SUM-OF-SQUARES ORTHOGONALITY AND COMPLETE SETS

by

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ABSTRACT

The concept of sum-of-squares orthogonality is explained in terms of what is known about factorial treatment design and analysis and Projective geometry. The idea is to clarify notions about the new geometry introduced by Federer (2003a, 2003b). Note that the geometry of prime numbers is included in the new geometry. Several new ideas such as semi-F-squares (row or column frequency squares), complete sets of combinations of regular and semi-F-squares, maximum number of F-squares when some are semi-F-squares, and proportionally orthogonal F-squares are required in the explanation. For factorials with an equal number for each combination, the property of orthogonality is explained in terms of an algebraic identity. Multiplicative and geometrical interaction ideas are used in explaining the relationships. It is shown how to construct pairwise combinatorially orthogonal Latin squares and F-squares. Then, using these concepts, it is shown how to construct complete sets of F-squares for any n, n a product of prime numbers. The associated orthogonal arrays are also presented. These arrays are useful for constructing experiment designs, fractional replicates, and codes.

Key words: Combinatorial orthogonality, sum-of-squares orthogonality, F-square, Latin square, semi-F-square, row frequency square, main effect, multiplicative interaction, geometrical interaction, complete sets of F-squares, fractional replication.

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INTRODUCTION

The relationships among the main effects and interaction effects from a factorial treatment design and their properties are given. The degrees of freedom and sum of squares obtained for these effects are orthogonal when the number of observations for all combinations of the factors is a constant number. Then it is shown how to relate the row by column interactions in an $n \times n$, n a prime power, square to pairwise orthogonal Latin squares. Instead of constructing Latin squares, it is shown how to construct pairwise combinatorially orthogonal F-squares, F(n, p), of order n and with p symbols. Complete sets of Latin squares and of F-squares are demonstrated. Then orthogonal arrays are constructed from these sets.

An F-square has been defined as an $n \times n$ square in which the p symbols appear n/p times in each row and n/p times in each column, F(n, p). This has been called a regular F-square by Federer (2003a, 2003b). He also defined proportionally orthogonal F-squares for the case where symbols occur a proportional rather than equal number of times in the rows and columns and has given squares where a symbol occurs more frequently with itself than with the other symbols. A semi-F-square was defined to be one for which the symbols occur equally frequent in rows (columns) but not in columns (rows). Pesotan *et al.* (2003) have denoted this type of square as a row (column) frequency square, RF(n, p) (CF(n, p)).

If the symbols in a pair of Latin squares or F-squares occur together equally frequent, this is called combinatorial orthogonality (Federer, 2003a, 2003b). Another kind of orthogonality has been described by Federer (2003a, 2003b). This is sum-of-squares orthogonality. The definition of sum-of-squares orthogonality is:

Definition: F-squares may be constructed from the interactions in a factorial treatment design. If the sums of squares and degrees of freedom for these F-squares add to the sum of squares and degrees of freedom for the interaction, this is called sum-of-squares orthogonality.

The interaction in a factorial has been denoted as a multiplicative interaction. This multiplicative interaction may be partitioned into a set of geometrical interaction components. The former type of interaction has implications and meaning for data from experiments. Geometrical interaction components have no practical interpretations but have geometrical properties useful for constructing codes, experiment designs, fractional replicates, etc. Originally geometrical interaction components were available only for prime powers. The new geometry introduced by Federer (2003a, 2003b) makes use of the geometrical interaction components for any value of n, n a product of prime numbers.

FACTORIAL TREATMENT DESIGN AND ANALYSIS

Given two or more factors with a specified number of levels of each factor, all possible combinations of the levels of the factors is known as a factorial treatment design. In particular, let the i^{th} of n factors be associated with k_i levels. Then there are $k_1 \times k_2 \times k_3 \times \ldots \times k_n$ total combinations of the n factors. To illustrate, consider a two factor factorial (two-way array) with r levels of factor row (factor A) and c levels of factor column (factor B). Let Y_{ij} be the response for the ij^{th} combination of the two factors, i = 1, 2, … , r, and j = 1, 2, …, c. Let $Y_{i.}$ be the total for the i^{th} level of factor row, $Y_{.j}$ the j^{th} total for factor column, and $Y_{..}$ the total of all rc combinations. Also, let y denote a mean value. A linear model for this situation is considered to be:

$$\begin{aligned} Y_{ij} &= \mu_{ij} + \xi_{ij} \\ &= \mu_{..} + (\mu_{i.} - \mu_{..}) + (\mu_{.j} - \mu_{..}) + (\mu_{ij} - \mu_{i.} - \mu_{.j} + \mu_{..}) + \xi_{ij} \\ &= \mu_{..} + \alpha_i + \beta_j + \alpha\beta_{ij} + \varepsilon_{ij} \end{aligned}$$

μ_{ij} is the true mean of the ijth combination of levels of the two factors, $\mu_{i.}$ is the average of the μ_{ij} summed over levels of factor B, $\mu_{.j}$ is the mean of the μ_{ij} summed over levels of factor A, $\mu_{..}$ is the average of all μ_{ij} , ξ_{ij} is a random error effect for combination ij distributed with mean zero and variance σ_ε^2, $\alpha_i = (\mu_{i.} - \mu_{..})$ is effect of the i^{th} level of factor A, $\beta_j = (\mu_{.j} - \mu_{..})$ is the effect of the j^{th} level of factor B, and $\alpha\beta_{ij} = (\mu_{ij} - \mu_{i.} - \mu_{.j} + \mu_{..})$ is the interaction effect of the ij^{th} combination of the two factors.

The following algebraic identity holds:

$$\Sigma_i \Sigma_j Y_{ij}^2 = Y_{..}^2 / rc + (\Sigma_i Y_{i.}^2/c - Y_{..}^2 / rc) + (\Sigma_j Y_{.j}^2 / r - Y_{..}^2 / rc) +$$

$$(\Sigma_i Y_{ij}^2 - \Sigma_i Y_{i.}^2 / c - \Sigma_j Y_{.j}^2 / r + Y_{..}^2 / rc) =$$

$$Y_{..}^2 + c\, \Sigma_i (y_{i.} - y_{..})^2 + r\, \Sigma_j (y_{.j} - y_{..})^2 + \Sigma_i \Sigma_j (Y_{ij} - y_{i.} - y_{.j} + y_{..})^2$$

A similar identity holds for partitioning the total degrees of freedom rc into degrees of freedom for the various effects. Thus,

$$rc = 1 + (r - 1) + (c - 1) + (r - 1)(c - 1)$$

Note that $\Sigma_i\alpha_i = \Sigma_j\beta_j = \Sigma_i\alpha\beta_{ij} = \Sigma_j\alpha\beta_{ij} = 0$ by definition of the means.

An analysis of variance table for the above is:

Source of Variation	Degrees of freedom	Sum of squares
Total	rc	$\Sigma_i \Sigma_j Y_{ij}^2$
Correction for mean	1	$Y_{..}^2 / rc$
Row	r - 1	$c\, \Sigma_i (y_{i.} - y_{..})^2$
Column	c - 1	$r\, \Sigma_j (y_{.j} - y_{..})^2$
Row × column	(r - 1)(c - 1)	$\Sigma_i \Sigma_j (Y_{ij} - y_{i.} - y_{.j} + y_{..})^2$

Since the $\Sigma_i (y_{i.} - y_{..}) = 0$, there is one restriction on the row sum of squares and there are only r - 1 ways in which the sum of squares can vary. Hence, the number of degrees of freedom is r - 1. For the row by column interaction, $\Sigma_i (Y_{ij} - y_{i.} - y_{.j} + y_{..}) = 0$ and $\Sigma_j (Y_{ij} - y_{i.} - y_{.j} + y_{..}) = 0$; hence, there are only (r - 1)(c - 1) ways in which the interaction sum of squares can vary. These sums of squares and degrees of freedom are disjoint, independent, uncorrelated, and orthogonal as there is no confounding among them.

These ideas extend to any number of factors. For example, consider a three factor, A, B, and C, factorial with levels a, b, and c for factors A, B, and C, respectively. An algebraic identity for the disjoint parts of the total sum of squares, where Y_{hij} is the response for the hij^{th} combination of levels of the three factors, is given below:

$$\Sigma_h \Sigma_i \Sigma_j Y_{hij}^2 = Y_{...}^2 / abc + (\Sigma_h Y_{h..}^2 / bc - Y_{...}^2 / abc) + (\Sigma_i Y_{.i.}^2 / ac - Y_{...}^2 / abc) +$$

$(\Sigma_h \Sigma_i Y_{hi.}^2 / c - \Sigma_h Y_{h..}^2 / bc - \Sigma_i Y_{.i.}^2 / ac + Y_{...}^2 / abc) + (\Sigma_j Y_{..j}^2 / ab - Y_{...}^2 / abc)$

$+ (\Sigma_h \Sigma_j Y_{h.j}^2 / b - \Sigma_h Y_{h..}^2 / bc - \Sigma_j Y_{..j}^2 / ab + Y_{...}^2 / abc) +$

$(\Sigma_i \Sigma_j Y_{.ij}^2 / a - \Sigma_i Y_{.i.}^2 / ac - \Sigma_j Y_{..j}^2 / ab + Y_{...}^2 / abc) +$

$(\Sigma_h \Sigma_i \Sigma_j Y_{hij}^2 + \Sigma_h Y_{h..}^2 / bc + \Sigma_i Y_{.i.}^2 / ac + \Sigma_j Y_{..j}^2 / ab - \Sigma_h \Sigma_i Y_{hi.}^2 / c -$

$\Sigma_i \Sigma_j Y_{.ij}^2 / a - \Sigma_h \Sigma_j Y_{h.j}^2 / b - Y_{...}^2 / abc)$

A linear model for the above three factor factorial is constructed in a similar manner as was done for the two factor factorial. A similar algebraic partitioning of the total degrees of freedom abc in the degrees of freedom corresponding to the various sums of squares above is:

$$abc = 1 + (a - 1) + (b - 1) + (a - 1)(b - 1) + (c - 1) + (a - 1)(c - 1) + (b - 1)(c - 1) + (a - 1)(b - 1)(c - 1)$$

An analysis of variance table for the above three factor factorial treatment design, using formulas for the means, is:

Source of variation	Degrees of freedom	Sum of squares
Total	abc	$\Sigma_h \Sigma_i \Sigma_j Y_{hij}^2$
Mean	1	$Y_{...}^2 / abc$
A	a - 1	$bc \Sigma_h (y_{h..} - y_{...})^2$
B	b - 1	$ac \Sigma_i (y_{.i.} - y_{...})^2$
A × B	(a - 1)(b - 1)	$c \Sigma_h \Sigma_i (y_{hi.} - y_{h..} - y_{.i.} + y_{...})^2$
C	c - 1	$ab \Sigma_j (y_{..j} - y_{...})^2$
A × C	(a - 1)(c - 1)	$b \Sigma_h \Sigma_i (y_{h.j} - y_{h..} - y_{..j} + y_{...})^2$
B × C	(b - 1)(c - 1)	$a \Sigma_i \Sigma_j (y_{.ij} - y_{.i.} - y_{..j} + y_{...})^2$
A × B × C	(a - 1)(b - 1)(c - 1)	$\Sigma_h \Sigma_i \Sigma_j (Y_{hij} + y_{h..} + y_{.i.} + y_{..j} - y_{hi.} - y_{h.j} - y_{.ij} - y_{...})^2$

The individual sums of squares in the above table are all disjoint and orthogonal. The degrees of freedom are explained in the same manner as for the two factor factorial. For the above properties to hold the number of observations for any combination ij or hij must be a constant. Unequal numbers of observations introduces confounding of effects and non-orthogonality.

N × N ARRAYS FOR N EQUAL A PRIME POWER

For n a prime power, properties of Projective and Euclidean geometries are available. In this case, the multiplicative interaction may be partitioned into its geometrical components of interaction. To illustrate, let n = p = 3, i = 0, 1, 2 and j = 0, 1, 2. The following analysis of variance table illustrates this partitioning:

Source of variation	Degrees of freedom	Sum of squares
Total	9	
Mean	1	
A	2	
B	2	
A × B	4	
AB	2	$(Y_{00} + Y_{12} + Y_{21})^2 / 3 + (Y_{01} + Y_{10} + Y_{22})^2 /3 + (Y_{02} + Y_{20} + Y_{11})^2 / 3 - Y_{..}^2 / 9$
AB^2	2	$(Y_{00} + Y_{11} + Y_{22})^2 / 3 + (Y_{02} + Y_{10} + Y_{21})^2 /3 + (Y_{01} + Y_{20} + Y_{12})^2 / 3 - Y_{..}^2 / 9$

The levels of AB are obtained as $i + j$ modulo(3) and the levels of AB^2 as $i + 2j$ modulo(3). The sums of squares for AB and AB^2 add to that for the A × B interaction sum of squares. Hence, they are not only combinatorially orthogonal components but they are also sum-of-squares orthogonal. In general for p a prime number or prime power levels for both of the factors, the A × B interaction with $(p - 1)^2$ degrees of freedom may be partitioned into (p - 1) geometrical components of the interaction each with (p - 1) degrees of freedom as

$$A \times B = AB + AB^2 + AB^3 + \ldots + AB^{p-1}$$

The levels of AB and AB^2 may be used to construct pairwise orthogonal Latin squares as follows:

LS1

Column	Row 0	1	2
0	0	1	2
1	1	2	0
2	2	0	1

LS2

Column	Row 0	1	2
0	0	2	1
1	1	0	2
2	2	1	0

Also, an orthogonal array may be constructed from the above as:

Row:	0	0	0	1	1	1	2	2	2
Column:	0	1	2	0	1	2	0	1	2
LS1:	0	1	2	1	2	0	2	0	1
LS2:	1	2	1	1	0	2	2	1	0

The first row of the array is for row numbers, the second row for columns, the third row for the first Latin square, and the fourth row for the second Latin square. There is a one-to-one relation between orthogonal arrays and the elements of the Projective geometry and complete sets of pairwise orthogonal Latin squares. In general there will be p - 1 geometrical components of the multiplicative interaction. The $(p - 1)^2$ degrees of freedom for the interaction of the two factors is partitioned into p - 1 components each with p - 1 degrees of freedom. These p - 1 components plus the row and column components lead to the p + 1 rows of an orthogonal array. The p^2 -1 degrees of freedom are partitioned into p + 1 components each with p - 1 degrees of freedom, or $(p^2 - 1)/ (p - 1) = p + 1$. These p - 1 geometrical components may be used to construct a complete set of pairwise orthogonal Latin squares, POLS(p, p - 1). This set is also sum-of-squares orthogonal.

When $n = p^k$, a prime power, marks of the field with addition and multiplication rules, are used to obtain the elements of a geometrical interaction component. For example the marks of the field for four are 0, 1, x, and x + 1. A POLS(4, 3) set is:

	Row					Row					Row			
Column	0	1	2	3	Column	0	1	2	3	Column	0	1	2	3
0	0	1	2	3	0	0	1	2	3	0	0	1	2	3
1	1	0	3	2	1	3	2	1	0	1	2	3	0	1
2	2	3	0	1	2	1	0	3	2	2	3	2	1	0
3	3	2	1	0	3	2	3	0	1	3	1	0	3	2

The corresponding orthogonal array is:

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

COMPLETE SETS OF F-SQUARES WITH P SYMBOLS, F(n, p)

When $n = p^k$, F-squares with p symbols (levels), F(n, p), may be constructed instead of Latin squares which are a special case of F-squares for k = 1. For example, let $n = 4 = 2^2$. $(4 - 1)^2 / (2 - 1) = 9$ F(4, 2)s may be constructed to form a complete set. A set of nine pairwise combinatorially orthogonal F(4, 2) squares is:

AC=F1	AD=F2	ACD=F3	BC=F4	BD=F5	BCD=F6
0 0 1 1	0 0 1 1	0 0 1 1	0 1 0 1	0 1 0 1	0 1 0 1
0 0 1 1	1 1 0 0	1 1 0 0	0 1 0 1	1 0 1 0	1 0 1 0
1 1 0 0	0 0 1 1	1 1 0 0	1 0 1 0	0 1 0 1	1 0 1 0
1 1 0 0	1 1 0 0	0 0 1 1	1 0 1 0	1 0 1 0	0 1 0 1

ABC=F7	ABD=F8	ABCD=F9
0 1 1 0	0 1 1 0	0 1 1 0
0 1 1 0	1 0 0 1	1 0 0 1
1 0 0 1	0 1 1 0	1 0 0 1
1 0 0 1	1 0 0 1	0 1 1 0

For the above, the column numbers are 00, 01, 10, and 11 for factors A and B. The row numbers are 00, 01, 10, and 11 for factors C and D. Thus the 16 combinations of the four factor factorial are those for a 2^4 factorial. The levels, 0 and 1, for the A × C multiplicative interaction are the same as for the geometrical interaction component AC. This one-to-one correspondence holds for $n = 2^k$. These levels form the F-square F1. The same procedure is used to construct F2 to F9. This is the maximum number, 9 / (2 - 1), that can be formed and thus forms a complete set. The following semi-F-squares may be formed from the rows and columns:

A	B	AB	C	D	CD
0 0 1 1	0 1 0 1	0 1 1 0	0 0 0 0	0 0 0 0	0 0 0 0
0 0 1 1	0 1 0 1	0 1 1 0	0 0 0 0	1 1 1 1	1 1 1 1
0 0 1 1	0 1 0 1	0 1 1 0	1 1 1 1	0 0 0 0	1 1 1 1
0 0 1 1	0 1 0 1	0 1 1 0	1 1 1 1	1 1 1 1	0 0 0 0

An orthogonal array with two rows of four symbols and nine rows of two symbols or an orthogonal array of $2^4 = 15$ rows with two symbols, 0 and 1, in each row could be formed from the above. The 15 row orthogonal array for the latter case is:

A:	0 0 1 1	0 0 1 1	0 0 1 1	0 0 1 1
B:	0 1 0 1	0 1 0 1	0 1 0 1	0 1 0 1
AB:	0 1 1 0	0 1 1 0	0 1 1 0	0 1 1 0
C:	0 0 0 0	0 0 0 0	1 1 1 1	1 1 1 1
D:	0 0 0 0	1 1 1 1	0 0 0 0	1 1 1 1
CD:	0 0 0 0	1 1 1 1	1 1 1 1	0 0 0 0
AC:	0 0 1 1	0 0 1 1	1 1 0 0	1 1 0 0
AD:	0 0 1 1	1 1 0 0	0 0 1 1	1 1 0 0
ACD:	0 0 1 1	1 1 0 0	1 1 0 0	0 0 1 1
BC:	0 1 0 1	0 1 0 1	1 0 1 0	1 0 1 0
BD:	0 1 0 1	1 0 1 0	0 1 0 1	1 0 1 0
BCD:	0 1 0 1	1 0 1 0	1 0 1 0	0 1 1 0
ABC:	0 1 1 0	0 1 1 0	1 0 0 1	1 0 0 1
ABD:	0 1 1 0	1 0 0 1	0 1 1 0	1 0 0 1
ABCD	0 1 1 0	1 0 0 1	1 0 0 1	0 1 1 0

This array is combinatorially orthogonal as well as sum-of-squares orthogonal.

COMPLETE SET OF F-SQUARES FOR N EQUAL A PRODUCT OF PRIMES

Federer (2003a, 2003b, 2003d) has demonstrated how to obtain complete sets of sum-of-squares orthogonal F-squares, SOSOFS, for all n equal to a product of prime numbers. This new geometry includes the case when n is a prime number but does not work for a prime power. He (2003c) also demonstrated that the set obtained was the maximum number that could be constructed. The F-squares for n not a prime number will be a combination of regular F-squares and semi-F-squares. It was further shown how to construct sum-of-squares orthogonal arrays from the complete sets. The method used was an adaptation of that for prime numbers.

To illustrate, let n = 6 = 2 × 3. Let the row numbers be represented by the two-level factor A by the three-level factor B; let the column numbers be designated by the factors C at two levels and D at three levels. Then the relation of the factorial effects and the resulting F-squares is depicted in the following analysis of variance table:

Source of variation	Degrees of freedom			F-square
Total	36			
Correction for mean	1			
Row	5			
A		1		FR1 = F(6, 2)
B		2		FR2 = F(6, 3)
A × B =AB		2		FR3 = F(6, 3)
Column	5			
C		1		FC1 = F(6, 2)
D		2		FC2 = F(6, 3)
C × D = CD		2		FC3 = F(6, 3)
Row × column	25			
A × C = AC		1		F1 = F(6, 2)
A × D = AD		2		F2 = F(6, 3)
A × C × D = ACD		2		F3 = F(6, 3)
B × C = BC		2		F4 = F(6, 3)
B × D		4		
BD			2	F5 = F(6, 3)
BD^2			2	F6 = F(6, 3)
B × C × D		4		
BCD			2	F7 = F(6, 3)
BCD^2			2	F8 = F(6, 3)
A × B × C =ABC			2	F9 = F(6, 3)
A × B × D		4		
ABD			2	F10 = F(6, 3)
ABD2			2	F11 = F(6, 3)
A × B × C× D		4		
ABCD			2	F12 = F(6, 3)
$ABCD^2$			2	F13 = F(6, 3)

The above F1 to F13 represent a complete set of F-squares. This is the maximum number that can be constructed from the 25 degrees of freedom and the associated sums of squares. In addition, three F-squares, FR1, FR2, and FR3, may be constructed from the row degrees of freedom and sum of squares and three F-squares, FC1, FC2, and FC3, from the column degrees of freedom and sum of squares. These 19 F-squares may be used to construct a 19 row by 36 column sum-of-squares orthogonal array. Also, a 15 row sum-of-squares orthogonal array with two rows of six symbols for the row and column numbers and 13 additional rows using F1 to F13. F-squares FR1, FR2, FR3, FC1, FC2, FC3, F2, F3, F4, and F9 are semi-F-squares. The remaining ones are regular F-squares.

A combinatorially orthogonal array of three rows of six symbols (0, 1, 2, 3, 4, 5) and seven rows of three symbols (0, 1, 2) is given in Federer (2003a, 2003b). He shows how to complete this set with three semi-F-squares, F(6, 3). This is a complete set and no larger sum-of-squares array can be constructed. The combinatorially orthogonal set has one Latin square and seven F(6, 3) squares. The complete orthogonal array for this last case is:

Row	000000	111111	222222	333333	444444	555555
Column	012345	012345	012345	012345	012345	012345
Treatment	012345	103254	234501	325410	450123	541032
F1	211002	201201	022110	012012	100221	120120
F2	012021	210102	121020	202110	021201	100212
F3	102012	211020	120102	021210	202101	010221
F4	121020	202110	021201	100212	012021	210102
F5	112200	001122	220011	001122	112200	220011
F6	112200	220011	001122	112200	001122	220011
F7	001122	112200	001122	220011	112200	220011
A×F1=F8	211002	201201	022110	120120	211002	201201
A×F2=F9	012021	210102	121020	010221	102012	211020
C×F3=F10	102120	211101	120210	021021	2 02212	010002

The first ten rows of the above array are pairwise combinatorially orthogonal as well as sum-of-squares orthogonal. The last three rows are only sum-of-square pairwise orthogonal as these are semi-F-squares.

COMMENTS

Federer (2003c) has determined the cardinality for complete sets of sum-of-squares orthogonal F-square of order n, a product of prime numbers. Constructing the additional F-squares from row and column numbers allows construction of sum-of-squares orthogonal arrays of maximum width and length n^2. Such arrays greatly increase the number of arrays useful for constructing codes, experiment designs, fractional replicates, etc. The sum-of-squares orthogonal arrays considerably increase the flexibility for codes with varying numbers of symbols in the arrays. Saturated main effect plans for factors at different levels may be constructed from the sum-of-squares orthogonal arrays. It is to be noted that the new geometry is used in the same manner as the one for prime numbers. The only difference is that the orthogonal arrays obtained are sum-of-squares orthogonal but not combinatorially orthogonal. Both types of orthogonality occur when n is a prime number.

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