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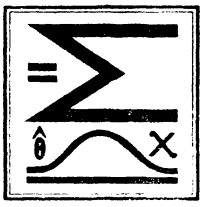

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INTERSITE TRANSFER OF AGROTECHNOLOGY

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Summary

The transferability of agrotechnology questions the feasibility of extrapolating a response-input relationship, estimated from experimental sites, to other sites with similar conditions. One specific example is testing the hypothesis that crop production technology is transferable within the soil family classification. The general approach to the transfer hypothesis incorporates into the data analysis the prediction of yields not used in the estimation of the transfer function. Three transfer models, using a second order response surface and measured site variable information, are formulated and yields for each experimental site are predicted using a transfer function estimated from the other sites. The resulting transfer residuals are compared with the ordinary within-site residuals. A prediction test statistic based on a sum of squares criterion is developed and shown to have a distribution of a ratio of independent quadratic forms. The transfer residual methodology for testing the transfer hypothesis is applied to data from the Benchmark Soils Project.

Key Words: Regression; Prediction; Extrapolation; Controlled and uncontrolled variables.

1. Introduction

Agrotechnology transfer is the extrapolation of a response-input relationship, estimated from a series of experiments, to new but similar sites. Agronomists have long been concerned with the analogous problem of making inferences to farmers' fields. The target population for transfer can be defined as a geographical area or defined by other criteria such as soil and past management information. Recommendations based on a relatively large number of site specific experiments, coupled with long-term experience of agronomists, has been the modus operandi for transferring agrotechnology. In less developed countries, however, a need presently exists to shorten the time and effort required for extensive site specific experimentation.

A major objective of the Benchmark Soils Project, established by U.S.A.I.D (Agency for International Development) in cooperation with the Universities of Hawaii and Puerto Rico, is to test the hypothesis that crop production technology is transferable from one tropical region to another on the basis of similarity of soils as indicated by the soil family in the Soil Taxonomy Classification Systems (Soil Survey Staff 1975). The soil family was selected for the hypothesis since the family classification integrates soil factors with the long-term environmental factors that influence crop yield. The theory is that experimental results, specifically the response of maize to applications of phosphorus and nitrogen, obtained from one country can be applied to sites on the same soil family in another country. Figure 1 schematically demonstrates the inferential structure of the project.

[Figure 1 here]

A straightforward statistical procedure for evaluating the transfer hypothesis is to test the homogeneity of the regression coefficiencts in the k

transfer functions relating response to the controlled variables at each of the k experimental sites. If the transfer function model is the same for all the selected sites, then agrotechnology can be transferred from one site to another through a common transfer function. Specifically, if the homogeneity hypothesis is not rejected, there is not sufficient evidence to indicate that a different model holds for each site. Then a common transfer function can be estimated and in this sense, the agrotechnology can be transferred.

In Figure 1, soil and long-term climatic constants are those factors inherent to the soil family classification. However, within the discrete soil family designations, soil properties do vary and cannot be held at a constant level. Certain soil properties might also vary due to past management. Unfortunately, the natural and man-made variability within the soil family usually cannot be controlled in field experimentation. Consequently, the homogeneity hypothesis usually will be rejected in practice. Interpreting this rejection to mean that agrotechnology isn't transferable can be faulty. The individual site response-input relationship can be affected by the specific biotic environment of the site. Only by measuring the uncontrolled site variables, and including them in the response-input relationship, will the response to the controlled variable be clearly focused.

In addition, a test of the transfer hypothesis should simulate the actual transfer of agrotechnology to sites where experimentation has not been carried out. Our approach is to predict the yields, denoted as $\hat{Y}_{(-i)}$, for one of k experimental sites using a transfer function estimated from the other (k-1) sites. This is then repeated for predicting the yields for each of the k sites based on a transfer function estimated from the other (k-1) sites. The transfer residuals, $Y_i - \hat{Y}_{(-i)}$, can be compared with the ordinary $Y_i - \hat{Y}_i$ residuals, calculated by fitting a response function individually to each of the k sites. The

specific objectives here are (i) to develop the transfer residual methodology for testing the transfer hypothesis and (ii) to demonstrate the methodology with yield and site variable results from maize transfer experiments on the thixotropic, isothermic soil family of Hydric Dystrandepts. The first step is the development of a test statistic for evaluating the transfer residuals.

2. The General Problem

Our approach utilizes a sum of squares criterion to compare the magnitude of the transfer residuals, $Y_i - \hat{Y}_{(-i)}$, to the ordinary within-site residuals, $Y_i - \hat{Y}_i$. In particular, Cady (1974) proposed the ratio of the pooled sum of squared transfer residuals to the pooled sum of squared within-site residuals; i.e.,

$$P = \sum_{i=1}^{k} \left(Y_i - \hat{Y}_{(-i)}\right)' \left(Y_i - \hat{Y}_{(-i)}\right) \Big/ \sum_{i=1}^{k} \left(Y_i - \hat{Y}_i\right)' \left(Y_i - \hat{Y}_i\right) \quad .$$

For two sites (P - 1) is a symmetrized version of Gardner's (1972) ratio bias statistic used for assessing the predictive ability of one sample for a second sample. In the more general case of k sites, P is the natural extension comparing the predictive ability of the ith site for itself with the predictive ability of the remaining (k - 1) sites.

Here we consider the distribution of the P statistic under several predictive models. Throughout, we assume that Y_i, $i = 1, \cdots, k$, arise as observed yields from an equally replicated quantitative treatment design common to all k sites. Further, assume that Y_i have a multivariate normal distribution with identity covariance matrix, I_n . Let Y denote the vector of all observations; i.e., $Y' = [Y_1' \vdots \cdots \vdots Y_k']$. Also, X (an $n \times p$ matrix) will denote the common design matrix with p variables including a column of ones. The non-constant columns of X have been centered at zero.

Model 1: The simplest predictive model is one in which a common response

remaining site. In Section 3, $(P-1)$ is expressed as a constant times a ratio of two quadratic forms, $Y'B_1Y$ and $Y'BY$, where B_1 is idempotent and of rank $p(k-1)$ and $B_1B=0$. The structure for B is given in (1) and B_1 in (3) of Section 3. It is also shown in Section 3 that $(P-1)$ is distributed as a constant times $F[p(k-1)],[k(n-p)]$.

Model 2: Often due to differences in weather, previous management practices, or other site specific variables, one would not expect a common response surface to fit all sites. However, it is conceivable that these differences may be explained by measured site variables. Attention is restricted to second-order response surfaces where the two linear factors are orthogonal. We assume that any differences among the true surfaces involve only (i) differences in mean yields which may be explained by site variables and (ii) differences in the linear response rates which may be explained by interactions with site variables. Once these site variables and interactions have been identified, the predictive ability of the equations, incorporating the site variable information, again can be investigated.

For this model, it is found that $(P-1)$ is no longer proportional to an F statistic, but is distributed as a constant times the ratio of a linear combination of independent χ^2 (1 d.f.) variables to an independent $\chi^2[k(n-p)\text{d.f.}]$ variable. In particular, the numerator of $P-1$ is proportional to a quadratic form $Y'B_2Y$ which, under the assumption of normality, is distributed as $\Sigma_{i=1}^{kn}\theta_i\chi^2_i$, where χ^2_i are independent χ^2 (1 d.f.) variables and θ_i, $i=1,\cdots,kn$ are the eigenvalues of B_2 (see Section 5). While $B_2B=0$, unlike the first predictive model, B_2 is not idempotent. Therefore the eigenvalues, while positive, are not restricted to be 0 or 1.

In general, the distribution of a linear combination of χ^2 variables does not exist in closed form. However, in a particular problem, once P has been computed from the data and the eigenvalues of B_2 have been determined, the attained significance level of P can be accurately estimated by Monte Carlo

Model 3: The last predictive model considered is one in which we prefer to allow unexplained differences in mean yield, yet explain any differences in response surfaces with interactions of site variables with linear response rates. Not surprisingly, we find that by centering the observed yields about the mean for that site, the results for Model 2 remain valid with simple modifications. In particular, the above results hold if we delete the column of ones from the design matrix for each site and correspondingly replace p with (p-1) in the numerator.

In each of the last two models the dimension of B_2 (B_3) is extremely large for moderate k and n . This makes direct numerical computations of the eigenvalues not feasible. Fortunately, this problem can be reduced to the computation of the eigenvalues of several matrices, each of dimension k, a problem readily handled by available computer packages (Section 5).

3. Common Response Surfaces

In the simplest model, we assume that a common response surface is to be fitted to all but one site and then used to predict for the remaining site. The predicted values $\hat{Y}_{(-i)}$, i = 1, ..., k, then take a simple form

$$\hat{Y}_{(-i)} = Xb_{(-i)} \quad ,$$

where X is the common design matrix and $b_{(-i)}$ is the vector of regression coefficients estimated from all but the ith site. Since we are fitting a common response surface,

$$b_{(-i)} = (k-1)^{-1}(X'X)^{-1}\sum_{j\neq i} X'Y_j \quad .$$

In order to derive the result given in Section 2 for Model 1, we need to write the combined vector of transfer residuals as AY; i.e.,

$$R_1 = \left[\left(Y_1 - \hat{Y}_{(-1)}\right)' \vdots \cdots \vdots \left(Y_k - \hat{Y}_{(-k)}\right)'\right]' = AY \quad .$$

Then $\sum_i \left(Y_i - \hat{Y}_{(-i)}\right)'\left(Y_i - \hat{Y}_{(-i)}\right) = Y'A'AY$ and the result follows if $[A'A - B]B = 0$, where B is defined by

$$\sum_{i=1}^{k} \left(Y_i - \hat{Y}_i\right)'\left(Y_i - \hat{Y}_i\right) = Y'BY \quad . \tag{1}$$

Since $\hat{Y}_i = P_X Y_i$, where $P_X = X(X'X)^{-1}X'$,

$$Y_i - \hat{Y}_{(-i)} = Y_i - (k-1)^{-1}P_X \sum_{j \neq i} Y_j = \left(I_n + (k-1)^{-1}P_X\right)Y_i - (k-1)^{-1}P_X \sum_{j=1}^{k} Y_j \quad .$$

Introducing Kronecker products and J_k, a $(k \times k)$ matrix of ones,

$$R_1 = \left[I_k \otimes \left(I_n + (k-1)^{-1}P_X\right)\right]Y - (k-1)^{-1}\left(J_k \otimes P_X\right)Y$$

and

$$A = \left[I_k \otimes \left(I_n + (k-1)^{-1}P_X\right)\right] - (k-1)^{-1}\left(J_k \otimes P_X\right) \tag{2}$$

is the required matrix.

Next, in order to identify the quadratic form, we note that

$$[k^2/(k-1)^2][A'A - B] = \left[\left(I_k - k^{-1}J_k\right) \otimes P_X\right]$$

is an idempotent matrix with rank $p(k-1)$. Since $B = [I_k \otimes (I_n - P_X)]$, $[A'A - B]B = 0$ and the two quadratic forms are independent. Setting

$$B_1 = \left(I_k - k^{-1}J_k\right) \otimes P_X \quad , \tag{3}$$

$$P\text{-}1 = \frac{k^2 Y'B_1 Y}{(k-1)^2 Y'BY} = \frac{k^2}{(k-1)^2} \frac{\chi^2[p(k-1)\text{d.f.}]}{\chi^2[k(n-p)\text{d.f.}]} = \frac{kp}{(k-1)(n-p)} F[p(k-1)],[k(n-p)] \quad .$$

4. Predictions Using Site Variable Information

Site variable information may be incorporated into the predictions to explain both differences in the mean yield and differences in the linear components of the response surfaces of various sites. The predicted values for the ith site based on the other (k-1) sites can again be represented as $\hat{Y}_{(-i)} = X_i b_{(-i)}$, where X_i is now the design matrix X augmented by the site variable information for the ith site and $b_{(-i)}$ is the vector of estimated regression coefficients estimated from the remaining sites using both X and the site variable information. As before, the combined vector of transfer residuals is written as a linear combination of Y, say R_2, and properties of the resulting quadratic form are investigated.

Let ℓ ($\ell < k - 1$) denote the number of site variables used to explain differences in intercepts. Then T_{il}, $i = 1, \cdots, k$ will denote a $[(k-1) \times \ell]$ matrix of site variables for all sites except the ith site which are used to explain the differences in intercepts. Without loss of generality, assume

that the columns of T_{i1} are centered at zero. Also, let $m_1(m_2) < k - 1$ be the number of variables used as interactions between sites and the first (second) linear design variable. Then $T_{i2}(T_{i3})$, $i = 1, \cdots, k$, will denote the $(k-1) \times m_1(m_2)$ matrix of centered interaction variables for all sites except the ith site.

Returning to $\hat{Y}_{(-i)}$, it follows that $b_{(-i)}$ is based on the data matrix

$$X_{(-i)} = \left[1_{(k-1)} \otimes X \vdots T_{i1} \otimes 1_n \vdots T_{i2} \otimes x_1 \vdots T_{i3} \otimes x_2\right] ,$$

where $x_1(x_2)$ is the linear component of the first (second) design variable. In particular $b_{(-i)} = \left(X_{(-i)}'X_{(-i)}\right)^{-1} X_{(-i)}'Y_{(-i)}$, where $Y_{(-i)}$ is the combined vector of yields excluding the ith site. Also, if we let $T_{ij\cdot 1}$ denote the row vector of centered site variables for the previously excluded ith site corresponding to the site variables in T_{ij}, $j = 1,2,3$ and $i = 1, \cdots, k$, then

$$X_i = \left[X \vdots T_{i1\cdot 1} \otimes 1_n \vdots T_{i2\cdot 1} \otimes x_1 \vdots T_{i3\cdot 1} \otimes x_2\right]$$

and $\hat{Y}_{(-i)} = X_i\left(X_{(-i)}'X_{(-i)}\right)^{-1} X_{(-i)}'Y_{(-i)}$.

With these definitions, it can be shown (Appendix 1) that the transfer residuals, R_2, can be expressed as

$$R_2 = \left\{A - \left[\left(T \otimes n^{-1}J_n\right) + \left(\gamma_1 \otimes P_1\right) + \left(\gamma_2 \otimes P_2\right)\right]\right\}\epsilon ,$$

where (i) A is as defined in (2), (ii) ϵ is a multivariate normal vector with mean vector zero and covariance matrix I_{nk}, (iii) $P_i = x_i(x_i'x_i)^{-1}x_i'$, $i = 1,2$, (iv) T is a $(k \times k)$ matrix with diagonal elements equal to zero and the remaining elements in the ith row given in order by $T_{i1\cdot 1}\left(T_{i1}'T_{i1}\right)^{-1} T_{i1}'$, $i = 1, \cdots, k$ and (v) $\gamma_1(\gamma_2)$ is a $(k \times k)$ matrix with diagonal elements equal to zero and the remaining elements in the ith row given in order by $T_{i2\cdot 1}\left(T_{i2}'T_{i2}\right)^{-1} T_{i2}'$ $\left[T_{i3\cdot 1}\left(T_{i3}'T_{i3}\right)^{-1} T_{i3}'\right]$. Notice that R_2 now involves both the design variables

through A, the site variables used to explain differences in intercepts through $T \otimes n^{-1}J_n$, and the interaction variables used to explain differences in the linear trend in the first (second) design variable through $\gamma_1 \otimes P_1$ $(\gamma_1 \otimes P_2)$.

The sum of squared transfer residuals can then be expressed as

$$R_2'R_2 = \epsilon'\left[A'A + k^2(k-1)^{-2}\left(C \otimes J_n\right) + k^2(k-1)^{-2}\left(D_1 \otimes P_1\right) + k^2(k-1)^{-2}\left(D_2 \otimes P_2\right)\right]\epsilon \quad ,$$

where $k^2(k-1)^{-2}C = n^{-1}T'T - n^{-1}k(k-1)^{-1}(T + T') + n^{-1}(k-1)(J_kT + T'J_k)$ and

$$k^2(k-1)^{-2}D_i = \gamma_i'\gamma_i - k(k-1)^{-1}\left[\gamma_i + \gamma_i'\right] + (k-1)\left(J_k\gamma_i + \gamma_i'J_k\right), \qquad i = 1,2 \quad .$$

From Section 3, recall that $A'A - B = k^2(k-1)^{-2}[(I_k - k^{-1}J_k) \otimes P_X]$ and define

$$B_2 = k^{-2}(k-1)^2(A'A - B) + \left(C \otimes J_n\right) + \left(D_1 \otimes P_1\right) + \left(D_2 \otimes P_2\right) \quad . \tag{4}$$

It now follows that

$$P - 1 = \left[\frac{k^2}{(k-1)^2}\,\frac{\epsilon'B_2\epsilon}{\epsilon'B\epsilon}\right] \quad .$$

The numerator and denominator are independent, if $B_2B = 0$. But since $P_XP_i = P_i$, $i = 1,2$ and $P_XJ_n = J_n$, $B_2B = 0$.

Model 3, allowing unexplained differences in mean yield over different sites, is a transfer function consisting of both design variables and site variable interactions with the linear design variables. It is now convenient to separate the design variables in X from the column of ones. In particular, $X_i = [X \vdots T_{i2\cdot1} \otimes x_1 \vdots T_{i3\cdot1} \otimes x_2]$, where X contains only design variables. Then, $Y_i = \beta_{i1} + X_i\beta + \epsilon_i$, where β is now redefined so as not to contain the common intercept and β_{i1} is the mean of the ith site. Since the columns of X are centered at zero, $\bar{y}_i = \beta_{i1} + \bar{\epsilon}_i$, and $Y_i - \bar{y}_1 1_n = X_i\beta + (I_n - n^{-1}J_n)\epsilon_i$.

Thus, adjusting the yields by the intrasite means eliminates the differences in intercepts. The transfer functions are then calculated by estimating β from only (k-1) sites, say $b_{(-i)}$, using the adjusted yields. These coefficients are used for calculating the transfer residuals for the excluded ith site. Following the method of generalized least squares and the previously outlined procedure (Appendix 1),

$$P - 1 = \frac{k^2}{(k-1)^2} \frac{Y'B_3Y}{Y'BY} \quad ,$$

where B_3 is found by deleting the $C \otimes J_n$ component from B_2 as given in (4).

5. Distributional Properties

In the previous two sections, we have found that for Model 2 and Model 3, respectively,

$$(P - 1) = \left[\frac{k^2}{(k-1)^2} \frac{\epsilon'B_i\epsilon}{\epsilon'B\epsilon} \right], \quad i = 2,3 \quad .$$

In addition it was shown that $B_iB = 0$, $i = 2,3$. Therefore, in each case, the numerator and denominator are independent. Also, since B is idempotent, the denominator is a $\chi^2[k(n-p)\text{d.f.}]$. In this section, we consider the distribution of the numerator. We will deal with B_2 directly, since the arguments are identical and the results are analogous for B_3 .

Since $E(\epsilon) = 0$, we have from Searle (1971), Theorem 2.2 that $\epsilon'B_2\epsilon \sim \sigma^2\Sigma_{i=1}^{kn}\theta_i\chi^2_i(1 \text{ d.f.})$ where $\chi^2_i(1 \text{ d.f.})$ are independent χ^2 random variables, each with 1 d.f., and θ_i are the eigenvalues of B_2 . Since this matrix is of dimension kn, we must find simplified expressions for the eigenvalues before proceeding to do any computations. First we will state the results for B_2 . If θ_i, $i = 1, \ldots, kn$ are the eigenvalues of B_2,

$$\theta_i = 1 + \mu_i \ , \qquad i = 1, \cdots, (k-1)(p)$$

and

$$\theta_i = 0 \ , \qquad i = [(k-1)p+1], \cdots, kn \ ,$$

where μ_i, $i = 1, \cdots, (k-1)$ are the nonzero eigenvalues of C, μ_i, $i = k, \cdots, 2(k-1)$ are the nonzero eigenvalues of D_1, μ_i, $i = 2(k-1)+1, \cdots, 3(k-1)$ are the nonzero eigenvalues of D_2, and $\mu_i = 0$, $i = 3(k-1)+1, \cdots, (k-1)p$. Thus we have reduced the problem of computing the eigenvalues of B_2 to the problem of computing the eigenvalues of C, D_1, and D_2 . Details are given in Appendix 2.

A similar argument for B_3 yields the following result: If θ_2 represent the eigenvalues of B_3, then $\theta_i = 0$, $i = [(k-1)(p-1)+1], \cdots, kn$ and $\theta_i = 1 + \mu_i$, $i = 1, \cdots, (k-1)(p-1)$, where μ_i, $i = 1, \cdots, (k-1)$ are the nonzero eigenvalues of D_1, μ_i, $i = k, \cdots, 2(k-1)$ are the nonzero eigenvalues of D_2 and $\mu_i = 0$, $i = 2(k-1)+1, \cdots, (k-1)(p-1)$.

6. Example

The Benchmark Soils Project is described by Silva and Beinroth (1978). As indicated in Section 1, a major objective of the project is to test the feasibility of transferring agrotechnology in the tropics on the basis of soil taxonomic units, thereby reducing the amount of site specific experimentation. Specifically, the hypothesis that an estimated response-input relationship can be transferred within the same soil family needs to be tested. This example uses data from five maize experiments on the Hydric Dystrandept soil family; two sites (PUC-K and BUR-B) are in the Philippines, two in Hawaii (KUC-C and KUK-D) and one in Indonesia (LPH-E). The same 13-point treatment design was used at each site, a partial 5 × 5 factorial with applied phosphorus and applied nitrogen as the controlled variables. An estimated second order response surface model in the two factors adequately

fits the treatment means. As expected, calculation of the P statistic for Model 1 resulted in rejection of the transfer hypothesis. Given here are the numerical details of calculating the P statistic under Model 3 which introduces site variable information in the transfer function as interactions between the site variables and the linear effects of applied phosphorus and applied nitrogen. Table 1 gives the basic site variable information, (EXTN = extractable soil nitrogen, MINT = average daily minimum temperature for eight weeks around tasseling and TRUOG = soil phosphorus), the within-site residual sum of squares (SS) based on fitting a response function to each site, and the transfer SS based on the transfer function estimated from the other sites. Four interactions are included in the transfer function, applied phosphorus with TRUOG and EXTN and applied nitrogen with MINT and EXTN.

[Insert Table 1 here]

From Table 1, we see that the prediction statistic is

$$P = \frac{126,433,780}{88,006,684} = 1.44 \quad .$$

In other words, a 44% increase in unexplained variability when predicting the ith site from the remaining sites is observed using the model with five design variables (quadratic polynomial) and four interactions with the site variables.

The next step is to assess whether this 44% increase is to be expected, or is so large as to contradict the ability to transfer results from one experiment to another. From Section 5, we have that

$$\frac{(k-1)^2}{k^2}(P-1) = 0.64\,(P-1) \sim \frac{\sigma^2 \sum_{i=1}^{20} \theta_i \chi^2_i(1 \text{ d.f.})}{\sigma^2 \chi^2(165 \text{ d.f.})}$$

where $20 = (k-1)(p-1)$ and $165 = k(n-p)$. The θ_i are the eigenvalues of B_3, χ^2_i (1 d.f.) are independent, $\theta_i = 1 + \mu_i$, $i = 1, \cdots, 8$ and $\theta_i = 1$, $i = 9, \cdots, 20$, where $\mu_1, \cdots, \mu_4$ are the nonzero eigenvalues of D_1 and $\mu_5, \cdots, \mu_8$ are the nonzero eigenvalues of D_2 .

Following the construction method outlined in Section 4, D_1 is computed from the site variables TRUOG and extractable nitrogen (EXTN). In particular, D_1 and its nonzero eigenvalues are:

$$D_1 = \begin{bmatrix} 3.070 & -1.837 & 0.267 & 0.462 & -1.963 \\ -1.837 & 0.440 & 0.659 & -0.507 & 1.245 \\ 0.267 & 0.659 & 0.657 & -1.470 & -0.113 \\ 0.462 & -0.507 & -1.470 & 1.145 & 0.370 \\ -1.963 & 1.245 & -0.113 & 0.370 & 0.461 \end{bmatrix} \quad \text{and} \quad \begin{aligned} \mu_1 &= 5.208 \\ \mu_2 &= 2.564 \\ \mu_3 &= -1.000 \\ \mu_4 &= -1.000 \end{aligned}$$

Similarly, D_2 is computed from minimum temperature (MINT) and extractable nitrogen (EXTN). This yields the eigenvalues

$$\mu_5 = 10.705, \quad \mu_6 = 1.666, \quad \mu_7 = -1.000, \quad \text{and} \quad \mu_8 = -1.000 \ .$$

Combining these facts we see that

$$0.64\ (P-1) \sim \sigma^2 \sum_{i=1}^{20} \theta_i \chi^2_i\ (1 \text{ d.f.}) / \sigma^2 \chi^2 (165 \text{ d.f.}) \ ,$$

where $\theta_i = 1 + \mu_i$, $i = 1, \cdots, 8$, and $\theta_i = 1$, $i = 9, \cdots, 20$.

We need to compare the observed value of $(k-1)^2/k^2(P-1) = .280$ with the quantiles of the distribution of $\Sigma_i \theta_i \chi^2_i$ (1 d.f.)$/\chi^2$(165 d.f.) . As stated earlier, the distribution of such a linear combination of χ^2_i (1 d.f.) as found in the numerator does not exist in closed form, while the denominator is an independent χ^2(165 d.f.) variable.

Even though no tables exist for the distribution of $[(k-1)^2/k^2](P-1)$, the attained significance level may be readily estimated by Monte Carlo

simulation. Using the fact that a standard normal variable squared is χ^2 (1 d.f.) and that the numerator and denominator are independent, many variables with the above distribution may be computed and the proportion which falls above the computed value of 0.280 recorded. This will give an accurate estimate of the attained significance level. In this example, we may make a further simplification. Since the d.f. of the denominator is so large, MS Residual is very close to σ^2, the unknown experimental error, with high probability. Rewriting

$$[(k-1)^2/k^2](P-1) \doteq \frac{\sigma^2 \sum_{i=1}^{20} \theta_i \chi^2_i(1 \text{ d.f.})}{165\sigma^2} \quad \text{or} \quad 165[(k-1)^2/k^2](P-1) \doteq \sum_{i=1}^{20} \theta_i \chi^2_i(1 \text{ d.f.}) \ .$$

This implies that we need only compare 165(.280) = 46.2 with the quantiles of $\Sigma_i \theta_i \chi^2_i$ (1 d.f.).

Ten thousand random variables with the distribution given above were generated. In particular, at each iteration, twenty standard normal random variables, say N_i, $i = 1, \cdots, 20$, were generated using GGUSN from the IMSL Statistical Package. Then each variable was formed as the linear combination of χ^2_i (1 d.f.) (N_i^2) variables given above. The attained significance level is 0.292, thereby giving evidence that the response surface for applied phosphorus and applied nitrogen can be transferred with an estimated transfer function including interactions between the site variables and the linear effects of the controlled variables.

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Appendix 1

Representation of the Sum of Squared Transfer Residuals for Model 2 and Model 3

Using the notation developed in Section 4 the combined vector of transfer residuals for Model 2, R_2, is developed by first considering the transfer residuals for one excluded site; e.g., site 1. Recall that

$$X_1 = \left[X \vdots T_{11\cdot 1} \otimes 1_n \vdots T_{12\cdot 1} \otimes x_1 \vdots T_{13\cdot 1} \otimes x_2 \right]$$

and

$$\hat{Y}_{(-1)} = X_1 \left(X_{(-1)}' X_{(-1)} \right)^{-1} X_{(-1)}' Y_{(-1)} = \Big[(k-1)^{-1} 1_{k-1}' \otimes P_X + T_{11\cdot 1} (T_{11}' T_{11})^{-1} T_{11}' \otimes n^{-1} J_n$$

$$+ T_{12\cdot 1} (T_{12}' T_{12})^{-1} T_{12}' \otimes P_1 + T_{13\cdot 1} (T_{13}' T_{13})^{-1} T_{13}' \otimes P_2 \Big] Y_{(-1)} \ ,$$

where J_n is an $(n \times n)$ matrix of ones and $P_i = x_i (x_i' x_i)^{-1} x_i'$, $i = 1, 2$. Note that $T_{1i\cdot 1} (T_{1i}' T_{1i})^{-1} T_{1i}'$, $i = 1, 2, 3$ are $[1 \times (k-1)]$ row vectors. Augmenting each by a zero in the first position, we can define the $(1 \times k)$ row vectors.

$$\tau_1 = \left[0 \vdots T_{11\cdot 1} \left(T_{11}' T_{11} \right)^{-1} T_{11}' \right], \qquad \gamma_{11} = \left[0 \vdots T_{12\cdot 1} \left(T_{12}' T_{12} \right)^{-1} T_{12}' \right]$$

and

$$\gamma_{12} = \left[0 \vdots T_{13\cdot 1} \left(T_{13}' T_{13} \right)^{-1} T_{13}' \right] \ .$$

Then

$$\hat{Y}_{(-1)} = \left[(k-1)^{-1} 1_{k-1}' \otimes P_X \right] Y_{(-1)} + \left[\tau_1 \otimes n^{-1} J_n + \gamma_{11} \otimes P_1 + \gamma_{12} \otimes P_2 \right] Y$$

and

$$Y_1 - \hat{Y}_{(-1)} = \left\{ \left[I_n \vdots -(k-1)^{-1} 1_{k-1}' \otimes P_X \right] - \left[\left(\tau_1 \otimes n^{-1} J_n \right) + \left(\gamma_{11} \otimes P_1 \right) + \left(\gamma_{12} \otimes P_2 \right) \right] \right\} Y \ .$$

Next define τ_i, γ_{i1}, and γ_{i2}, $i = 2, \cdots, k$, analogously to τ_1, γ_{11}, and γ_{12};

e.g., τ_2 is the $(1 \times k)$ row vector formed from $T_{21 \cdot 1}(T_{21}'T_{21})^{-1}T_{21}'$ with a zero element inserted as the second element, γ_{21} is the $(1 \times k)$ row vector formed from $T_{22 \cdot 1}(T_{22}'T_{22})^{-1}T_{21}'$ with a zero element inserted as the second element, and γ_{22} is defined similarly. Then

$$R_2 = \left[\left(Y_1 - \hat{Y}_{(-1)}\right)' \vdots \left(Y_2 - \hat{Y}_{(-2)}\right)' \vdots \cdots \vdots \left(Y_k - \hat{Y}_{(-k)}\right)'\right]'$$

$$= \left\{A - \left[\left(T \otimes n^{-1}J_n\right) + \left(\gamma_1 \otimes P_1\right) + \left(\gamma_2 \otimes P_2\right)\right]\right\} Y$$

where A is defined in (2),

$$T = \begin{bmatrix} \tau_1 \\ \hline \tau_1 \\ \hline \vdots \\ \hline \tau_k \end{bmatrix}, \qquad \gamma_1 = \begin{bmatrix} \gamma_{11} \\ \hline \gamma_{21} \\ \hline \vdots \\ \hline \gamma_{k1} \end{bmatrix}, \qquad \text{and} \qquad \gamma_2 = \begin{bmatrix} \gamma_{12} \\ \hline \gamma_{22} \\ \hline \vdots \\ \hline \gamma_{k2} \end{bmatrix}.$$

At this point it is convenient to note that since we assume that, including site variables and site variable interactions, a common response surface fits all sites,

$$Y_i - \hat{Y}_{(-i)} = \left(X_i\beta + \epsilon_i\right) - X_i\left(X_{(-i)}'X_{(-i)}\right)^{-1}X_{(-i)}'\left[X_{(-i)}\beta + \epsilon_{(-i)}\right]$$

$$= \epsilon_i - X_i\left(X_{(-i)}'X_{(-i)}\right)^{-1}X_{(-i)}'\epsilon_{(-i)} \quad ,$$

where $\epsilon_{(-i)}$ is the combined vector of all errors excluding the ith site. Therefore,

$$R_2 = \left\{A - \left[T \otimes n^{-1}J_n\right] + \left(\gamma_1 \otimes P_1\right) + \left(\gamma_2 \otimes P_2\right)\right]\right\} \underline{\epsilon} \quad ,$$

where $\underline{\epsilon}$ is the combined vector of errors.

Next, consider the sum of squared transfer residuals for Model 2. With

the above representation,

$$R_2'R_2 = \epsilon'\Big\{A'A - A'\Big[\Big(T\otimes n^{-1}J_n\Big) + \sum_{i=1}^{2}\Big(\gamma_i\otimes P_i\Big)\Big] - \Big[\Big(T'\otimes n^{-1}J_n\Big) + \sum_{i=1}^{2}\Big(\gamma_i\otimes P_i\Big)\Big]A$$

$$+ \Big[\Big(T'\otimes n^{-1}J_n\Big) + \sum_{i=1}^{2}\Big(\gamma_i'\otimes P_i\Big)\Big]\Big[\Big(T\otimes n^{-1}J_n\Big) + \sum_{i=1}^{2}\Big(\gamma_i\otimes P_i\Big)\Big]\Big\}\epsilon \quad .$$

Since X contains a column of ones, $P_X J_n = J_n$ and

$$A'\Big(T\otimes n^{-1}J_n\Big) = k(k-1)^{-1}\Big(T\otimes n^{-1}J_n\Big) - (k-1)^{-1}\Big[J_k T\otimes n^{-1}J_n\Big] \quad .$$

Similarly, since $P_X P_i = P_i$, $i = 1, 2$,

$$A'\Big(\gamma_i\otimes P_i\Big) = k(k-1)^{-1}\Big(\gamma_i\otimes P_i\Big) - (k-1)^{-1}\Big(J_k\gamma_i\otimes P_i\Big) \quad .$$

Next, $(T'\otimes n^{-1}J_n)(T\otimes n^{-1}J_n) = (T'T\otimes n^{-1}J_n)$ and, since $P_1P_2 = 0$,

$$\Big[\sum_{i=1}^{2}\Big(\gamma_i'\otimes P_i\Big)\Big]\Big[\sum_{i=1}^{2}\Big(\gamma_i\otimes P_i\Big)\Big] = \sum_{i=1}^{2}\Big(\gamma_i'\gamma_i\otimes P_i\Big) \quad .$$

Combining these facts, we have that $R_2'R_2$ is as expressed in Section 4.

As noted in Section 4, X, X_i, $X_{(-i)}$, and β must be modified in Model 3 so as not to contain intercept terms. The combined vector of adjusted yields, excluding the i<u>th</u> site, can then be written as

$$X_{(-i)}\beta + \Big[I_{(k-1)}\otimes\Big(I_n - n^{-1}J_n\Big)\Big]\epsilon_{(-i)}, \qquad i = 1, \cdots, k \quad .$$

Since the adjusted yields are not independent, we follow the methods of generalized least squares. Noting that the covariance matrix of the adjusted yields is given by $[I_{(k-1)}\otimes(I_n - n^{-1}J_n)]$, which is idempotent, and that $[I_{(k-1)}\otimes(I_n - n^{-1}J_n)]X_{(-i)} = X_{(-i)}$,

$$b_{(-i)} = \left(X_{(-i)}'X_{(-i)}\right)^{-1} X_{(-i)}'\left[I_{(k-1)} \otimes \left(I_n - n^{-1}J_n\right)\right]\left\{X_{(-i)}\beta + \left[I_{(k-1)} \otimes \left(I_n - n^{-1}J_n\right)\right]\epsilon_{(-i)}\right\}$$

$$= \beta + \left(X_{(-i)}'X_{(-i)}\right)^{-1} X_{(-i)}'\epsilon_{(-i)}, \qquad i = 1, \cdots, k \quad .$$

Therefore

$$Y_i - \hat{Y}_{(-i)} = \left(I_n - n^{-1}J_n\right)\epsilon_i - X_i\left(X_{(-i)}'X_{(-i)}\right)^{-1} X_{(-i)}'\left[I_{(k-1)} \otimes \left(I_n - n^{-1}J_n\right)\right]\epsilon_{(-i)} \quad .$$

Following the arguments for R_2, the transfer residuals are given by

$$R_3 = \left[A - \left(\gamma_1 \otimes P_1\right) - \left(\gamma_2 \otimes P_2\right)\right]\left[I_k \otimes \left(I_n - n^{-1}J_n\right)\right]\underline{\epsilon} \quad ,$$

where A is defined as in (2) but using the redefinition of X and $P_X = X(X'X)^{-1}X'$. Since $P_X 1_n = 0$, we have

$$A\left[I_k \otimes \left(I_n - n^{-1}J_n\right)\right] = \left[I_k \otimes \left(I_n - n^{-1}J_n\right)\right]\left[\left(I_k - k^{-1}J_k\right) \otimes P_X\right]$$

$$= \left[I_k - k^{-1}J_k\right] \otimes P_X \quad .$$

Also, since the columns of T_{j2} and T_{j3}, $j = 1, \cdots, k$, are centered at zero, $\gamma_1 J_k = \gamma_2 J_k = 0$,

$$\left[\gamma_1 \otimes P_1\right]\left[\left(I_k - k^{-1}J_k\right) \otimes P_X\right] = \left(\gamma_1 \otimes P_1\right)$$

and

$$\left[\gamma_2 \otimes P_2\right]\left[\left(I_k - k^{-1}J_k\right) \otimes P_X\right] = \left(\gamma_2 \otimes P_2\right) \quad .$$

Combining these facts, we have that

$$R_3 = \left[A - \left(\gamma_1 \otimes P_1\right) - \left(\gamma_2 \otimes P_2\right)\right]\epsilon \quad .$$

Following the argument used for Model 2, we can show that

$$P\text{-}1 = \left[\frac{k^2}{(k-1)^2} \frac{Y'B_3Y}{Y'BY} \right] ,$$

where

$$B_3 = k^{-2}(k-1)^2\left[\left(A'A - B\right) + \left(D_1 \otimes P_1\right) + \left(D_2 \otimes P_2\right)\right] \quad \text{and} \quad B_3B = 0 \quad .$$

Appendix 2

Eigenvalues of B_2 and B_3

First we state some useful properties of the matrices involved in B_2; i.e., for

$$B_2 = \left[\left(I_k - k^{-1}J_k\right) \otimes P_X + \left(C \otimes J_n\right) + \left(D_1 \otimes P_1\right) + \left(D_2 \otimes P_2\right)\right] \quad ,$$

$$\text{(i)} \quad \left[I_k - k^{-1}J_k\right]\left[I_k - k^{-1}J_k\right] = \left[I_k - k^{-1}J_k\right] ;$$

$$\text{(ii)} \quad \left[\left(I_k - k^{-1}J_k\right) \otimes P_X\right]\left(C \otimes J_n\right) = \left(C \otimes J_n\right) ;$$

and

$$\text{(iii)} \quad \left[\left(I_k - k^{-1}J_k\right) \otimes P_X\right]\left(D_i \otimes P_i\right) = \left(D_i \otimes P_i\right) \quad .$$

The first relationship shows that $[I_k - k^{-1}J_k]$ is idempotent. Therefore the eigenvalues of $[I_k - k^{-1}J_k]$ are either 0 or 1 . Since the rank of $[I_k - k^{-1}J_k]$ is (k-1), there are exactly (k-1) eigenvalues which are 1 and one eigenvalue which is zero. Since P_X is also idempotent with rank p, P_X has p eigenvalues which are 1 and [n-p] eigenvalues which are zero. Combining these two facts, it follows from Bellman (1970), Theorem 12.4, that $[(I_k - k^{-1}J_k) \otimes P_X]$ has (k-1)(p) eigenvalues which are one and the remaining eigenvalues are zero.

Next we want to show that the nonzero eigenvalues of B_2 are the nonzero eigenvalues of $[(I_k - k^{-1}J_k) \otimes P_X]$ plus the eigenvalues of $[(C \otimes J_n) + (D_1 \otimes P_1)$

$+ (D_2 \otimes P_2)]$. Since $(C \otimes J_n)$, $(D_i \otimes P_i)$, $i = 1, 2$, and $[I_k - k^{-1}J_k]$ are symmetric matrices, (ii) and (iii) imply that $[I_k - k^{-1}J_k]$ and $[(C \otimes J_n) + (D_1 \otimes P_1) + (D_2 \otimes P_X)]$ commute. From Bellman (1970), Theorem 4.5, this yields the useful result that there exists a matrix N such that $N'N = I$ and

$$N'\left\{\left[\left(I_k - k^{-1}J_k\right) \otimes P_X\right] + \left(C \otimes J_n\right) + \left(D_1 \otimes P_1\right) + \left(D_2 \otimes P_2\right)\right\}N = \operatorname{diag}\left(\lambda_i + \mu_i\right)$$

where λ_i are the eigenvalues of $[(I_k - k^{-1}J_k) \otimes P_X]$ and μ_i are the eigenvalues of $[(C \otimes J_n) + (D_1 \otimes P_1) + (D_2 \otimes P_2)]$. Note that $\theta_i = \lambda_i + \mu_i$, $i = 1, \cdots, kn$.

Now there exists a square matrix U such that $P_X U = U$ and $U'U = I_k$. Without loss of generality we may assume that

$$U = \left[n^{-1/2}1_k \vdots \|x_1\|^{-1}x_1 \vdots \|x_2\|^{-1}x_2 \vdots U_0\right] \quad ,$$

where $\|x_i\| = (\Sigma_j x_{ij}^2)^{1/2}$. Also let $W = w_{(ij)}$, where for $i = 1, \cdots, k$ and $j = 1, \cdots, (k-1)$, $w_{ij} = [(i-1) + i^2]^{-1/2}$, for $j < i$, $w_{ij} = -i[(i-1) + i^2]^{-1/2}$, for $j = i$, and $w_{ij} = 0$ for $j > i$. Then $W'W = I_{k-1}$ and $[I_k - k^{-1}J_k]W = W$. That is, W are the eigenvectors of $(I_k - k^{-1}J_k)$ corresponding to the nonzero eigenvalues. Our goal is to construct the eigenvectors which correspond to the nonzero eigenvalues of $[I_k - k^{-1}J_k] \otimes P_X$. But

$$\left[\left(I_k - k^{-1}J_k\right) \otimes P_X\right]\left(W \otimes U\right) = W \otimes U$$

and we have the required eigenvectors. Contained in the proof of Theorem 4.5 of Bellman (1970) is the fact that the μ_i's corresponding to nonzero λ_i's; say, $\lambda_i = 1, \cdots, (k-1)(n-p)$ are the eigenvalues of

$$\left(W' \otimes U'\right)\left[\left(C \otimes J_n\right) + \left(D_1 \otimes P_1\right) + \left(D_2 \otimes P_2\right)\right]\left(W \otimes U\right)$$

$$= \left[W'CW \otimes U'J_nU\right] + \left[W'D_1W \otimes U'P_1U\right] + \left[W'D_2W \otimes U'P_2U\right] \quad .$$

Now $U'J_nU$ is zero except for the first diagonal element which is equal to n. Also $U'P_1U(U'P_2U)$ is zero except for second (third) diagonal element which is one. Combining these facts, we see that the eigenvalues of

$$\left[W'CW \otimes U'J_nU\right] + \left[W'D_1W \otimes U'P_1U\right] + \left[W'D_2W \otimes U'P_2U\right]$$

is the set of values found by taking eigenvalues of $W'D_1W$, of $W'D_2W$ and of the eigenvalues of $W'CW$ multiplied by n. From this latter result and the definition of C, without loss of generality, we may assume $n = 1$ when computing the eigenvalues.

Finally, we note that $1_k \otimes U$ is the eigenvector of $(I_k - k^{-1}J_k) \otimes P_X$ corresponding to the one zero eigenvalue. But

$$[1_k' \otimes U'] \left[\left(C \otimes J_n\right) + \left(D_1 \otimes P_1\right) + \left(D_2 \otimes P_2\right)\right] [1_k \otimes U] = 0 \quad ,$$

therefore the eigenvalues of $[(C \otimes J_n) + (D_1 \otimes P_1) + (D_2 \otimes P_2)]$ corresponding to the zero eigenvalue of $[I_k - k^{-1}J_k]$ are identically zero. A similar argument yields the results for B_3.

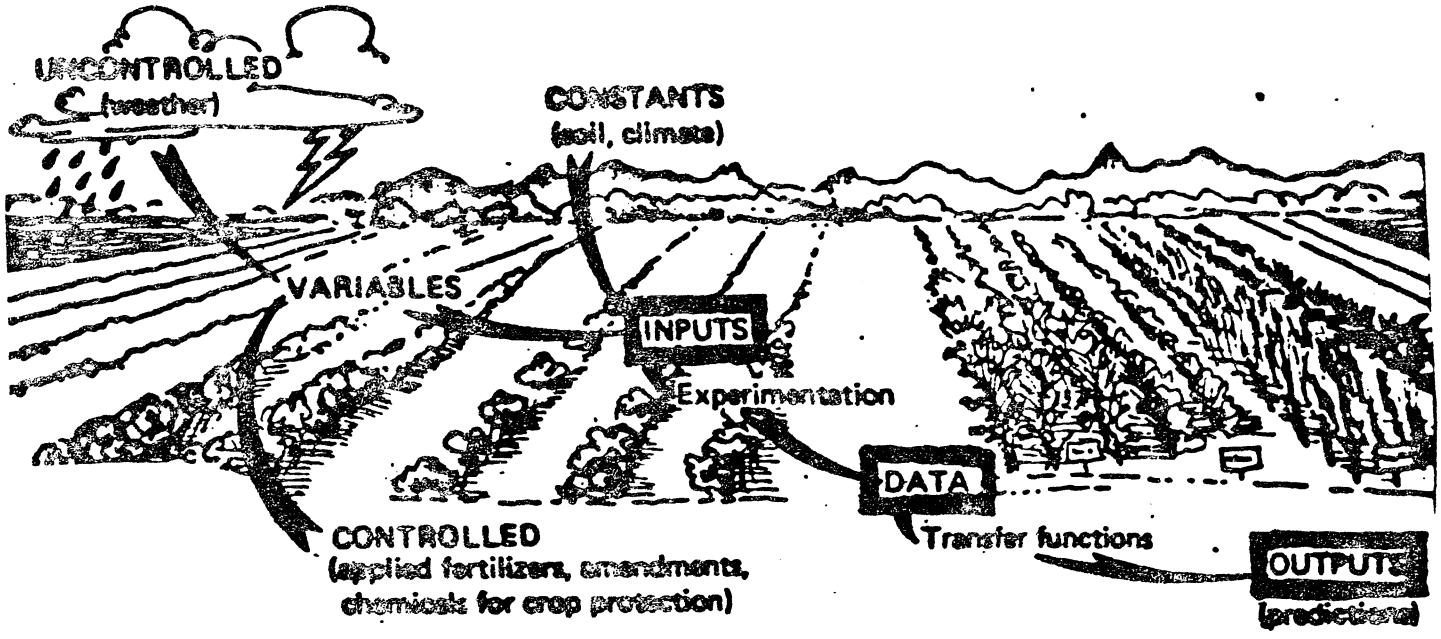

Figure 1

Schematic of Input Factors and Steps Required

to Implement the Benchmark Soils Project

TABLE 1

Site Variable Data, Residual Sum of Squares

and Transfer Sum of Squares

Site	EXTN	MINT	TRUOG	SS Residual	SS Transfer
PUC-K	79	23.00	10	5,869,074	14,700,000
BUR-B	29	21.50	5	25,055,220	36,584,690
KUK-C	46	18.83	74	13,602,420	18,695,610
KUK-D	29	17.90	62	25,599,730	32,792,720
LPH-E	119	16.76	23	17,880,240	23,660,760
				88,006,684	126,433,780