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Chapter 3

A Comparison of Discrete and Continuous Models in Agricultural Production Analysis

Types of Experimental Procedures

Historical Review

IN a recent review article (1), this writer traced the development of multifactor experimental procedures. A brief resumé of this development seems desirable at this time: In the first multifactor experiments, a single factor was varied at a time. For example, with five factors, one might plan 5ℓ experiments, in which each of the factors in turn was used at ℓ levels while the other four factors were held at some starting level. Fisher (14) and Yates (25) encouraged the use of complete factorials and developed a large number of special designs involving them. In a complete factorial, all combinations of the factor levels are used, e.g., ℓ^5 for the above experiment. These designs were developed for experiments in which the experimental error could not be neglected. In order to estimate the magnitude of this error in each experiment, the experiment had to be repeated several times, e.g., r. These factorial designs were formed largely for useful field experiments in which sequential experimentation would be less than the laboratory experiments, and the factors were often of the discrete type, e.g., varieties or rations.

Because of the large number of factor combinations required in many field experiments, it was felt that some form of incomplete block design was needed to reduce the experimental error. This resulted in the so-called confounded designs, e.g., with 2^k, 3^k, 3×2^k, $3^k \times 2$, 4^k designs. These are described by Yates (26). More complicated factorial designs have been constructed by Nair (21, 22), Bose (4), Finney (13), and Li (20), among others.

When physical scientists and engineers became interested in multifactor experiments, they found that complete and confounded factorials required too many experimental units, especially since the experimental errors were often much lower than in field experiments. One method of reducing the number of experimental units was to use higher order interaction effects to estimate the error and hence avoid repetition of the design. Fisher (14) and Cornish (9) described the analysis of the singly replicated unconfounded factorial design and used the higher order

interactions for this purpose. Jeffreys (17) and Kempthorne (18) have advance justifications for this approach. Then Finney (11, 12), Plackett and Burman (23), Kempthorne (18), Rao (24), and Davies and Hay (10) developed the fractional replication designs, based on using parts of the confounded designs. Yates (25) and Hotelling (16) had already mentioned the use of such designs.

Some General Considerations of Factorial Experiments

The results of multifactor experiments are usually summarized in various two- and more-way tables of means and an analysis of variance. For example, let us assume there are two factors (A and B), one with p and the other with q groups, each of the pq classes having r samples. Some characteristic, such as yield, is measured for each of the pqr samples. The results are summarized in a (p x q) table of class means ($\bar{Y}_{ij}$) with the corresponding (p + q) border means ($\bar{A}_i$ and $\bar{B}_j$).

		B				
		1	2	. . .	q	
A	1	$\bar{Y}_{11}$	$\bar{Y}_{12}$	. . .	$\bar{Y}_{1q}$	$\bar{A}_1$
	2	$\bar{Y}_{21}$	$\bar{Y}_{22}$	. . .	$\bar{Y}_{2q}$	$\bar{A}_2$
	.	.	.		.	.
	.	.	.		.	.
	.	.	.		.	.
	p	$\bar{Y}_{p1}$	$\bar{Y}_{p2}$	. . .	$\bar{Y}_{pq}$	$\bar{A}_p$
		$\bar{B}_1$	$\bar{B}_2$	. . .	$\bar{B}_q$	$\bar{Y}$

For example, the border means for A represent averages over all B-groups. There are two circumstances under one or both of which these A-means are of importance:

1. Differences between B-groups are the same for all A-groups, i.e., there is no AB interaction.
2. The experimenter desires to make inferences regarding A only when averaged over these particular B-groups.

If item 1 is true, one can set up the following model to represent the yield for a given sample:

(1) Y = (mean) + (A effect) + (B effect) + (error).

The A and B effects are estimated by computing the deviations of group means from the general mean, e.g.,

$$A_1 \text{ effect} = \bar{A}_1 - \bar{Y}.$$

The errors are assumed to be normally and independently distributed

with zero means and same variances, σ^2. In this case, analysis of variance is:

Source of Variation	d. f.	S. S.	M. S.
A	p-1	SSA	MSA
B	q-1	SSB	MSB
Residual	(p-1)(q-1)	SSI	MSI
Error	(r-1) pq	SSW	s^2

In the above analysis of variance, SSA = $qr \sum \bar{A}_i^2 - pqr \bar{Y}^2$ and SSB = $pr \sum \bar{B}_j^2 - pqr \bar{Y}^2$. The residual sum of squares measures the failure of the A and B effects to be additive, i.e., presence of AB interaction. It is computed as:

$$r \sum \bar{Y}_{ij}^2 - pqr \bar{Y}^2 - SSA - SSB .$$

The error variance, σ^2, is estimated from the variability within classes. The mean squares are all computed by dividing the sums of squares by the corresponding degrees of freedom. One can test for the existence of interaction by use of $F = MSI/s^2$. Presumably, if this is significant, inferences about A effects must be confined to averages over these q B-groups. Otherwise one should consider the general model:

(2) $$Y = (\text{class mean}) + (\text{error}) .$$

Then each of the *pq* classes is considered separately and the simple analysis of variance is:

Source of Variation	d. f.	S. S.	M. S.
Treatments	pq-1	SST	MST
Error	(r-1) pq	SSW	s^2

$SST = r \sum \bar{Y}^2 - pqr \bar{Y}^2$

The same procedures can be followed for more than two classification variables. In this it is advisable to look at the individual contributions to the interaction: AB, AC, BC ... ABC ... . In many cases it is even possible to subdivide SSA, for example, into pertinent single degree of freedom contracts; hence, SS(AB) can also be subdivided. This subdivision of SSI is useful in detecting particular aspects of nonadditivity which may be concealed in blanket tests of MSI/s^2. For more exact discussion of these problems, see Chapter 20 of Anderson and Bancroft (2).

Extension of Factorial Experimentation to Continuous Variables

In the past, even though the factors could be varied continuously, most analyses of experimental data have followed the same procedures as for discrete classifications. For example, if one had an experiment to study the effect of nitrogen (n) and potash (k) on the yield of corn, one might consider a simple 2 x 2 experiment with four treatment combinations: low n and k (00); low n and high k (02); high n and low k (20); and high n and high k (22).[1] Suppose each treatment were randomly assigned to r plots. The usual summary procedure would be to form the four-treatment totals and means in 2 x 2 tables. The totals are indicated as follows:

		Potash: low	Potash: high	
Nitrogen	low	(00)	(02)	N_0
	high	(20)	(22)	N_2
		K_0	K_2	G

The border totals are indicated by capital letters, with G for the grand total.

If one were unwilling to make any assumptions about the comparability of the four treatments, he would look only at the four-cell mean (cell totals divided by r) and use model 2 and the accompanying analysis.

If the experimenter feels that the effect of increased n or k is the same regardless of the level of the other element, he would use an adaptation of model 1 as follows:

(1′) Y = (mean) ± (n effect) ± (k effect) ± (error),

where the + sign refers to high level plots and the - to low level plots. For example, the average or expected yield for a plot receiving high n and low k is:

$$(\text{mean}) + (n \text{ effect}) - (k \text{ effect}) .$$

The n effect, for example, represents the expected increase in yield due to high n over the average of high and low n, and is estimated by

$$\frac{N_2 - N_0}{4_r} = \frac{N_2}{2r} - Y .$$

The analysis of variance is the same as for model 1. The residual can be used to test the adequacy of the additive model 1′, i.e., test for the existence of an (NK) interaction. If this residual is significant, the

[1] 0 is used for the low level and 2 is used for the high level, so that 1 may be introduced as a middle level.

Source of Variation	Sum of Squares = Mean Square
N	$\frac{(N_2 - N_0)^2}{4r}$
K	$\frac{(K_2 - K_0)^2}{4r}$
Residual	$\frac{[(00)-(02)-(20)+(22)]^2}{4r}$

effect of increased n is not the same for low and for high k (and vice versa). Hence it is necessary to interpret each cell mean separately, i.e., use model 2.

Continuing this aping of the models for discrete factors, the following general model has been constructed for the 2 x 2 experiment:

(3) Y = (mean) ± (n effect) ± (k effect) ± (nk interaction effect) + (error), where the interaction effect receives a plus sign for the (0,0) and (2,2) plots and a minus sign for the (0,2) and (2,0) plots. For example, the expected yield for a plot receiving high n and low k is:

(mean) + (n effect) - (k effect) - (nk interaction effect).

The interaction effect is estimated by:

$$\frac{(00) - (02) - (20) + (22)}{4r}.$$

If the response surface can be approximated by a simple mathematical function, it seems more logical to estimate the parameters of this function instead of main effects and interactions. In the present example, consider the following continuous model:

(4) $$Y = \beta_0 + \beta_1 X_1 + \beta_2 X_2 + \beta_{12} X_1 X_2 + (\text{error}).$$

X_1 and X_2 represent the respective levels of nitrogen and potash as deviations from the mean level in the experiment ($X = -1$ for low and $X = +1$ for high level); β_0 is the expected yield for n and k midway between the amounts applied in the experiment ($X_1 = X_2 = 0$); β_1 and β_2 are linear effects of added n and k; β_{12} is the interaction parameter. Using model 4, the cell totals (of r plots each) have these expectations:

	low k (X_2=-1)	high k (X_2=1)	Total
low n (X_1=-1)	$r(\beta_0-\beta_1-\beta_2+\beta_{12})$	$r(\beta_0-\beta_1+\beta_2-\beta_{12})$	$2r(\beta_0-\beta_1)$
high n (X_1=1)	$r(\beta_0+\beta_1-\beta_2-\beta_{12})$	$r(\beta_0+\beta_1+\beta_2+\beta_{12})$	$2r(\beta_0+\beta_1)$
Total	$2r(\beta_0-\beta_2)$	$2r(\beta_0+\beta_2)$	$4r\,\beta_0$

The estimators of the β's in equation 4 are:

Parameter	Estimator
β_1	$b_1 = \frac{N_2 - N_0}{4r}$
β_2	$b_2 = \frac{K_2 - K_0}{4r}$
β_{12}	$b_{12} = \frac{(00)-(02)-(20)+(22)}{4r}$
β_0	$b_0 = G/4r = \bar{Y}$.

The variance of each estimator is $\sigma^2/4r$. Note that these estimators are the same as for the effects of model 3. β_1, for example, measures the average difference in yield per unit change in n for these two k treatments, i.e., the change in Y for a unit change in X_1, neglecting interaction.[2] Also the analysis of variance produces the same three orthogonal sums of squares for treatments, using either models 3 or 4.

Hence it appears that models 3 and 4 are identical. However, there is a very important difference. Model 3 makes no assumption regarding the shape of the response surface, but model 4 implies a definite continuity of response; hence, one would feel free to use the results of model 4 to interpolate between the actual levels used in the experiment. If he did use model 3 for this purpose, he would actually be assuming the continuous model 4. One is often tempted to extrapolate the results beyond the levels used in the experiment; such extrapolation assumes the same response surface holds beyond the experimental levels. In other words, one uses model 2 or 1 if he does not wish to assume a quadratic response surface, but uses model 4 if experience or theory indicates such a surface would be satisfactory.

If the design is spread out so that the low and high levels differ by $2d$ units (instead of 2), b_i will have a denominator of $4rd$ and b_{12} a denominator of $4rd^2$. Hence the variance of b_i is reduced by a factor of d^2 and b_{12} by a factor of d^4. The only reason for not using extremely divergent levels is that the response surface may have a different shape at extremely large or small fertilizer applications.

If the continuous model 4 is used, it seems unreasonable to include a quadratic term involving X_1X_2 without also including terms involving X_1^2 and X_2^2. The shape of a response surface such as model 4 is rather grotesque. In other words one would be more likely to consider the following general quadratic model:

$$(5) \quad Y = \beta_0 + \beta_1X_1 + \beta_2X_2 + \beta_{12}X_1X_2 + \beta_{11}X_1^2 + \beta_{22}X_2^2 + (\text{error}) .$$

[2] It should be clear that the difference between low and high levels is a two-unit change, e.g., if low is 50 pounds per plot and high is 100 pounds per plot, a unit change is 25 pounds and β_1 and β_2 measure the linear effects of 25-pound increases.

If model 5 is the true continuous model, the expectations of the cell totals are:

	low k (X_2=-1)	high k (X_2=1)	Total
low n(X_1=-1)	$r(\beta_0-\beta_1-\beta_2+\beta_{11}+\beta_{22}+\beta_{12})$	$r(\beta_0-\beta_1+\beta_2+\beta_{11}+\beta_{22}-\beta_{12})$	$2r(\beta_0-\beta_1+\beta_{11}+\beta_{22})$
high n(X_1=1)	$r(\beta_0+\beta_1-\beta_2+\beta_{11}+\beta_{22}-\beta_{12})$	$r(\beta_0+\beta_1+\beta_2+\beta_{11}+\beta_{22}+\beta_{12})$	$2r(\beta_0+\beta_1+\beta_{11}+\beta_{22})$
Total	$2r(\beta_0-\beta_2+\beta_{11}+\beta_{22})$	$2r(\beta_0+\beta_2+\beta_{11}+\beta_{22})$	$4r(\beta_0+\beta_{11}+\beta_{22})$

It turns out that the estimates of β_1, β_2, and β_{12} are the same as for model 4 and are not mixed up with the quadratic terms (β_{11} and β_{22}), i.e., they are unbiased estimates. However, there is no method of estimating β_0, β_{11}, or β_{22}, since their sum is estimated by $\bar{Y}$. Hence this analysis indicates that it is safe if only statements are made regarding the treatments used in the experiment and no attempt is made to predict the results for other fertilizer levels.

Of course the solution to the above dilemma is to add other levels of n and k. The traditional design to estimate quadratic effects is the 3 x 3 complete factorial with the three levels of n and k equally spaced.[3] Assuming the middle values of n and k are the averages of the low and high levels used in the 2 x 2 experiment, i.e., if the low and high applications were 50 and 100 pounds per plot, the middle application would be 75 pounds per plot. In the factorial setup, the levels are designated as 0, 1, and 2 with X = -1, 0, 1, respectively. Henceforth, factor combination will be designated by the levels used, e.g., (-1, -1). Assuming r plots per cell and using model 5, the expectations for the (-1, -1), (-1, 1), (1, -1) and (1, 1) totals would be as before. The expectations for the other five class totals and the border totals would be:

(-1, 0)	$r(\beta_0 - \beta_1 + \beta_{11})$
(0, -1)	$r(\beta_0 - \beta_2 + \beta_{22})$
(0, 0)	$r\,\beta_0$
(0, 1)	$r(\beta_0 + \beta_2 + \beta_{22})$
(1, 0)	$r(\beta_0 + \beta_1 + \beta_{11})$
N_0	$3r(\beta_0 - \beta_1 + \beta_{11}) + 2r\,\beta_{22}$
N_1	$3r\,\beta_0 + 2r\,\beta_{22}$
N_2	$3r(\beta_0 + \beta_1 + \beta_{11}) + 2r\,\beta_{22}$
K_0	$3r(\beta_0 - \beta_2 + \beta_{22}) + 2r\,\beta_{11}$
K_1	$3r\,\beta_0 + 2r\,\beta_{11}$
K_2	$3r(\beta_0 + \beta_2 + \beta_{22}) + 2r\,\beta_{11}$
G	$9r\,\beta_0 + 6r\,(\beta_{11} + \beta_{22})$

[3]Equal spacing enables one to analyze linear and quadratic components in a simple manner, but it is not an essential, or even the most efficient, method of spacing.

The following estimators and variances are obtained:

Parameter	Estimator	Variance of Estimator
β_1	$b_1 = (N_2-N_0)/6r$	$\sigma^2/6r$
β_2	$b_2 = (K_2-K_0)/6r$	$\sigma^2/6r$
β_{12}	$b_{12} = [(-1,-1) - (-1,1) - (1,-1) + (1,1)]/4r$	$\sigma^2/4r$
β_{11}	$b_{11} = (N_2-2N_1+N_0)/6r$	$\sigma^2/2r$
β_{22}	$b_{22} = (K_2-2K_1+K_0)/6r$	$\sigma^2/2r$
β_0	$b_0 = [5(N_1+K_1)-(N_0+N_2+K_0+K_2)]/18r$	$5\ \sigma^2/9r$

Note that b_1, b_2, and b_{12} are the same as before; also, if the levels are (-d,0,d), the variances for the linear coefficients are again reduced by a factor of d_2 and for the quadratic and interaction coefficients by a factor of d^4.

The analysis of variance is as follows (ℓ stands for linear and q for quadratic component):

Effect	d.f.	M. S.
N_ℓ	1	$(N_2-N_0)^2/6r$
K_ℓ	1	$(K_2-K_0)^2/6r$
$N_\ell K_\ell$	1	$[(-1,-1)-(-1,1)-(1,-1)+(1,1)]^2/4r$
N_q	1	$(N_2-2N_1+N_0)^2/18r$
K_q	1	$(K_2-2K_1+K_0)^2/18r$
Residual	3	$[SST - SS(N_\ell + K_\ell + \ldots + K_q)]/3$
Error	9(r-1)	$s^2 = SSW/9(r-1)$

The residual mean square can be used to test for the adequacy of the model. If the 3 x 3 complete factorial is used, it turns out that these three degrees of freedom can be subdivided into three orthogonal components, which measure $N_\ell K_q$, $N_q K_\ell$, and $N_q K_q$ interaction effects [$\beta_{122}X_1X_2^2 + \beta_{112}X_1^2X_2 + \beta_{1122}X_1^2X_2^2$ is added to model 5].

Once again a factorial model similar to model 3 can be constructed with the same linear and quadratic effects as in model 5. However, there seems little reason for estimating such effects unless one is willing to assume a quadratic response surface. If he does not wish to assume a quadratic response surface, he has two possible factorial models:

1. Model 2 with nine treatments

2. Model 1′ with two effects for each factor: above and below the middle application or referred to either the high or low application.[4]

The analysis based on model 1′ would include a sum of squares attriutable to the interactions, giving a test of the adequacy of the model. These remarks hold for any number of factors and levels per factor.

If there is a mixture of classification variables (e.g., varieties) and continuous variables, a combined factorial and continuous model can be set up and analyzed in a manner analogous to covariance. This would assume that the parameters for the continuous variables were the same for each discrete classification; a test of this hypothesis can also be constructed.

The Use of Blocking Methods to Reduce Experimental Error

The use of blocking methods in the previous discussion has not been considered because they only complicate the presentation without altering any of the conclusions. However, one must consider the blocking procedure if there is confounding. Unfortunately, the procedures used in constructing such designs have been based on confounding certain parts of the higher order interactions which are not related to higher degree components. For example, the so-called I and J parts of the NK interaction in a 3 x 3 experiment do not pertain to any one of the four degree components, $N_\ell N_\ell$, $N_\ell K_q$, $N_q K_\ell$, or $N_q K_q$. One would prefer a design which minimized the confounding on $N_\ell K_\ell$.

A bulletin now in press by Binet, Leslie, Weiner, and Anderson (3) presents the confounding patterns in terms of degree components. This bulletin should be of use in three ways:

1. It presents short-cut methods of analyzing these confounded experiments when degree components are of interest.
2. Several new confounded designs are presented.
3. It presents the confounding patterns for various designs, so the reader can select the design which will be best for his problem.

To illustrate the procedures, suppose the nine treatments in the 3 x 3 experiment were put in 3 blocks of 3 plots each. One such arrangement would be (the treatments refer to levels, and B_i are block totals):

Block		
1	2	3
(1,-1)	(-1,-1)	(0,-1)
(-1,0)	(0,0)	(1,0)
(0,1)	(1,1)	(-1,1)
B_1	B_2	B_3

[4] Cf. Anderson and Bancroft (2), Section 20.5.

If b'_j represents the mean of the j-th block, then two block contrasts are formed:

$$2C_1 = b'_3 - b'_1 \text{ and } 6c_2 = b'_3 - 2b'_2 + b'_1 .$$

The least squares equations for the two block and four NK effects are:

C_1	$N_\ell K_q$	$N_q K_\ell$	C_2	$N_\ell K_\ell$	$N_q K_q$	Yield Sum
6	-6	6	0	0	0	$B_3 - B_1$
-6	12	0	0	0	0	$(N_\ell K_q)$
6	0	12	0	0	0	$(N_q K_\ell)$
0	0	0	18	-6	-18	$B_1 - 2B_2 + B_3$
0	0	0	-6	4	0	$(N_\ell K_\ell)$
0	0	0	-18	0	36	$(N_q K_q)$

The yield sum for $N_\ell K_q$, for example, is:

$$[(1,1) - 2(1,0) + (1,-1)] - [(-1,1) - 2(-1,0) + (-1,-1)] .$$

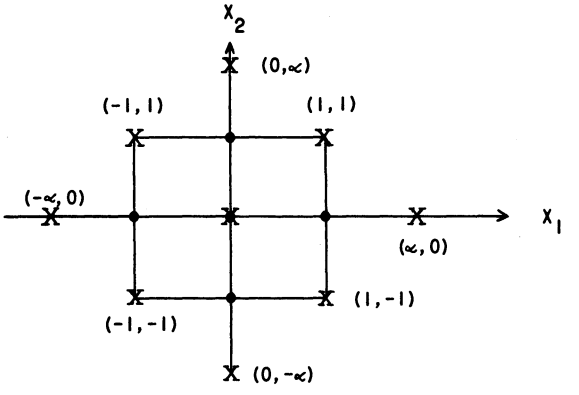
The usual procedure in analyzing these results would be to assume the block contrasts and $N_\ell K_\ell$ were the only real effects. This leaves only one contrast for testing the model, since there are only four degrees of freedom in the above six equations. The method of analysis proposed in the bulletin is the abbreviated Doolittle method, which is also discussed in detail by Anderson and Bancroft (2). Obviously there is no estimate of error from this experiment. If such an estimate is needed, another replicate should be used, preferably one which has a different confounding pattern, as indicated in the bulletin.

For experiments with many factors, it is often possible to estimate the pertinent contrasts by use of fractional designs.

Special Designs To Estimate Parameters of Response Surfaces

The material by Binet et al. (3) furnishes a method of using existing confounded factorial designs to estimate the important degree components. However, for most experiments in which the experimenter has evidence that a smooth response surface is suitable, he should consider designs especially constructed to estimate the parameters of this surface and not to estimate class means for a classification model. Box (5) developed some general design principles for estimating the parameters of planar surfaces.

Box and Wilson (8) proposed a new design for estimating quadratic surfaces which gives more information on the quadratic effects and less on the high-degree effects. Their *composite design* would push the (0,1), (0,-1), (1,0), and (-1,0) points α units from the center of the design as indicated in figure 3.1.



• 3 X 3 DESIGN
X COMPOSITE DESIGN

Fig. 3.1 — The Box and Wilson composite design for estimating quadratic surfaces.

If $\alpha = 2$, the expectations of the totals for the four altered cells are:

(-2,0)	$r\,(\beta_0 - 2\beta_1 + 4\beta_{11})$
(0,-2)	$r\,(\beta_0 - 2\beta_2 + 4\beta_{22})$
(0,2)	$r\,(\beta_0 + 2\beta_2 + 4\beta_{22})$
(2,0)	$r\,(\beta_0 + 2\beta_1 + 4\beta_{11})$

In this case one cannot analyze the results as for a 3 x 3 table, because it is an incomplete 5 x 5 factorial experiment. Here one must use the general least-squares approach. The matrix for the normal equations is:

	Coefficients of Estimators						Right hand side
Equation	b_0	b_1	b_2	b_{12}	b_{11}	b_{22}	
b_0	9r	0	0	0	12r	12r	G
b_1	0	12r	0	0	0	0	$g_1 = SX_1Y$
b_2	0	0	12r	0	0	0	$g_2 = SX_2Y$
b_{12}	0	0	0	4r	0	0	$g_{12} = SX_1X_2Y$
b_{11}	12r	0	0	0	36r	4r	$g_{11} = SX_1^2Y$
b_{22}	12r	0	0	0	4r	36r	$g_{22} = SX_2^2Y$

In the preceding, for example, $g_1 = (1,1) + 2(2,0) + (1,-1) - (-1,1) - 2(-2,0) - (-1,-1)$, where (1,1), etc., stand for class totals. The solutions and variances[5] of the estimators are:

		Variance of Estimator ($X\sigma^2/r$)		
Parameter	Estimator	Composite	3 x 3	3 x 3 (Adjusted)
β_1	$g_1/12r$	1/12	1/6	1/12
β_2	$g_2/12r$	1/12	1/6	1/12
β_{12}	$g_{12}/4r$	1/4	1/4	1/16
β_{11}	$(30g_{11} + 18g_{22} - 64G)/384r$	5/64	1/2	1/8
β_{22}	$(30g_{22} + 18g_{11} - 64G)/384r$	5/64	1/2	1/8
β_0	$(10G - 3g_{11} - 3g_{22})/18r$	5/9	5/9	5/9

One gets the impression that there is a tremendous reduction in variances of estimators by use of the composite design instead of the 3 x 3 factorial. However, most of this gain is the natural result of using a wider range of X's; the incompleteness of the factorial in the composite design is not responsible for all the gain. This was indicated for the 2 x 2 experiment. One could adjust the coordinates of the 3 x 3 design so that the spread is the same as for the composite design. The variance of the coordinates for the latter (with $\alpha = 2$) is $[2(4) + 4(1) + 3(0)]/9 = 4/3$. Let the new coordinates for the 3 x 3 design be (-d,0,d), so that the variance of these coordinates is $2d^2/3 = 4/3$; or $d = \sqrt{2}$. Hence, the variances of linear terms are reduced by 1/2 and of quadratic terms by 1/4. Therefore, the composite design has improved the quadratic estimators at the expense of the interaction one. Box and Wilson (8) show that this is desirable in estimating the optimal factor combination.

Another criterion of the relative efficiency of two different designs in estimating the parameters of a response surface would be the amount of information used to estimate the high degree coefficients, which are assumed to be unimportant.

Box and Hunter (7) have advanced another principle of a good surface-fitting design; it should be rotatable; i.e., the accuracy of the estimates of the parameters should not depend on the orientation of the design with respect to the true surface itself. They have constructed several incomplete factorial designs which meet this requirement.

Mason discusses in Chapter 5 some recent experiments in which the composite designs have been used.

[5]These are obtained by inverting the left-hand matrix. The abbreviated Doolittle or square-root method is usually used, although special pattern matrices can be used.

Sequential Experimentation

Much of the impetus for the Box-Wilson paper (8) came from a need to develop sequential procedures for determining optimal factor combinations. Various procedures have been summarized in Anderson's review article (1). Since then, Box (6) has published an extensive discussion of the entire problem. Although the use of these sequential methods may be somewhat limited in fertilizer experiments because of the length of time needed to obtain results, it probably would be desirable to develop a more systematic procedure of utilizing past experience in designing future experiments.

Better methods are needed to pool data from a series of experiments. Researchers should be encouraged to spend more time on these problems.

Some Special Comparisons of Discrete and Continuous Models

Comparison of Discrete Model 2 and Quadratic Model 5 Using 3 x 3 Design

1. *The quadratic model is correct.* In this case the estimated average yield for plots receiving X_1 units of N and X_2 units of K (measured from the mean level) is:

$$\hat{Y} = b_0 + b_1X_1 + b_2X_2 + b_{12}X_1X_2 + b_{11}X_1^2 = b_{22}X_2^2 .$$

In order to obtain the sampling variance of $\hat{Y}$, it requires the variances of the estimators given previously and the covariances. All of these could be obtained by inverting the matrix of sums of squares and products of the regression variables in the normal equations. This matrix is as follows:

	b_0	b_1	b_2	b_{12}	b_{11}	b_{22}
b_0	9r	0	0	0	6r	6r
b_1	0	6r	0	0	0	0
b_2	0	0	6r	0	0	0
b_{12}	0	0	0	4r	0	0
b_{11}	6r	0	0	0	6r	4r
b_{22}	6r	0	0	0	4r	6r

Since b_0, b_{11}, and b_{12} are the only correlated variables, consider them separately in a 3 x 3 matrix A, which when multiplied by its inverse C is the identity matrix.

$$A \begin{bmatrix} 9r & 6r & 6r \\ 6r & 6r & 4r \\ 6r & 4r & 6r \end{bmatrix} \cdot C \begin{bmatrix} C_1 & C_2 & C_2 \\ C_2 & C_3 & C_4 \\ C_2 & C_4 & C_3 \end{bmatrix} = \begin{bmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \end{bmatrix}$$

There are only four different elements of C. These can be determined quite simply as follows:

$$\left.\begin{aligned} 9r\,C_1 + 12r\,C_2 &= 1 \\ 6r\,C_1 + 10r\,C_2 &= 0 \end{aligned}\right\} \quad C_2 = -1/3r;\ C_1 = 5/9r$$

$$\left.\begin{aligned} 6r\,C_2 + 6r\,C_3 + 4r\,C_4 &= 1 \\ 9r\,C_2 + 6r\,C_3 + 6r\,C_4 &= 0 \end{aligned}\right\} \quad \begin{aligned} C_4 &= -1/2r - \frac{3C_2}{2} = 0 \\ C_3 &= 1/6r - C_2 = 1/2r \end{aligned}$$

Hence the matrix of variances and covariances of the b's is:

$$\frac{\sigma^2}{r}\begin{bmatrix} 5/9 & 0 & 0 & 0 & -1/3 & -1/3 \\ 0 & 1/6 & 0 & 0 & 0 & 0 \\ 0 & 0 & 1/6 & 0 & 0 & 0 \\ 0 & 0 & 0 & 1/4 & 0 & 0 \\ -1/3 & 0 & 0 & 0 & 1/2 & 0 \\ -1/3 & 0 & 0 & 0 & 0 & 1/2 \end{bmatrix}$$

The variance of $\hat{Y}$ is:

$$\sigma^2(\hat{Y}) = \frac{\sigma^2}{r}\left[5/9 + 1/6\,(X_1^2 + X_2^2) + 1/4\,(X_1^2X_2^2) + 1/2\,(X_1^4 + X_2^4) - 2/3\,(X_1^2 + X_2^2)\right]$$

$$= \frac{\sigma^2}{r}\left[5/9 + 1/2\,(X_1^4 + X_2^4 - X_1^2 - X_2^2) + 1/4\,X_1^2X_2^2\right] .$$

If the discrete model is used, every mean will have a sampling variance of σ^2/r. For even the most divergent points ($\pm 1, \pm 1$),

$$\sigma^2(\hat{Y}) = 29\,\sigma^2/36r$$

which is less than σ^2/r. Hence, if the quadratic model is correct, even the yields at the experimental points are estimated more accurately from the regression model instead of the simple average yield at that point. Of course $\hat{Y}$ is even more accurate for the other five points.

The same conclusions hold for comparing two mean yields. The largest variance using $\hat{Y}$ is the comparison of (1,1) and 1,-1), which is $5\,\sigma^2/3r$, as compared to $2\,\sigma^2/r$ for model 2. Many of the comparisons using $\hat{Y}$ have much lower variances than this.

The results might be even more favorable if another design were used.

2. *The quadratic model is biased.* Suppose the true model is model 5 plus $\beta\,X_1^3$. In this case $\hat{Y}$ is too small by β when $X_1 = 1$ and too large by β when $X_1 = -1$. Some mean differences would be biased by 2β, others by β, and others not at all. However, the estimates using

model 2 would be unbiased. The problem of whether to use the biased estimates depends on a comparison of the suspected magnitude of the bias and the variances mentioned above. This problem may be even more serious if the form of the response equation is radically different from the quadratic, e.g., if it is exponential or logistic.

Returning to the bias of βX_1^3, it should be mentioned that at least one of the other β's will also be biased if this term is not considered in the estimation procedure (when $\beta \neq 0$); for example:

$$E(b_1) = \beta_1 + \beta \ .$$

β is called an *alias* of β_1. Box and Wilson (8) consider possible aliases in evaluating various designs. It is possible to construct designs so that possible aliases will not have much effect on the estimates. This may be one of the chief reasons why agricultural experimenters have not considered continuous models. Hildreth (15) has considered an estimation procedure which is built on model 2, but uses certain inequality restrictions on the production function. The estimation procedure used by Hildreth is discussed in Chapter 4.

Pseudo-Interactions in Some Factorial Experiments

The tendency to follow the mechanical procedure of analyzing factorial experiments in terms of main effects and interactions can result in serious loss of information, often of a misleading nature. As an example, consider an experiment involving two levels of nitrogen (coded n = -1 and 1) and two different cover crops to be plowed under. Suppose C_1 supplies no nitrogen to the soil, whereas C_2 supplies 2 units of n (coded n = -1 and 1). In addition, the two crops supply other unspecified nutrients. Assume that the yield is a quadratic function of n plus some additive amount due to the unspecified nutrients in the soil and furnished by the two crops: $\beta_0 - \gamma$ for C_1 and $\beta_0 + \gamma$ for C_2 (γ may be positive or negative). Hence the model is:

$$Y = \beta_0 + \beta_1 n + \beta_{11} n^2 \pm \gamma + (\text{error}) \ ,$$

where γ is added for C_2 plots and subtracted for C_1 plots.[6] The expected class and border total yields are:

	Crop 1	Crop 2	Total
n = -1	$r(\beta_0 - 2\beta_1 + 4\beta_{11} - \gamma)$	$r(\beta_0 + \gamma)$	$2r(\beta_0 - \beta_1 + 2\beta_{11})$
n = 1	$r(\ _0 - \ )$	$r(\beta_0 + 2\beta_1 + 4\beta_{11} + \gamma)$	$2r(\beta_0 + \beta_1 + 2\beta_{11})$
	$2r(\beta_0 - \beta_1 + 2\beta_{11} - \gamma)$	$2r(\beta_0 + \beta_1 + 2\beta_{11} + \gamma)$	$4r(\beta_0 + 2\beta_{11})$

[6]The center of the system is now one unit more than the average of the two nitrogen levels.

The estimators and their variances are:

Parameter	Estimator	Variance
β_1	$(N_1 - N_{-1})/4r$	$\sigma^2/4r$
β_{11}	$[(-1,1)-(-1,2)-(1,1)+(1,2)]\ /8r$	$\sigma^2/16r$
γ	$[(-1,2)-(1,1)]\ /2r$	$\sigma^2/2r$
β_0	$[(-1,2)+(1,1)]\ /2r$	$\sigma^2/2r$

Compare these results with those obtained by use of traditional factorial methods.

Effect	Yield	E(Yield)	E(MS)
Nitrogen	N_1-N_{-1}	$4r\beta_1$	$4r\beta_1^2+\sigma^2$
Crop	C_2-C_1	$4r(\gamma+\beta_1)$	$4r(\gamma+\beta_1)^2+\sigma^2$
N x C	$(-1,1)-(-1,2)-(1,1)+(1,2)8r\beta_{11}$		$16r\beta_{11}^2+\sigma^2$

An N x C interaction is indicated if there is a quadratic effect of nitrogen; also the crop effect will be mixed up with the linear effect of nitrogen (this is satisfactory if one only wants to test for differences in yields and not to determine basic causes of such differences). But a major criticism is a failure to provide a method of estimating the quadratic effect of nitrogen. The N x C interaction effect is the least squares estimate of β_{11}, but this fact is concealed in a routine factorial analysis of variance.

This is a very simple illustration of the need for more basic models in discussing responses to treatments. Classification models may conceal basic response patterns. One might consider this problem when three instead of two levels of n were used. In this case the factorial estimate of β_{11} probably would be inefficient, because of neglect of the information from the N x C interaction.

Yates (26) presents a 2^3 experiment with 4 replications, the factors being N, K, and D (dung). Levels were none and some, the latter being 0.45 cwt. N per acre, 1.12 cwt. K_2O per acre, and 8 tons of D per acre. Assume that this amount of dung supplies the same as the "some" of n and k, plus "some" other nutrients (called d). Code these data with -1 for none and +1 for some. Hence, the values of the variables for the various plots are:[7]

[7]A unit of nitrogen is 0.225 cwt., of potash is 0.56 cwt., and of dung is 4 tons: the center is at 0.45 N, 1.12 K and 4 D.

N	K	D	n	k	d	Yield of 4 plots
0	0	0	-2	-2	-1	425
1	0	0	0	-2	-1	426
0	1	0	-2	0	-1	1118
1	1	0	0	0	-1	1203
0	0	1	0	0	1	1283
1	0	1	2	0	1	1396
0	1	1	0	2	1	1673
1	1	1	2	2	1	1807

Assume a quadratic equation in n and k, with d appearing linearly. Hence:

$$(6) \qquad Y = \beta_0+\beta_1 n+\beta_2 k+\beta_{11} n^2+\beta_{22} k^2+\beta_{12} nk+\beta_3 d+ (\text{error}) \ .$$

Because this experiment was not designed to estimate quadratic effects, it turns out that if a complete quadratic model was used with $\beta_{33}d^2$, $\beta_{13}nd$, and $\beta_{23}kd$ included, the following pairs of coefficients could not be separated: β_0 and β_{33}; β_{11} and β_{13}; and β_{22} and $\beta 23$. In other words the constant and d^2, n^2, and nd and k^2 and kd are aliases. It is assumed here that d is essentially a residual variable, which is unlikely to have any effect and especially not a quadratic one; however, one cannot be sure which of two aliases is responsible for an effect.

The matrix for the least squares equations for model 6 is:

b_0	b_1	b_2	b_{11}	b_{22}	b_{12}	b_3	Yield Sum
32	0	0	64	64	32	0	9,331
	64	32	0	0	0	32	3,320
		64	0	0	0	32	5,258
			256	128	128	0	18,984
				256	128	0	17,324
					128	0	8,928
						32	2,987

The forward solution of the abbreviated Doolittle method is as follows:

	b_0	b_1	b_2	b_{11}	b_{22}	b_{12}	b_3	Yield
	32	0	0	64	64	32	0	9331
b_0	1	0	0	2	2	1	1	9331/32
		64	32	0	0	0	32	3320
b_1		1	1/2	0	0	0	1/2	3320/64
			48	0	0	0	16	3598
b_2			1	0	0	0	1/3	3598/48
				128	0	64	0	322
b_{11}				1	0	1/2	0	322/128
					128	64	0	-1338
b_{22}					1	1/2	0	-1338/128
						32	0	105
b_{12}						1	0	105/32
							32/3	383/3
b_3							1	383/3

The variance-covariance matrix and the estimates are:

$$\frac{\sigma^2}{128}\begin{bmatrix} 16 & 0 & 0 & -4 & -4 & 4 & 0 \\ & 4 & 0 & 0 & 0 & 0 & -4 \\ & & 4 & 0 & 0 & 0 & -4 \\ & & & 2 & 1 & -2 & 0 \\ & & & & 2 & -2 & 0 \\ & & & & & 4 & 0 \\ & & & & & & 12 \end{bmatrix}$$

	Estimates
b_0	310.75
b_1	10.41**
b_2	70.97**
b_{11}	.88
b_{22}	-12.09**
b_{12}	3.28
b_0	11.97*

Since the error variance in the experiment was 347.01 (with 21 degrees of freedom), $\sigma^2/128$ is estimated by 2.71. This is multiplied by the diagonal terms to obtain the estimated variances for the estimates. All linear terms and the quadratic term for k are significant (b_3 barely so at the 5% level) while b_{12} is about the same size as its standard error. The sum of squares can be compared with those of Yates as follows:

Effect	Yates	Here[8]
N_ℓ	3,465.3	172,225.0
K_ℓ	161,170.0	269,700.1
N_q and $N_\ell D_\ell$	810.0	810.0
K_q and $K_\ell D_\ell$	13,986.3	13,986.3
$N_\ell K_\ell$	344.5	344.5
D_ℓ	278,817.8	1,528.0
$N_\ell K_\ell D_\ell$	124.0	124.0

This is only an illustrative example, however, and should serve as an example of the procedure. There may be some questions concerning the use of the coded values. These are put in so that the estimators will be as nearly uncorrelated as possible; this enables one to better evaluate the usefulness of various predictors in the model. Box and Wilson (8) generally follow this procedure.

Problem of Adjustment for Available Nutrients With Continuous Models

One of the major needs in the determination of fertilizer response surfaces is a method of adjusting for nutrients available in the soil before the experiment is started. In a single experiment, it is usually assumed that the variation in basic levels is random, with the average level being taken account of by the constant term. If there are no essential differences between the basic levels in the plots for each of the treatments, the results of the experiment can be used to indicate treatment contrasts. However, if a continuous model such as the quadratic model 5 is used, the experimenter should be careful about extending the results to plots with different available nutrients.

If the effect of the available nutrients is to merely increase the actual levels of X, the results can be converted to a prediction equation in terms of the available plus added nutrients. In order to simplify the results, consider a quadratic prediction equation for an experiment involving only one nutrient,

$$E(X) = \beta_0 + \beta_1 X + \beta_{11} X^2 \,, \tag{7}$$

where X is the added amount of the nutrient. The actual amount (available plus added) of the nutrient in an experiment is designated as $N = X + d$ ($X = N - d$). Then:

$$E(N) = (\beta_0 - \beta_1 d + \beta_{11} d^2) + (\beta_1 - 2\beta_{11} d)\, N + \beta_{11} N^2 \,. \tag{8}$$

Now try to apply the results of this experiment to a farm. The

[8]These are not adjusted sums of squares; i.e., N_ℓ is not adjusted for K_ℓ or D_ℓ; K_ℓ is not adjusted for D_ℓ; and N_q and K_q not for $N_\ell K_\ell$. Note the N_q = Yates' $N_\ell D_\ell$ and the K_q = Yates' $K_\ell D_\ell$, as indicated above.

predicted yield if X is applied is E(X). Suppose the value of d for this farm is d_0 ($N = X + d_0$); then the expected yield when X is added should be:

$$F(X) = (\beta_0 - \beta_1 d + \beta_{11} d^2) + (\beta_1 - 2\beta_{11} d)(X + d_0) + \beta_{11}(X + d_0)^2$$

$$= [(\beta_0 - \beta_1(d - d_0) + \beta_{11}(d - d_0)^2] + [\beta_1 - 2\beta_{11}(d - d_0)]X + \beta_{11}X^2 .$$

The bias in using E (X) instead of F (X) is:

$$E(X) - F(X) = (d - d_0)(\beta_1 + 2\beta_{11} X) - (d - d_0)^2 \beta_{11} . \tag{9}$$

One might suppose that even though the predicted yield is biased, at least the difference between the predicted yields for two different levels of farm application would be unbiased. Even this is not true. The bias in the predicted increase in yield for an application of X_2 instead of X_1 is $2\beta_{11}(X_2 - X_1)(d - d_0)$, which will be negative for $X_2 > X_1$ and $d > d_0$, since B_{11} is expected to be negative; hence, one would tend to underestimate the effect of added nutrients if the available nutrients at the farm are less than at the experimental plots.

These problems become further aggravated when one attempts to combine the results of experiments at two locations with different values of d. Suppose $d = d_1$ for one location and $d = d_2$ for a second location, but the same rates of application are used in each experiment, e.g., X = -1, 0, 1. If a quadratic model is used, the experimental model E(N) is:

$$E(N) = \beta_0^* + \beta_1^* N + \beta_{11}^* N^2 , \tag{10}$$

where β_0^*, β_1^* and β_{11}^* can be found from model 8 above. The values of the β^* are assumed to be the same for each experiment (neglecting other nutrients in this discussion); however, the values of β_0 and β_1 in model 7 are not the same. Let β_1' and β_1'' represent the values of β_1 in experiments 1 and 2, respectively.

Then solving for the β's in terms of the β^*'s, yields:

$$\beta_0' = \beta_0^* + d_1\beta_1^* + d_1^2\beta_{11}^* \text{ and } \beta_0'' = \beta_0^* + d_2\beta_1^* + d_2^2\beta_{11}^* ;$$

$$\beta_1' = \beta_1^* + 2d_1\beta_{11}^* \text{ and } \beta_1'' = \beta_1^* + 2d_2\beta_{11}^* .$$

On the basis of the above results, the experimenter would make one of two incorrect decisions if he did not take account of the inequality of the available nutrients for the two experiments:

1. He would conclude that the true response pattern was different at the two localities and publish two predition equations, each of which represents an inefficient use of the data in estimating the basic parameters. This may prevent the savings in extension work which overall recommendations entail. However, the biases mentioned above are less likely to be so important, because the experimenter realizes his prediction equation is different for different locations.

2. If the experimental error is large compared with $(d_2 - d_1)$, he might conclude that the differences in the estimates of the β's was a

chance difference, and use average β's for his prediction equation. This would produce the biased results mentioned above. However, the important point here is that the estimates of the parameters are quite inefficient because the large spread in N over both experiments is neglected. There is uncertainty as to which incorrect procedure is worse, since this is a matter of weighing the extra costs of a wide variety of recommendations against the inefficiencies and biases of over-all recommendations.

To illustrate the fact that one can obtain more information regarding the response surface by combining the two experiments, suppose only two levels of X (X = -1 and 1) are used for each experiment but the available coded levels are $d_1 = -1$ and $d_2 = 1$. If single estimates are made for each experiment, no estimator of β_{11} will be available; hence, if β_{11} is not zero, the separate estimators of the linear coefficient will be biased. However, in this case, the pooled estimator of β_1 will be unbiased because $d_1 + d_2 = 0$. Also, in this case, the objective is to compare the response surfaces in terms of the total nutrients (X + d). The number of plots for each level of N and the estimators of β_1^* and their expected values when $\beta_{11}^* \neq 0$:

	N				
Experiment	-2	0	2	b_1^*	$E(b_1^*)$
1	r	r		$(N_0-N_{-2})/2r$	$\beta_1^* - 2\beta_{11}^*$
2		r	r	$(N_2-N_0)/2r$	$\beta_1^* + 2\beta_{11}^*$

In both experiments, $\sigma^2(b_1^*) = \sigma^2/2r$. The pooled estimate of β_1^* is unbiased and has $\sigma^2(b_1^*) = \sigma^2/4r$.

If a combined analysis is made, $b_{11}^* = (N_2 - N_0 + N_{-2})/8r$, where N_0 is the sum of the yields of the $2r$ plots with N = 0; $\sigma^2(b_{11}^*) = \sigma^2/16r$. In this case $b_1^* = (N_2 - N_{-2})/4r$ with $\sigma^2(b_1^*) = \sigma^2/8r$; note that this variance is one-half the pooled variance. Even if the experimenter wants to assume different values of β_0^* in each experiment because of unequal amounts of other nutrients, he obtains the same estimate of β_{11}^* from the combined data, and the above pooled estimate of β_1^*.

If a more complicated model is considered, such as an exponential or logistic model, the experimenter will probably find that the inclusion of the available nutrients in the model is just as important. It may be that one of the reasons for obtaining such unrealistic production functions from combined data is the failure to adjust for the available nutrients. Also, this may account for the divergent shape of combined response surfaces when various mathematical forms are used. Someone might make studies similar to these for the more complicated production models.

If one can obtain more efficient and more nearly unbiased estimates by adjusting for available nutrients in several experiments in a combined analysis, why is this not done more often? In many cases, the answer may be lack of knowledge of how to make even the simple

combined analyses. However, the real answer may be generally more complimentary to experimenters:

1. Statisticians have not developed easy and efficient estimation procedures for the more complicated models.
2. Procedures for determining available nutrients are not too well developed.
3. It is often difficult to calibrate available and applied nutrients.
4. Even though only a few nutrients are added in the experiment, admustments must be made for all available nutrients. This may result in a much more complicated analysis.
5. Research has not been well coordinated. As a result, computations may be complicated and total levels may not be spread out very much in the various experiments.
6. Adjustments for weather factors are also needed, especially when combining data from several years. Crop-weather and soil-weather relationships are even more poorly known than are crop-nutrient relationships.

Much of the computing difficulty will probably be relieved as more use of electronic computers is made. Hence, it should be recommended that coordination of efforts in the direction of setting up realistic models and measuring and calibrating available nutrients is needed.

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