.

Represent the 32 units as combinations of five two-level unit factors $\mathcal{W}_1, \mathcal{W}_2, \mathcal{W}_3, \mathcal{W}_4, \mathcal{S}$.

whole-plot contrasts: the effects that do not involve $\mathcal{S}$

subplot contrasts: the effects that involve $\mathcal{S}$

Represent the 32 units as combinations of five two-level unit factors $\mathcal{W}_1, \mathcal{W}_2, \mathcal{W}_3, \mathcal{W}_4, \mathcal{S}$.

whole-plot contrasts: the effects that do not involve $\mathcal{S}$

subplot contrasts: the effects that involve $\mathcal{S}$

$$
\begin{array}{cc}
 & \begin{array}{ccccc} \mathcal{S} & \mathcal{W}_1 & \mathcal{W}_2 & \mathcal{W}_3 & \mathcal{W}_4 \end{array} \\
K = & \begin{bmatrix} 1 & 0 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 & 0 \\ 0 & 0 & 1 & 0 & 0 \\ 1 & 0 & 0 & 1 & 0 \\ 1 & 0 & 0 & 0 & 1 \end{bmatrix} \begin{array}{c} S \\ A \\ B \\ T \\ U \end{array}
\end{array}
$$

Five independent generators stu, a, b, t, and u are identified from the columns of K.

(1)	a	b	ab	t	at
stu	$astu$	$bstu$	$abstu$	su	asu

etc.

s^n split-plot factorial designs with s^q whole-plots each containing s^{n-q} subplots

s is a prime number or power of a prime number

n_1 of the n treatment factors are whole-plot factors and the other $n_2 = n - n_1$ treatment factors are subplot factors.

Theorem Each complete s^n factorial split-plot design can be constructed by using a design key of the form

$$\boldsymbol{K} = \begin{bmatrix} \boldsymbol{I}_{n-q} & \boldsymbol{0}_{n-q,q} \\ \boldsymbol{B} & \boldsymbol{I}_q \end{bmatrix},$$

where $\boldsymbol{B}$ is $q \times (n-q)$, the first $n-q$ columns of $\boldsymbol{K}$ correspond to $\mathcal{S}_1, \cdots, \mathcal{S}_{n-q}$, and the last q columns correspond to $\mathcal{W}_1, \cdots, \mathcal{W}_q$.

The first $n-q$ rows of $\boldsymbol{K}$ correspond to subplot treatment factors.

The next n_1 rows correspond to whole-plot treatment factors, and if $n_1 < q$, the last $q - n_1$ rows correspond again to sub-plot treatment factors.

All the first n_1 rows of $\boldsymbol{B}$ are zero, and if $n_1 < q$, the last $q - n_1$ rows of $\boldsymbol{B}$ are nonzero.

Theorem Each complete s^n factorial split-plot design can be constructed by using a design key of the form

$$\boldsymbol{K} = \begin{bmatrix} \boldsymbol{I}_{n-q} & \boldsymbol{0}_{n-q,q} \\ \boldsymbol{B} & \boldsymbol{I}_q \end{bmatrix},$$

where $\boldsymbol{B}$ is $q \times (n-q)$, the first $n-q$ columns of $\boldsymbol{K}$ correspond to $\mathcal{S}_1, \cdots, \mathcal{S}_{n-q}$, and the last q columns correspond to $\mathcal{W}_1, \cdots, \mathcal{W}_q$.

The first $n-q$ rows of $\boldsymbol{K}$ correspond to subplot treatment factors.

The next n_1 rows correspond to whole-plot treatment factors, and if $n_1 < q$, the last $q - n_1$ rows correspond again to sub-plot treatment factors.

All the first n_1 rows of $\boldsymbol{B}$ are zero, and if $n_1 < q$, the last $q - n_1$ rows of $\boldsymbol{B}$ are nonzero.

This dates back to the construction of block designs in Das (1964).

$$
\begin{array}{rc}
 & \begin{array}{ccccc} \mathcal{S} & \mathcal{W}_1 & \mathcal{W}_2 & \mathcal{W}_3 & \mathcal{W}_4 \end{array} \\
K = & \begin{bmatrix} 1 & 0 & 0 & 0 & 0 \\ * & 1 & 0 & 0 & 0 \\ * & 0 & 1 & 0 & 0 \\ * & 0 & 0 & 1 & 0 \\ * & 0 & 0 & 0 & 1 \end{bmatrix}
\begin{array}{c} S \\ A \\ B \\ T \\ U \end{array}
\end{array}
$$

$$\begin{array}{cc} \mathcal{S}\ \mathcal{W}_1\mathcal{W}_2\mathcal{W}_3\mathcal{W}_4 & \\ K = \begin{bmatrix} 1 & 0 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 & 0 \\ 0 & 0 & 1 & 0 & 0 \\ 1 & 0 & 0 & 1 & 0 \\ 1 & 0 & 0 & 0 & 1 \end{bmatrix} & \begin{array}{c} S \\ A \\ B \\ T \\ U \end{array} \end{array}$$

There is only one design up to isomorphism.

If the treatment combinations are generated by using the generators determined by the columns of the design key matrix and are arrangeed in the Yates order, then the first s^{n-q} in the generated sequence are in the same whole-plot, and each succeeding set of s^{n-q} treatment combinations are also in the same whole-plot.

If the treatment combinations are generated by using the generators determined by the columns of the design key matrix and are arrangeed in the Yates order, then the first s^{n-q} in the generated sequence are in the same whole-plot, and each succeeding set of s^{n-q} treatment combinations are also in the same whole-plot.

$$K^{-1} = \begin{bmatrix} \boldsymbol{I}_{n-q} & \boldsymbol{0} \\ -\boldsymbol{b}_1^T & \\ \vdots & \boldsymbol{I}_q \\ -\boldsymbol{b}_q^T & \end{bmatrix}$$

$s = 2$: $K^{-1} = K$

$s = 2$: $K^{-1} = K$

$$K^{-1} = \begin{array}{c} \begin{array}{ccccc} \mathsf{S} & \mathsf{A} & \mathsf{B} & \mathsf{T} & \mathsf{U} \end{array} \\ \begin{bmatrix} 1 & 0 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 & 0 \\ 0 & 0 & 1 & 0 & 0 \\ 1 & 0 & 0 & 1 & 0 \\ 1 & 0 & 0 & 0 & 1 \end{bmatrix} \end{array} \begin{array}{c} \\ \mathcal{S}_1 \\ \mathcal{W}_1 \\ \mathcal{W}_2 \\ \mathcal{W}_3 \\ \mathcal{W}_4 \end{array}$$

$s = 2$: $K^{-1} = K$

$$K^{-1} = \begin{array}{cc} \begin{array}{ccccc} \mathrm{S} & \mathrm{A} & \mathrm{B} & \mathrm{T} & \mathrm{U} \end{array} & \\ \begin{bmatrix} 1 & 0 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 & 0 \\ 0 & 0 & 1 & 0 & 0 \\ 1 & 0 & 0 & 1 & 0 \\ 1 & 0 & 0 & 0 & 1 \end{bmatrix} & \begin{array}{c} \mathcal{S}_1 \\ \mathcal{W}_1 \\ \mathcal{W}_2 \\ \mathcal{W}_3 \\ \mathcal{W}_4 \end{array} \end{array}$$

In general, independent splitting words can identified from the last $q - n_1$ rows of K.

The block structure, design requirements, independent generators, and splitting words are all built in the design key template.

The block structure, design requirements, independent generators, and splitting words are all built in the design key template.

No need to

1. check independence of splitting words;

The block structure, design requirements, independent generators, and splitting words are all built in the design key template.

No need to

1. check independence of splitting words;

2. check that no main effect of a subplot treatment factor is confounded with whole-plot contrasts;

The block structure, design requirements, independent generators, and splitting words are all built in the design key template.

No need to

1. check independence of splitting words;

2. check that no main effect of a subplot treatment factor is confounded with whole-plot contrasts;

3. solve equations to find the treatment combinations in the first whole-plot.

Blocked split-plot designs

s^n design with s^q whole-plots each containing s^{n-q} subplots, where there are n_1 whole-plot treatment factors, $n_2 = n - n_1$ subplot treatment factors, and the s^q whole-plots are divided into s^g blocks each of size s^{q-g}.

Block structure: $s^g / s^{q-g} / s^{n-q}$

Blocked split-plot designs

s^n design with s^q whole-plots each containing s^{n-q} subplots, where there are n_1 whole-plot treatment factors, $n_2 = n - n_1$ subplot treatment factors, and the s^q whole-plots are divided into s^g blocks each of size s^{q-g}.

Block structure: $s^g/s^{q-g}/s^{n-q}$

McLeod and Brewster (2004) proposed three construction methods: pure whole-plot blocking, separation, and mixed blocking.

Represent the s^n units by the combinations of n s-level unit factors

$\mathcal{S}_1, \cdots, \mathcal{S}_{n-q}, \mathcal{W}_1, \cdots, \mathcal{W}_{q-g}, \mathcal{B}_1, \cdots, \mathcal{B}_g$

Three strata

Represent the s^n units by the combinations of n s-level unit factors

$\mathcal{S}_1, \cdots, \mathcal{S}_{n-q}, \mathcal{W}_1, \cdots, \mathcal{W}_{q-g}, \mathcal{B}_1, \cdots, \mathcal{B}_g$

Three strata

A treatment main effect is confounded with a block (respectively, whole-plot) contrast if its unit alias does not involve any of $\mathcal{S}_1, \cdots, \mathcal{S}_{n-q}$, $\mathcal{W}_1, \cdots, \mathcal{W}_{q-g}$ (respectively, involves at least one of $\mathcal{W}_1, \cdots, \mathcal{W}_{q-g}$ but not any of $\mathcal{S}_1, \cdots, \mathcal{S}_{n-q}$), and is orthogonal to block and whole-plot contrasts if its unit alias involves at least one of $\mathcal{S}_1, \cdots, \mathcal{S}_{n-q}$.

$$
\boldsymbol{K} = \begin{bmatrix} \boldsymbol{I}_{n-q} & \boldsymbol{0}_{n-q,q-g} & \boldsymbol{0}_{n-q,g} \\ & \boldsymbol{I}_{q-g} & \boldsymbol{0}_{q-g,g} \\ \boldsymbol{B} & & \\ & \boldsymbol{C} & \boldsymbol{I}_{g} \end{bmatrix},
$$

where $\boldsymbol{B}$ is $q \times (n-q)$, $\boldsymbol{C}$ is $g \times (q-g)$, the first $n-q$ columns of $\boldsymbol{K}$ correspond to $\mathcal{S}_1, \cdots, \mathcal{S}_{n-q}$, the next $q-g$ columns correspond to $\mathcal{W}_1, \cdots, \mathcal{W}_{q-g}$, the last g columns correspond to $\mathcal{B}_1, \cdots, \mathcal{B}_g$, the first $n-q$ rows of $\boldsymbol{K}$ correspond to subplot treatment factors, the next n_1 rows correspond to whole-plot treatment factors, and all the remaining rows correspond to subplot treatment factors if $n_1 < q$.

$$K = \begin{bmatrix} I_{n-q} & 0_{n-q,q-g} & 0_{n-q,g} \\ & I_{q-g} & 0_{q-g,g} \\ B & & \\ & C & I_g \end{bmatrix},$$

where B is $q \times (n-q)$, C is $g \times (q-g)$, the first $n-q$ columns of K correspond to $\mathcal{S}_1, \cdots, \mathcal{S}_{n-q}$, the next $q-g$ columns correspond to $\mathcal{W}_1, \cdots, \mathcal{W}_{q-g}$, the last g columns correspond to $\mathcal{B}_1, \cdots, \mathcal{B}_g$, the first $n-q$ rows of K correspond to subplot treatment factors, the next n_1 rows correspond to whole-plot treatment factors, and all the remaining rows correspond to subplot treatment factors if $n_1 < q$.

Furthermore, the first n_1 rows of B are zero, all the last $q-n_1$ rows of B are nonzero if $n_1 < q$, and all the first $n_1-(q-g)$ rows of C are nonzero if $n_1 > q-g$.

For constructing an s^{n-p} fractional factorial design, we can add p rows to a design key for the complete factorial of $n-p$ basic factors, one for each added factor.

Two treatment factorial effects are aliased if and only if their unit aliases are aliased.

Given the defining relation of the fraction, the row of the design key associated with each added factor can be obtained as a linear combination of the rows corresponding to the basic factors whose interaction is used to define the given factor.

Need to check that the constraints imposed by the block structures are observed. For instance, if no treatment main effects are to be confounded with block contrasts, then one needs to make sure their unit aliases are not block contrasts.

Experiments with multiple processing stages

Levels of treatment factors are assigned at different stages. At each stage, the experimental units are divided into disjoint groups. All the units in the same group are assigned the same level of each factor whose levels are set at that stage.

2^4 experiment, four stages, four groups at each stage

2^4 experiment, four stages, four groups at each stage

0	0	0	0	1	1	1	1
1	0	0	1	3	1	3	2
0	0	1	0	2	1	2	4
1	0	1	1	4	1	4	3
0	1	0	1	1	3	3	3
1	1	0	0	3	3	1	4
0	1	1	1	2	3	4	2
1	1	1	0	4	3	2	1
0	0	1	1	1	2	2	2
1	0	1	0	3	2	4	1
0	0	0	1	2	2	1	3
1	0	0	0	4	2	3	4
0	1	1	0	1	4	4	4
1	1	1	1	3	4	2	3
0	1	0	0	2	4	3	1
1	1	0	1	4	4	1	2

Wu (1989) showed that for even n, the $2^n - 1$ columns of a saturated regular 2-level design of size 2^n can be decomposed into $(2^n - 1)/3$ disjoint groups of size three such that any column is the sum of the other two columns in the same group. For odd n, one can only construct up to $(2^n - 5)/3$ disjoint groups.

1	2	3	4	1, 1234, 234	2, 124, 14	12, 3, 123	134, 13, 4
0	0	0	0	1	1	1	1
1	0	0	1	3	1	3	2
0	0	1	0	2	1	2	4
1	0	1	1	4	1	4	3
0	1	0	1	1	3	3	3
1	1	0	0	3	3	1	4
0	1	1	1	2	3	4	2
1	1	1	0	4	3	2	1
0	0	1	1	1	2	2	2
1	0	1	0	3	2	4	1
0	0	0	1	2	2	1	3
1	0	0	0	4	2	3	4
0	1	1	0	1	4	4	4
1	1	1	1	3	4	2	3
0	1	0	0	2	4	3	1
1	1	0	1	4	4	1	2

1	2	3	4	$1, 1234, 234$	$2, 124, 14$	$12, 3, 123$	$134, 13, 4$
0	0	0	0	1	1	1	1
1	0	0	1	3	1	3	2
0	0	1	0	2	1	2	4
1	0	1	1	4	1	4	3
0	1	0	1	1	3	3	3
1	1	0	0	3	3	1	4
0	1	1	1	2	3	4	2
1	1	1	0	4	3	2	1
0	0	1	1	1	2	2	2
1	0	1	0	3	2	4	1
0	0	0	1	2	2	1	3
1	0	0	0	4	2	3	4
0	1	1	0	1	4	4	4
1	1	1	1	3	4	2	3
0	1	0	0	2	4	3	1
1	1	0	1	4	4	1	2

$$(0,0,0) \to 1, (0,1,1) \to 2, (1,0,1) \to 3, (1,1,0) \to 4$$

1	2	3	4	1, 2, 12	3, 4, 34	13, 24, 1234	23, 124, 134
0	0	0	0	1	1	1	1
1	0	0	0	3	1	3	2
0	1	0	0	2	1	2	4
1	1	0	0	4	1	4	3
0	0	1	0	1	3	3	3
1	0	1	0	3	3	1	4
0	1	1	0	2	3	4	2
1	1	1	0	4	3	2	1
0	0	0	1	1	2	2	2
1	0	0	1	3	2	4	1
0	1	0	1	2	2	1	3
1	1	0	1	4	2	3	4
0	0	1	1	1	4	4	4
1	0	1	1	3	4	2	3
0	1	1	1	2	4	3	1
1	1	1	1	4	4	1	2

Choose one contrast from each group and relabel them as 1, 2, 3, and 4, respectively.

Choose one contrast from each group and relabel them as 1, 2, 3, and 4, respectively.

Ranjan, Bingham and Dean (2009) used the method of collineation of projective spaces.

Choose one contrast from each group and relabel them as 1, 2, 3, and 4, respectively.

Ranjan, Bingham and Dean (2009) used the method of collineation of projective spaces.

Suppose 1, 3, 24, and 134 are to be relabeled as 1, 2, 3, and 4, respectively.

Choose one contrast from each group and relabel them as 1, 2, 3, and 4, respectively.

Ranjan, Bingham and Dean (2009) used the method of collineation of projective spaces.

Suppose 1, 3, 24, and 134 are to be relabeled as 1, 2, 3, and 4, respectively.

$$
\begin{array}{cc}
 & \begin{array}{cccc} \mathbf{1} & \mathbf{2} & \mathbf{3} & \mathbf{4} \end{array} \\
\mathsf{K} = & \left[\begin{array}{cccc} 1 & 0 & 0 & 0 \\ 0 & 0 & 1 & 0 \\ 0 & 1 & 0 & 1 \\ 1 & 0 & 1 & 1 \end{array}\right]
\begin{array}{c} \mathbf{1} \\ \mathbf{2} \\ \mathbf{3} \\ \mathbf{4} \end{array}
\end{array} .
$$

1	2	3	4	1, 2, 12	3, 4, 34	13, 24, 1234	23, 124, 134
0	0	0	0	1	1	1	1
1	0	0	0	3	1	3	2
0	1	0	0	2	1	2	4
1	1	0	0	4	1	4	3
0	0	1	0	1	3	3	3
1	0	1	0	3	3	1	4
0	1	1	0	2	3	4	2
1	1	1	0	4	3	2	1
0	0	0	1	1	2	2	2
1	0	0	1	3	2	4	1
0	1	0	1	2	2	1	3
1	1	0	1	4	2	3	4
0	0	1	1	1	4	4	4
1	0	1	1	3	4	2	3
0	1	1	1	2	4	3	1
1	1	1	1	4	4	1	2

1	2	3	4	1, 2, 12	3, 4, 34	13, 24, 1234	23, 124, 134
0	0	0	0	1	1	1	1
1	0	0	0	3	1	3	2
0	1	0	0	2	1	2	4
1	1	0	0	4	1	4	3
0	0	1	0	1	3	3	3
1	0	1	0	3	3	1	4
0	1	1	0	2	3	4	2
1	1	1	0	4	3	2	1
0	0	0	1	1	2	2	2
1	0	0	1	3	2	4	1
0	1	0	1	2	2	1	3
1	1	0	1	4	2	3	4
0	0	1	1	1	4	4	4
1	0	1	1	3	4	2	3
0	1	1	1	2	4	3	1
1	1	1	1	4	4	1	2

Replace the generators with those obtained from the columns of K.

1	2	3	4	1, 1234, 234	2, 124, 14	12, 3, 123	134, 13, 4
0	0	0	0	1	1	1	1
1	0	0	1	3	1	3	2
0	0	1	0	2	1	2	4
1	0	1	1	4	1	4	3
0	1	0	1	1	3	3	3
1	1	0	0	3	3	1	4
0	1	1	1	2	3	4	2
1	1	1	0	4	3	2	1
0	0	1	1	1	2	2	2
1	0	1	0	3	2	4	1
0	0	0	1	2	2	1	3
1	0	0	0	4	2	3	4
0	1	1	0	1	4	4	4
1	1	1	1	3	4	2	3
0	1	0	0	2	4	3	1
1	1	0	1	4	4	1	2