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The U.S. Department of Agriculture has used response-surface techniques as applied by Baker and Bargmann (1981) to plant process simulation models as an aid in the identification of interrelationships among yield and various single-valued and functional parameters. Orthogonal cubic surfaces have provided insight into higher order relationships as well as a measure of the relative sensitivity of yield to experimentally determined parameter values. Several examples investigate the effectiveness of those higher order surfaces and illustrate how less precise (and less costly) measurements may be possible in building and using these simulation models.

KEY WORDS: Response surfaces; Experimental design; Statistical computation.

1. INTRODUCTION

The application of response-surface techniques to plant process simulation (PPS) models was initiated by the U.S. Department of Agriculture (USDA) as an analytic tool by which agronomists, agricultural engineers, and other plant scientists could identify more clearly the structure of their plant process models and the effectiveness of those models in mimicking the actual growth of a specific kind of plant or plants. In addition, the sensitivities of various responses could be identified with respect to model inputs, parameters, and substructures.

Plant modelers have had two basic objectives—to study the individual plant processes and their adaptation to various stresses and to predict biological yield. Parameter values for the differential equations and for the functional expressions are determined either by experimentally derived regression equations or by calibration. In most cases, the plant is grown on a daily time step, where the biomass is generated as a function of heat units or calendar days. The plant may be stressed as it reacts to initial and daily input of environmental variables, such as maximum and minimum temperatures, solar radiation, and precipitation. Various models permit application of fertilizers, pesticides, and herbicides and irrigation treatments.

The USDA Statistical Reporting Service currently uses regression models to estimate final gross yield and to make early and midseason forecasts of final yield. One potential application of PPS models is forecasting on the basis of early-season weather conditions, observed plant-part information, and simulated future weather. PPS models are validated by using the techniques and criteria in Wilson et al. (1980).

In our study of the structure of a PPS model (after validation), we have been concerned about the degree of interrelationships between model variables and parameters and about the sensitivity of yield to various factors. In a previous paper (Baker and Bargmann 1981), we discussed our first application of response-surface techniques to PPS models. Many of the resultant surfaces were not quadratic, but linear with large errors. Cubic effects were studied to determine whether such fine structure is required to exhibit the relationships. With the derivation and application of a scaled orthogonal central composite design, we are able to detect higher order relationships (in the model) and the sensitivity of the yield response to these relationships (as represented in the given model).

Let us first consider the derivation of an orthogonal cubic central composite design. Then we shall apply this orthogonal cubic design to a PPS model and discuss the resulting equations. The information from these equations will be contrasted with the information from the corresponding quadratic designs.

2. BACKGROUND

Most of the early research with response surfaces (e.g., Box 1954, Box and Hunter 1957, Draper 1960, and Gardiner et al. 1959) was concerned with the classes of second- and third-order designs that are rotatable. Box and Hunter (1957) addressed the topic of orthogonality for second-order designs only; they referred to the bias introduced if higher order terms are nonnegligible. There are many more such terms in a cubic model than in linear or quadratic models.

Gardiner et al. (1959) derived rotatable third-order designs without consideration of orthogonality. The use of central composite designs permits sequential methods for progressing to higher order surfaces. Derringer (1969), for example, discussed this procedure for up to third-order designs. Later authors have investigated other criteria for response-surface designs, including minimum bias estimation (e.g., Thompson 1973), *D* and *G* efficiency (e.g., Lucas 1976), and minimum point designs (e.g., M. J. Box and Draper 1974). G. E. P. Box and Draper (1982) suggested that power transformations can be used both to ascertain the degree of the response surface necessary for a good fit of the data and (with the transformed variables) to reduce the design to a lower degree. In their discussion they derived relationships in a cubic response-surface model. Montgomery and Bettencourt (1977) discussed the use of response-surface methodology for computer simulations in the context of system optimization for multiple responses. Smith and Mauro (1982) described strategies available for the analysis of large

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Table 1. Parameters and Definitions

Parameter	Definition
k	Number of factors
r	Number of replications at the center point (0, 0, . . .)
Lattice points	The 3^k points of the complete 3^k design
$n = 3^k + 2^*k + (r - 1)$	Number of observations
$a^2 = (n^*3^{k-2})^{1/2} - 3^{k-1}$	The squares of the nonzero factor levels at the star points (dependent on k and r)
$\gamma = 2^*(3^{k-2}/n)^{1/2}$ $= 2^*(a^2 + 3^{k-1})/n$	The correction for quadratic terms
$\delta = (3^{k-1} + a^4)/(3^{k-1} + a^2)$	The correction for cubic terms

Table 2. Minimal Values for n and Associated Values for a, γ, and δ

k	n	a	γ	δ
2	13	.7782	.5547	.9338
3	33	.9746	.6030	.9952
4	89	1.1410	.6360	1.0139
5	253	1.2845	.6534	1.0130
6	741	1.4113	.6612	1.0081

NOTE: For seven or more factors, fractional factorials are available (e.g., see John 1971, p. 143) that leave all terms up to and including cubics unaliased with other terms of degree three or less.

numbers of variables when factor screening procedures are employed.

3. THIRD-ORDER CENTRAL COMPOSITE DESIGNS WITH ALL EFFECTS ORTHOGONAL

As in the familiar second-order central composite design, the levels at which the "star points" are to be chosen ($+a$ and $-a$ for one factor with all other factors held constant at the central level) are completely determined if the design is to be orthogonal. A design variation is available if the center point is repeated r times (it should be noted, however, that the center point is one of the lattice points in the 3^k design, so an additional $r - 1$ readings should be made at this point if a different a is desired). For the present application the center point is given the weight r, since in most cases, for current PPS models, the response will be deterministic when the input levels are set. In the following set of formulas, each factor has been standardized so that the elements of the $X'X$ matrix will be 1 in the diagonal (except, of course, the constant term, which is estimated by the grand mean). Table 1 contains parameters and definitions for the design, and Table 2 contains the resulting values.

Table 3 presents the definition of standardized orthogonal linear, quadratic, and so forth, effects using the parameters defined in Table 1. With these definitions, all diagonal elements of $X'X$ (except the first) are 1.

The estimates of the coefficients for the standardized orthogonal effects are obtained from the responses at the 3^k lattice points, the center point(s), and the $2k$ star points. The 3^k lattice points are subjected to the extended Yates algorithm for 3^k factorial designs with the following modification: In the third cycle, where the Yates algorithm requires (High + Low − 2 · Middle) for each triple, the special application for this design uses just (High + Low). Thus after recording the responses to the lattice points in extended Yates order (−1, −1, −1; 0, −1, −1; 1, −1, −1; 1, 0, −1; 0, 0, −1; . . . ; 1, 1, 1) and dividing them into triples, the first 3^{k-1} entries of the next column are the sums of each triple (cycle 1: High + Middle + Low), the second 3^{k-1} entries are the differences of last minus first in each triple (cycle 2: High − Low), and the third 3^{k-1} entries are the modified sums (cycle 3: High + Low, instead of the usual High − 2 · Middle + Low). This procedure is performed k times. In Table 4, $E(a)$ denotes the entry in the final (k + 1st) column in the row corresponding to level (0, −1, −1, . . .) of this extended Yates tableau, $E(a^q)$ is the entry in row (1, −1, −1, . . .), $E(ab)$ is in row (0, 0, −1, −1, . . .), $E(ab^q)$ is in row (0, 1, −1, −1, . . .), and $E(abc)$ is in row (0, 0, 0, −1, . . .) of the final column of the extended Yates tableau. X_+ and X_- denote the responses for the star points, with factor X, at $+a$ and $-a$, respectively. G is the grand total.

For $k = 2$, the resulting response equation can be expressed as

$$\begin{aligned} z = {} & G/n + A_x \cdot X \text{ (linear)} + A_y \cdot Y \text{ (linear)} \\ & + A_{xy} \cdot XY \text{ (linear–linear)} \\ & + A_{xx} \cdot X \text{ (quadratic)} + A_{yy} \cdot Y \text{ (quadratic)} \\ & + A_{xxx} \cdot X \text{ (cubic)} \\ & + A_{yyy} \cdot Y \text{ (cubic)} + A_{xyy} \cdot XY \text{ (linear–quadratic)} \\ & + A_{yxx} \cdot YX \text{ (linear–quadratic)}, \end{aligned}$$

where the coefficients (e.g., A_x) are evaluated as in Table 4 and the orthogonal polynomials are defined as in Table 3.

The significance of each effect can be assessed by dividing each of these coefficients by the square root of the mean squared error (MSE) and comparing the result with t tables. Effects of degree 4 and higher and any replications are regarded as residual terms.

As in the case of a second-order design, replication of the center point permits other choices of the value a of the star

Table 3. Definitions of Standardized Orthogonal Effects for k Factors

Effect	Standardized Orthogonal Effect
X (linear)	$(n\gamma)^{-1/2} \cdot x$
X (quadratic)	$\{2(a^4 + 3^{k-2})\}^{-1/2} \cdot (x^2 - \gamma)$
X (cubic)	$(2a \cdot \lvert 1 - a^2 \rvert)^{-1} \cdot (n\gamma/3^{k-1})^{1/2} \cdot (x^2 - \delta) \cdot x$
XY (linear–linear)	$(4 \cdot 3^{k-2})^{-1/2} \cdot xy$
XY (linear–quadratic)	$(4 \cdot 3^{k-3})^{-1/2} \cdot x \cdot \{(y^2 - \gamma) - 2 \cdot (x^2 - \delta)/[3 \cdot (1 - a^2)]\}$
XYZ (linear–linear–linear)	$(8 \cdot 3^{k-3})^{-1/2} \cdot xyz$ ($k \geq 3$)

Table 4. Estimates of Coefficients of Orthogonal Effects for k Factors

Effect	*Coefficient*
X (linear)	$(n\gamma)^{-1/2} \cdot [E(a) + \alpha(X_+ - X_-)]$
X (quadratic)	$\{2(\alpha^4 + 3^{k-2})\}^{-1/2} \cdot \{E(a^q) + \alpha^2(X_+ + X_-) - \gamma^* G\}$
X (cubic)*	$(3^{k-1} n\gamma)^{-1/2} \cdot (\alpha E(a) - 3^{k-1}(X_+ - X_-)) \cdot \text{sgn}(1 - \alpha^2)$
XY (linear–linear)	$(4 \cdot 3^{k-2})^{-1/2} \cdot E(ab)$
XY (linear–quadratic)	$(4 \cdot 3^{k-3})^{-1/2} \cdot \{E(ab^q) - (2/3) \cdot E(a)\}$
XYZ (linear–linear–linear)	$(8 \cdot 3^{k-3})^{-1/2} \cdot E(abc)$ $(k \geq 3)$

* $\text{sgn}(x) = 1$, if $x > 0$; 0, if $x = 0$; -1, if $x < 0$.

point, while retaining the complete orthogonality property. The estimation procedure will then place additional weight on the center point observations. Because of this weighting of a central observation, we suggest keeping the choice of α within modest bounds of its minimal value. From the equation relating α and n in Table 1, we obtain

$$n = (\alpha^2 + 3^{k-1})^2 / 3^{k-2}.$$

Thus if $k = 3$ and $\alpha = 1.141$, then $n = 35.4$; for exact orthogonality, $n = 35$ (i.e., two extra replications of the center point) would require an α of 1.117.

For the purpose of illustrating the procedure, a numerical example has been included in the Appendix. (The computer program ORTCUB and instructions for its use can be obtained from the authors.)

4. APPLICATIONS OF CUBIC DESIGNS

The first example is presented to illustrate the procedure and interpretation of orthogonal cubic response surfaces when applied to PPS models. The second example illustrates the actual use of the procedure to decide, for a given PPS model, whether a cubic response surface is required or whether the much cheaper quadratic response surface would be adequate to explain the interaction of input variables or parameters and their effect on predicted yield.

4.1 A Florida Soybean Model

Scientists at the University of Florida (Gainesville) are constructing several versions of a soybean PPS model. For a given location, variety, and soil, these models "grow" a soybean plant on a daily basis, using known physiological relationships, experimentally derived relationships, and observed daily weather data. The farm operator can enter different combinations of management practices and pest regimes.

For our sensitivity analysis with cubic response surfaces, we used the research version of the model SOYGRO (Wilkerson et al. 1981). Weather inputs of maximum daily temperature (A), minimum daily temperature (B), and solar radiation (C) were the factors.

Table 5. Yates Order Seed Weight Responses for SOYGRO Example: Florida Soybean Model, 1980 Weather, 10% Deviation

411	423	415	416	416	407	415	410	401
431	442	436	436	434	428	434	428	419
443	455	448	448	450	438	447	443	435
436	428	442	429	416	449			

When three factors are used in a deterministic central composite design, 33 data points are required, including 6 star points at a distance of .9746 from the design center. The +1 and −1 levels of the three factors represent a 10% fluctuation in the daily values with the observed weather values as the center point settings. The point (−1, 0, 1), for example, represents days when the maximum temperature was reduced by 10% each day, the minimum daily temperature remained the same, and the solar radiation increased by 10% for each day. In the northern panhandle of Florida, for some design points, if minimum daily temperature is increased by 10%, say, it will be larger than the maximum daily temperature when it is decreased by 10%; the minimum and maximum temperatures are both set to the average of the two calculated temperatures in these cases. Seed weight in g/m^2 (SEEDWT) is the recorded response.

Actual 1980 weather data from Gainesville were entered as input to drive the simulation of the growth process of Bragg soybeans. The simulated seed weights are listed in Table 5 in Yates order for the lattice, followed by seed weights at the star points A_-, A_+, B_-, B_+, C_-, and C_+; the values for α, γ, and δ and the definitions of the orthogonal expressions are given in Table 6. The coefficients of the orthogonal effects and the statistical significance of their contributions appear in Table 7.

The orthogonal cubic response surface for seed weight shows that the effect of solar radiation (C) is very strong, with a linear coefficient of more than 16% of the calibrated model response; this large contribution is masked in the quadratic response-surface equation (5%). When the orthogonal factors' contri-

Table 6. Orthogonal Cubic Parameters and Expressions for SOYGRO Example

$N = 33$

$\alpha^2 = .9498$

$\alpha = .9746$

$\gamma = .6030$

$\delta = .9952$

X-LINEAR = .224 * X

X-QUADRATIC = .3580 * (X² − .6030)

X-CUBIC = 15.21 * X * (X² − .9952)

XY-LINEAR.LINEAR = .2887 * X * Y

XYZ-LIN.LIN.LIN = .3536 * X * Y * Z

XY-LIN.QUAD = .5000 * (X * (Y² − .6030)
  − 13.29 * X * (X² − .9952))

Table 7. Output From ORTCUB (A, B, C, Response = SEEDWT): 1980 Gainesville Weather, 10% Deviation

Effect	Orthogonal Coefficients	Resp. Eq. Coefficients	T for Ho, Parameter = 0	Pr > |T|
Mean	430.594	435.986	—	—
A	−14.202	−2.159	−14.47	.1415E-08
A(2)	−13.981	−5.005	−14.74	.1716E-08
A(3)	1.735	−2.340	1.829	.0905
B	−18.710	−3.665	−19.72	.4530E-10
A B	−15.820	−4.567	−16.68	.3713E-09
A(2) B	7.578	3.789	7.988	.2273E-05
B(2)	−1.686	−.603	−1.777	.0990
B(2) A	4.403	2.202	4.642	.4615E-03
B(3)	3.796	−3.315	4.001	.1508E-02
C	72.700	22.361	76.63	.1186E-17
A C	.436	.126	.459	.6535
A(2) C	−.672	−.336	.708	.4912
B C	.670	.199	.707	.4923
A B C	.574	.203	.604	.5559
B(2) C	−.208	−.104	.219	.8299
C(2)	−9.312	−3.333	−9.816	.2230E-06
C(2) A	−.081	−.040	−.085	.9325
C(2) B	1.608	.804	1.695	.1139
C(3)	−.768	−5.827	−.809	.4330

NOTE: SS regression, 6471.28; SSE, 11.70; R^2, .998; MS regression, 340.59; MSE, .900; Root MSE, .949; DF regression, 19; DF error, 13.

butions to seed weight are ordered, nine terms are significant (at the .05 level), with B(3) the last significant term. The quadratic–linear interactions between A and B are also significant.

In comparison, the quadratic surface (Table 8) has five significant terms and is basically linear, with A–B interaction. C has a linear coefficient that is less than 4% of the predicted center point response. The quadratic effects of A and C are not significant in this response surface.

The presence of higher order terms and interactions provide a clearer picture of the sensitivity of seed weight to the weather factors in the model. It may yet be difficult to interpret these interaction terms physically, but the behavior of the response is more precisely defined.

The prediction errors for both the quadratic and cubic models are very small and have not been presented; there is little variation in the seed weight for this particular combination of environmental data, and both models have a good fit. The cubic model has provided us with a more revealing description of the relationship between seed weight and the environmental variables.

4.2 A Texas Wheat Model

The Maas and Arkin (1980) wheat model TAMW was chosen to investigate the need for further refinement of response-surface models. Four factors were chosen with $a = 1.25$ to describe this PPS model for winter wheat grown in Temple, Texas, in 1978–1979. Results were obtained for one response—yield—for 89 points in the cubic central composite design with four factors. The 25 points used to determine the quadratic response surface are a subset of these 89 points.

Table 9 presents the coefficients of the response equation that, in the cubic surface, are significant at the .05 level. The

Table 8. SAS Output PROC GLM for Quadratic Response Surface: 1980 Gainesville Weather, 10% Deviation

Parameter	Estimate	T for Ho, Parameter = 0	Pr > |T|	S Er of Estimate
Intercept	435.678	285.75	.0001	1.525
A	−2.661	−2.89	.0341	.920
B	−3.203	−3.48	.0176	.920
C	16.290	17.66	.0001	.920
A * B	−4.367	−4.27	.0080	1.024
A * C	.341	.33	.7526	1.024
B * C	.137	.13	.8988	1.024
A * A	−4.320	−2.29	.0703	1.884
B * B	−.807	−.43	.6862	1.884
C * C	−3.542	−1.88	.1188	1.884

NOTE: SS regression, 3,120.15; SSE, 41.92; R^2, .987; MS regression, 346.68; MSE, 8.38; Root MSE, 2.90; DF regression, 9; DF error, 5.

maximum relative error in prediction of the observed value from the quadratic response surface was less than 2.75%, and with only one exception, the bias of prediction from the quadratic design is in the same direction as the bias from the cubic equation. Despite the significance of some of the cubic effects in the response equation, the quadratic model seems to describe quite adequately the behavior of the plant growth simulation model for this environmental scenario.

This last illustration describes the actual situation for which the orthogonal cubic procedure was designed. We found that for these weather conditions, and for the prediction of yield (rather than other responses, such as number of heads), the quadratic response equation was sufficient.

It should be noted that if the number of control variables to be studied simultaneously is three or fewer, then the extra effort to obtain simulation runs for a cubic design is so small that the refined model should be employed. It is for the very complex PPS models and for widely differing weather conditions that studies of this kind should be made, for then the additional runs that are required may be both expensive and unnecessary.

Table 9. 1979 Temple Wheat Data—Response-Surface Equations With $a = 1.25$

Term	Coefficient		
	Quadratic	Cubic	Orthogonal Cubic*
Intercept	5.206	5.213	5.1557
A	1.288	1.150	9.5880
B	.221	.227	1.6760
C	−.059	.070	−.4344
D	1.030	1.031	7.7960
A(2)	−.121	−.140	−.6683
A D	.259	.254	1.5230
B D	.044	.044	.2663
C(2)	ns	.046	.2175
A B	ns	.027	.1637
A C	ns	.019	.1120
B C	ns	.011	.0635
C D	ns	−.010	−.0618
C(3)		−.147	−.1871
C(2) A		.071	.2463
A(2) C		.043	.1480
A(2) D		−.029	−.0993

* With $a = 1.25$, the center point carries a weight of 2.65 to ensure complete orthogonality.

Table A.1. Extended Yates Table

Effect	*T*	*A*	*B*	*C*
1	71	354	1,326	4,968
a	132	448	1,698	546
a^q	151	524	1,944	3,252
b	108	441	232	672
ab	160	580	166	−60
a^qb	180	677	148	468
b^q	131	504	852	3,270
ab^q	182	670	1,112	380
a^qb^q	211	770	1,288	2,140
c	108	80	170	618
ac	157	72	236	−84
a^qc	176	80	266	436
bc	165	68	0	96
abc	200	50	−20	−40
a^qbc	215	48	−40	64
b^qc	200	72	120	396
ab^qc	229	44	164	−56
a^qb^qc	248	32	184	280
c^q	129	222	878	3,270
ac^q	174	288	1,118	380
a^qc^q	201	342	1,274	2,140
bc^q	200	284	160	436
abc^q	226	380	116	−40
a^qbc^q	244	448	104	304
b^qc^q	241	330	564	2,152
ab^qc^q	256	444	732	264
$a^qb^qc^q$	273	514	844	1,408
A	166.4			
A_+	214.6			
B	158.6			
B_+	228.1			
C	161.6			
C_+	225.1			

NOTE: Underscores indicate sets of three numbers used in calculation.

Table A.2. Printout of Computer Program ORTCUB for the Orthogonal Cubic Response Design Numerical Example: Coefficients of Orthogonals and of the Response Equation for Standardized Levels

	Orthogonal Coefficients	*Coefficients* for %*	*Resp. Eq. Coefficients*	*Coefficients* for %*
Mean	185.5	92.764	200.0	100.
A	132.9	66.468	20.00	10.0
A(2)	−27.93	−13.968	−10.00	−5.00
A(3)	7.32	3.6599	5.000	2.50
B	165.8	82.922	30.00	15.0
A B	−17.32	−8.6603	−5.000	−2.50
A(2) B	10.00	5.0000	5.000	2.50
B(2)	−19.56	−9.7778	−7.000	−3.50
B(2) A	8.000	4.0000	4.000	2.00
B(3)	2.14	1.0710	6.000	3.00
C	152.4	76.210	25.00	12.5
A C	−24.25	−12.124	−7.000	−3.50
A(2) C	12.00	6.0000	6.000	3.00
B C	27.71	13.856	8.000	4.00
A B C	−14.14	−7.0711	−5.000	−2.50
B(2) C	−8.000	−4.0000	−4.000	−2.00
C(2)	−19.56	−9.7778	−7.000	−3.50
C(2) A	8.000	4.0000	4.000	2.00
C(2) B	−6.000	−3.0000	−3.000	−1.50
C(3)	2.273	1.1367	8.000	4.00

* Responses are expressed as a percentage of the response at the center point.

APPENDIX: NUMERICAL EXAMPLE

Let T be the observed treatment value for each of the combinations of three factors in a cubic design. Examples of calculating estimates (G = grand total):

$$G = 6{,}122.4$$

$$\text{Mean} = G/33 = 185.5.$$

The extended Yates table (Table A.1) is different, in the last cycle, from the standard three-level Yates table; note that the first number in the last block of the A column is just 71 + 151 (instead of 71 + 151 − 2 × 132, as in the lattice design without star points).

By Table 4,

$$\text{A linear} = (33 * .6030)^{-1/2} * (546 + a * (214.6 - 166.4)) = 132.9$$

$$\text{A quadratic} = (2 * (a^4 + 3))^{-1/2} * (3{,}252 + a^2 * (166.4 + 214.6) - \gamma * 6{,}122.4) = -27.93$$

$$\text{A cubic} = (9 * 33 * \gamma)^{-1/2} * (a * 546 - 9 * (214.6 - 166.4)) = 7.34$$

$$\text{AB}(1 - 1) = (4 * 3)^{-1/2} * (-60) = -17.32$$

$$\text{AB}^2(1 - q) = (4)^{-1/2} * (380 - 2 * 546/3) = 8$$

$$\text{ABC}(1 - 1 - 1) = 8^{-1/2} * (-40) = -14.14.$$

If the coefficient of the orthogonal quadratic effect in A is multiplied by .3580, the value −10 (response equation coefficient of x^2) is obtained. In the same manner, multiplication of the estimates by the expressions in Table 3 produces the coefficients of x, $x^2 - \gamma$, and so forth.

Table A.2 contains both the orthogonal coefficients and the final response equation coefficients for these data.

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