

13.5.5 Quadratic Simplexes

A simplex most usually produces m coefficients in m runs. Historically, that simplex contains only linear terms, and Section 13.5.2 showed an example. However, if the points at the simplex vertices were augmented with midpoints on each edge, it would contain exactly the $m(m+1)/2$ runs needed to calculate both linear and quadratic coefficients. In general, quadratic simplexes are not orthogonal in the factors, but using the inverse matrix square root, one may always find orthogonal components that render the coefficients independent. One may generate quadratic simplexes as follows.

1. Begin with an appropriate RVS design, linear and orthogonal in $m+1$ points.
2. Average the coordinates of each of the $m(m+1)/2$ pairs to create $m(m+1)/2$ new coordinates associated with the midpoint of each edge of the simplex.
3. Subtract the mean value of the sum from each quadratic component break the interaction with a_0 .
4. Observe $\mathbf{X}^T\mathbf{X}$ after this procedure; it may reveal further means for generating additional orthogonal components. Notwithstanding, at least a portion of quadratic matrix may remain nonorthogonal.
5. Use $\mathbf{S}^{-1}$ to generate orthogonal components for those remaining via $\mathbf{W} = \sqrt{m(m+1)/2} \cdot \mathbf{XS}^{-1}$. The multiplier is not strictly necessary but serves to generate a first column of 1s for $\mathbf{W}$. In such a case, $\mathbf{W}^T\mathbf{W}$ generates a diagonal matrix having diagonal entries of value $m(m+1)/2$ and zeroes elsewhere. Without the multiplier, the diagonal elements will be unity.

Example 13.5-2: A Quadratic Simplex in Three Factors.

Problem Statement:

1. Construct a quadratic simplex in three factors per the procedure above. Show the matrix $\mathbf{X}$, orthogonalized to the extent convenient
2. Show also $\mathbf{S}^{-1}$ and $\mathbf{W}$ to complete the orthogonalization of $\mathbf{X}$.
3. Show that $\mathbf{W}$ is orthogonal.
4. Using $\mathbf{XS}^{-1}$, write out the equation $\hat{\mathbf{y}} = \mathbf{Wb}$ in terms of the components and coefficients for $\hat{\mathbf{y}} = \mathbf{Xa}$

Solution:

In the present case, the linear quadratic simplex in three factors is identical to the half fraction of the two-level factorial design and this will be the case whenever $m = 2^n - 1$. However, the quadratic simplex adds middle edge points.

1. Table 13.5-1 shows $\mathbf{X}$ for the full quadratic simplex. Note that Columns 11, 22, and 33 have been transformed by Column $kk = x_k^2 - 3/5$ to avoid interactions with a_0 . Additionally, an inspection of $\mathbf{X}^T\mathbf{X}$ showed the interactions to be affected by their complementary main effects. Hence, the interaction columns were transformed via $x_jx_k - 2/3 x_h$, yielding the revised $\mathbf{X}^T\mathbf{X}$ of Table 13.5-2. Figure 13.5-2 gives the disposition in factor space.

Table 13.5-1

The X Matrix for the Quadratic Simplex in Three Factors

	Factors									
Pt	0	1	2	3	11	22	33	12	13	23
1	1	1	-1	-1	2/5	2/5	2/5	-1/3	-1/3	1/3
2	1	-1	1	-1	2/5	2/5	2/5	-1/3	1/3	-1/3
3	1	-1	-1	1	2/5	2/5	2/5	1/3	-1/3	-1/3
4	1	1	1	1	2/5	2/5	2/5	1/3	1/3	1/3
12	1	0	0	-1	-3/5	-3/5	2/5	2/3	0	0
13	1	0	-1	0	-3/5	2/5	-3/5	0	2/3	0
23	1	-1	0	0	2/5	-3/5	-3/5	0	0	2/3
14	1	1	0	0	2/5	-3/5	-3/5	0	0	-2/3
24	1	0	1	0	-3/5	2/5	-3/5	0	-2/3	0
34	1	0	0	1	-3/5	-3/5	2/5	-2/3	0	0

Table 13.5-2

The X^TX Matrix for the Quadratic Simplex in Three Factors

	0	1	2	3	11	22	33	12	13	23
0	10									
1		6								
2			6							
3				6						
12					12/5	2/5	2/5			
13					2/5	12/5	2/5			
23					2/5	2/5	12/5			
11								4/3		
22									4/3	
33										4/3

2. An examination of Table 13.5-2 reveals that the adjusted effects are orthogonal except for the pure quadratics, which are mutually biased. The inverse matrix, $\mathbf{S}^{-1}$, of Table 13.5-3 shows the required transformations*.

Examining the pure quadratic block, one notes that $\left(\frac{\sqrt{5}}{12} + \frac{\sqrt{2}}{3}\right)\left(x_h^2 - \frac{3}{5}\right) + \left(\frac{\sqrt{5}}{12} - \frac{\sqrt{2}}{6}\right)\left(x_j^2 + x_k^2 - \frac{6}{5}\right)$ gives orthogonal components. Dividing by $\left(\frac{\sqrt{5}}{12} + \frac{\sqrt{2}}{3}\right)$ one might also normalize the orthogonal component as $\left(x_h^2 - \frac{3}{5}\right) + \left(\frac{\sqrt{10}-4}{\sqrt{10}+8}\right)\left(x_j^2 + x_k^2 - \frac{6}{5}\right)$. Table 13.5-4 shows $\mathbf{W} = \sqrt{10} \cdot \mathbf{XS}^{-1}$.

* Excel and Real-Statistics algorithms sometime have difficulty calculating matrix inverses, roots, and eigenvectors for matrices having repeated eigenvalues, which happens to be the case here for $\mathbf{X}^T\mathbf{X}$ [verifiable via =EigVal($\mathbf{X}^T\mathbf{X}$)]. The solution in such cases is to parse $\mathbf{X}^T\mathbf{X}$ into orthogonal and non-orthogonal blocks. For the orthogonal elements of $\mathbf{X}^T\mathbf{X}$, the inverse square root of each diagonal element corresponds to the proper one for $\mathbf{S}^{-1}$. For the nonorthogonal block (e.g., pure quadratics), one may apply =MINVERSE(MSQRT()) without issues to find the inverse square root of that matrix block. This allows one to assemble $\mathbf{S}^{-1}$ in piecewise fashion without discombobulating Excel.

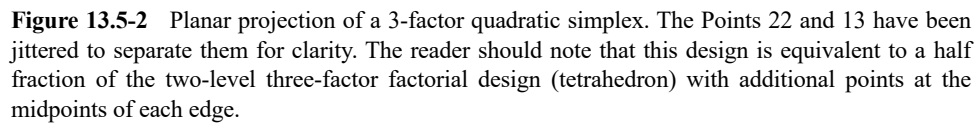


Table 13.5-3
The S^{-1} Matrix for the Quadratic Simplex in Three Factors

	0	1	2	3	11	22	33	12	13	23
0	$1/\sqrt{10}$									
1	$1/\sqrt{6}$									
2	$1/\sqrt{6}$									
3	$1/\sqrt{6}$									
12					$\sqrt{5/12} + \sqrt{2/3}$	$\sqrt{5/12} - \sqrt{2/6}$	$\sqrt{5/12} - \sqrt{2/6}$			
13					$\sqrt{5/12} - \sqrt{2/6}$	$\sqrt{5/12} + \sqrt{2/3}$	$\sqrt{5/12} - \sqrt{2/6}$			
23					$\sqrt{5/12} - \sqrt{2/6}$	$\sqrt{5/12} - \sqrt{2/6}$	$\sqrt{5/12} + \sqrt{2/3}$			
11								$\sqrt{3/2}$		
22								$\sqrt{3/2}$		
33								$\sqrt{3/2}$		

Table 13.5-4

The W Matrix for the Quadratic Simplex in Three Factors

	Factors									
Pt	w_0	w_1	w_2	w_3	w_{11}	w_{22}	w_{33}	w_{12}	w_{13}	w_{23}
1	1	a	$-a$	$-a$	b	b	b	$-e$	$-e$	e
2	1	$-a$	a	$-a$	b	b	b	$-e$	e	$-e$
3	1	$-a$	$-a$	a	b	b	b	e	$-e$	$-e$
4	1	a	a	a	b	b	b	e	e	e
12	1	0	0	$-a$	$-c$	$-c$	d	f	0	0
13	1	0	$-a$	0	$-c$	d	$-c$	0	f	0
23	1	$-a$	0	0	d	$-c$	$-c$	0	0	f
14	1	a	0	0	d	$-c$	$-c$	0	0	$-f$
24	1	0	a	0	$-c$	d	$-c$	0	$-f$	0
34	1	0	0	a	$-c$	$-c$	d	$-f$	0	0

Here, $a = \sqrt{15}/3$, $b = \sqrt{2}/2$, $c = \sqrt{2\sqrt{10} + 7}/3$, $d = \sqrt{22 - 4\sqrt{10}}/3$, $e = \sqrt{30}/6$, and $f = \sqrt{30}/3$. Note that $\mathbf{W}$ is identical to $\mathbf{X}$ with a change in substitutions: $a = 1$, $b = 2/5$, $c = 3/5$, $d = 2/5$, $e = 1/3$, and $f = 2/3$.

3. As shown

Table 13.5-5

The $\mathbf{W}^T \mathbf{W}$ Matrix for the Quadratic Simplex Showing That $\mathbf{W}$ is Orthogonal.

	w_0	w_1	w_2	w_3	w_{11}	w_{22}	w_{33}	w_{12}	w_{13}	w_{23}
w_0	10									
w_1		10								
w_2			10							
w_3				10						
w_{11}					10					
w_{22}						10				
w_{33}							10			
w_{12}								10		
w_{13}									10	
w_{23}										10

4. The equations in w and in x follow, the latter explicitly showing the orthogonal components in x that render those coefficients independent.

$$\hat{y} = w_0 + \sum_{k=1}^3 b_k w_k + b_{kk} w_{kk} + \sum_{j < k}^2 \sum_k^3 b_{jk} w_{jk}$$

$$\begin{aligned} \hat{y} = a_0 + \sum_{k=1}^3 a_k x_k + \sum_{h=1}^3 a_{hh} \left[\left(x_h^2 - \frac{3}{5} \right) + \frac{\sqrt{10} - 4}{\sqrt{10} + 8} \left(x_{j \neq h, k}^2 + x_{k \neq h, j}^2 - \frac{6}{5} \right) \right] \\ + \sum_{j < k}^2 \sum_k^3 b_{jk} \left(x_j x_k - \frac{1}{3} x_{h \neq j \neq k} \right) \end{aligned}$$