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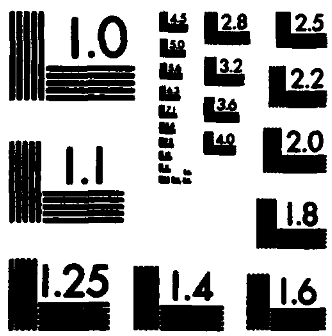

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ROLE OF THE PAPADAKIS ESTIMATOR IN ONE- AND TWO-DIMENSIONAL FIELD TRIALS

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ABSTRACT

Field trials when observations are correlated with those in neighboring or nearby plots in one and two dimensions are analyzed using simultaneous autoregressive models. The relationships between the maximum likelihood solutions and the corresponding well-known Papadakis estimators are clarified and it is shown that the maximum likelihood solutions are, for specific types of designs, easier to obtain directly then by iterating on the Papadakis estimator as has been suggested. A simulation study compares the different models and methods for one and two dimensions.

Note: In spite of its earlier number, MRC Technical Summary Report No. 2650 is a sequel to this report.

AMS (MOS) Subject Classifications: 62K10

Key Words: Correlated plot yields, Maximum likelihood estimator, Papadakis estimators, Simultaneous autoregressive field model

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SIGNIFICANCE AND EXPLANATION

The problem of analyzing data from field trials when observations in neighboring or nearby plots are correlated is an important one which has been extensively examined over the years. In 1937, Papadakis suggested a sensible but mysterious treatment estimator form whose role, and relationship to the corresponding maximum likelihood estimator has been debated for forty-odd years. These matters are here clarified for certain one-and two-dimensional designs under certain simultaneous autoregressive models. Some simulation results are also given.

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ROLE OF THE PAPADAKIS ESTIMATOR IN ONE- AND TWO-DIMENSIONAL FIELD TRIALS

N. R. Draper and D. Faraggi

1. INTRODUCTION

The analysis of field trials when observations in nearby or neighboring plots are correlated has received extensive study over a number of years. Early work was done by Papadakis (1937); his suggested method of model estimation has been regarded as the standard procedure and its consequences have been re-examined by a number of authors including Atkinson (1969), Bartlett (1978), Martin (1982), Wilkinson, Eckert, Hancock and Mayo (1983); for examples using the Papadakis method, see Kempton and Howes (1981). It has been pointed out by Atkinson (1969), Bartlett (1978), Ripley (1978, discussion to Bartlett, 1978) and Martin (1982) that the Papadakis estimator is an approximation to a maximum likelihood estimator. The contexts of their remarks differed somewhat. Atkinson (1969) was discussing the one-dimensional "plots in a line" case, following up work by Williams (1952). Bartlett suggested iterating the Papadakis procedure in one and two dimensions. Ripley (1978) provided a matrix expression for the maximum likelihood estimator for one and two dimensions, and showed its equivalence to generalized least squares. For additional discussion see Ripley (1981,

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pp. 88-97). Martin (1982) also used a matrix formulation and showed that Bartlett's iterative Papadakis procedure converged to the maximum likelihood estimator in certain circumstances.

The present paper considers the one-and two-dimensional situations in matrix form. We clarify the nature of the Papadakis estimator in general and show its relationship to the maximum likelihood estimators arising from two types of error correlation structure. We show further that in certain cases maximum likelihood solutions are obtainable sufficiently straightforwardly, so that the Papadakis estimator is not actually needed.

In general, we assume all one-dimensional designs to be circular in the sense that the nth plot will be supposed to be to the left of the first plot, as would be the case if the string of plots formed a collar on a mountain peak. A practical approximation to such an arrangement might involve adding additional treatments before and after the plot string, setting the treatment of plot n in a "0 plot" and setting the treatment of plot 1 in an "(n+1) plot". See, for example, Dyke and Shelley (1976) or Draper and Guttman (1980).

Similarly, two-dimensional designs are assumed to be torus designs, wrapped around in both dimensions, as assumed by Martin (1982).

2. ONE DIMENSION, ONE SIDED ERROR STRUCTURE

2.1 The First Order Autoregressive Model.

We suppose, following Williams (1952) and Atkinson (1969), that an experimental design consists of a string of adjacent plots used to examine t treatments. Each treatment will occur m times. If each treatment occurs c times adjacent to every other treatment, the design is called a Type II(a) design (by Williams, 1952). If $c = 2$, $t = m + 1$. Note that these designs are assumed to be circular.

We suppose a directional association exists between errors in the following sense. Let there be n response observations $y_1, y_2, \ldots, y_n$ in plot sequence from left to right. The assumed model is

$$y_i = \alpha_s + x_i, \quad i = 1, \ldots, n \quad s = 1, \ldots, t \tag{2.1.1}$$

where α_s denotes the effect of the s^{th} treatment. Furthermore

$$x_i = \rho x_{i-1} + \varepsilon_i \tag{2.1.2}$$

where $\varepsilon = (\varepsilon_1, \varepsilon_2, \ldots, \varepsilon_n)' \sim N(0, I\sigma^2)$.

A first order autoregressive relationship between the x's is assumed instead of the usual independent and identically normal distribution assumption. The joint distribution of $x_1, x_2, \ldots, x_n$ is

$$f(x_1, x_2, \ldots, x_n) =$$

$$\left(\frac{1}{2\pi\sigma^2}\right)^{n/2} (1 - \rho^2)^{\frac{1}{2}} \exp\left[\frac{-1}{2\sigma^2} \left\{x_1^2 + x_n^2 + (1 + \rho^2)\right.\right.$$

$$\left.\left. \cdot \sum_{i=2}^{n-1} (x_i^2) - 2\rho \sum_{i=1}^{n-1} (x_i x_{i+1})\right\}\right]; \qquad (2.1.3)$$

see Koopmans (1942) and Box and Jenkins (1976, p. 276.) The maximum likelihood estimator for ρ can be found in several steps. From the derivative of the log likelihood with respect to ρ we obtain

$$\hat{\sigma}^2 = \frac{(1 - \hat{\rho}^2)}{\hat{\rho}} \left[\sum_{i=1}^{n-1} (x_i x_{i+1}) - \hat{\rho} \sum_{i=1}^{n-1} (x_i^2)\right] \qquad (2.1.4)$$

which is the maximum likelihood of σ^2 in terms of $\hat{\rho}$. Secondly, from the derivative of the log likelihood with respect to σ^2 and a substitution for σ^2 by its maximum likelihood estimator (2.1.4) we find

$$\frac{\hat{\rho}}{1+\hat{\rho}^2} = n\left[\sum_{i=1}^{n-1} x_i x_{i+1} - \hat{\rho} \sum_{i=2}^{n-1} x_i^2\right] \times$$

$$\left[x_1^2 + x_n^2 + (1+\hat{\rho}^2) \sum_{i=2}^{n-1} x_i^2 - 2\hat{\rho} \sum_{i=1}^{n-1} x_i x_{i+1}\right]^{-1} \qquad (2.1.5)$$

which can be solved iteratively for $\hat{\rho}$. To find the maximum likelihood estimator of the effect of the s^{th} treatment α_s, substitute $x_i = y_i - \alpha_s$ into (2.1.3); the Jacobian is the identity matrix. This gives

$$-\hat{\sigma}^2 \frac{\partial L}{\partial \alpha_s} = (1+\hat{\rho}^2) \sum_{[i]=s} (y_i - \hat{\alpha}_s)$$

$$- \hat{\rho} \sum_{[i\pm 1]=s} (y_i - \hat{\alpha}_{[i]}) = 0, \qquad (2.1.6)$$

and the maximum likelihood estimator of α_s is

$$\hat{\alpha}_s^w = m^{-1}\left\{\sum_{[i]=s} y_i - \frac{\hat{\rho}}{1+\hat{\rho}^2} \sum_{[i\pm 1]=s} (y_i - \hat{\alpha}_i)\right\}, \qquad (2.1.7)$$

where the w acknowledges Williams (1952).

Note that $\sum_{[i]=s} y_i$ is used to denote the sum of all the responses from the plots receiving treatment s. So

$\sum_{[i\pm 1]=s} y_i$ is the sum of the responses from the plots adjacent to the plots receiving treatment s.

2.2 The Papadakis Procedure

Papadakis (1937) suggested a sensible but somewhat mysterious estimation procedure described by Atkinson (1969). The corrected yield of the i^{th} plot receiving treatment s is defined by

$$y_i^* = y_i - m^{-1} \sum_{[i]=s} y_i \tag{2.2.1}$$

The concomitant variable δ_i is defined as

$$\delta_i = (y_{i-1}^* + y_{i+1}^*)/2 \,. \tag{2.2.2}$$

The Papadakis estimator of the effect of treatment s is then

$$\hat{\alpha}_s^p = m^{-1}\left\{\sum_{[i]=s} y_i - \hat{\beta}\sum_{[i]=s}\delta_i\right\} =$$

$$= m^{-1}\left\{\sum_{[i]=s} y_i - \frac{\hat{\beta}}{2}\left[\sum_{[i\pm 1]=s}(y_i - m^{-1}\sum_{[i]=s} y_i)\right]\right\} \tag{2.2.3}$$

where

$$\hat{\beta} = \sum_{i=1}^{n} \delta_i y_i^* \Big/ \sum_{i=1}^{n} \delta_i^2 \,. \tag{2.2.4}$$

and p acknowledges Papadakis (1937).

Atkinson (1969) showed that the expectation of $\hat{\beta}$ when using a large sample approximation to x_i and taking the expectation of the ratio to be the ratio of expectations is $E(\hat{\beta}) = 2\rho/(1+\rho^2)$. Comparison of the two estimators (2.1.7) and (2.2.3) implies the Papadakis estimator $\hat{\alpha}_s^p$ is an approximation to the maximum likelihood estimator $\hat{\alpha}_s^w$, with $\hat{\alpha}_{s\pm 1}$ in the maximum likelihood estimator corresponding to $m^{-1}\sum_{[i]=s\pm 1} y_i$ in the Papadakis estimator, and $\hat{\rho}/(1+\hat{\rho}^2)$ in the maximum likelihood estimator replaced by $\hat{\beta}/2$ in the Papadakis estimator.

2.3 The Estimators in Matrix Form

Both the MLE and the Papadakis estimator can be written more conveniently in matrix form. Define T to be the design matrix of size t by n whose s^{th} row contains 1 in the i^{th} column if treatment s is applied to the i^{th} plot and zeroes otherwise. For example, for the design (1,2,3,4)(2,3,1,4)(3,1,4,2), the T matrix will be

$$\underset{4\times 12}{T} = \begin{bmatrix} 1 & 0 & 0 & 0 & 0 & 0 & 1 & 0 & 0 & 1 & 0 & 0 \\ 0 & 1 & 0 & 0 & 1 & 0 & 0 & 0 & 0 & 0 & 0 & 1 \\ 0 & 0 & 1 & 0 & 0 & 1 & 0 & 0 & 1 & 0 & 0 & 0 \\ 0 & 0 & 0 & 1 & 0 & 0 & 0 & 1 & 0 & 0 & 1 & 0 \end{bmatrix}. \quad (2.3.1)$$

Then, with an obvious matrix and vector notation,

$$\underset{n\times 1}{Y^*} = \underset{n\times 1}{Y} - m^{-1} \underset{n\times t}{T'} \underset{t\times n}{T} \underset{n\times 1}{Y} = (\underset{n\times n}{I} - m^{-1} \underset{n\times t}{T'} \underset{t\times n}{T}) \underset{n\times 1}{Y} \quad (2.3.2)$$

where $Y^* = (y_1^*, y_2^*, \ldots, y_n^*)'$, $Y = (y_1, y_2, \ldots, y_n)'$ so that the treatment averages are $m^{-1}TY$. To get the concomitant vector δ we define the neighbor-specification matrix N of size n by n whose i^{th} row contains 1 in positions j for which plot j is adjacent to plot i, and zeroes otherwise.

In our example it will be:

$$\underset{12\times 12}{N} = \begin{bmatrix} 0 & 1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 1 \\ 1 & 0 & 1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 1 & 0 & 1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 1 & 0 & 1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 1 & 0 & 1 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 1 & 0 & 1 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 1 & 0 & 1 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 1 & 0 & 1 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 1 & 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 1 & 0 & 1 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 1 & 0 & 1 \\ 1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 1 & 0 \end{bmatrix} \qquad (2.3.3)$$

Then $\underset{n\times 1}{\delta} = \frac{1}{2} NY^*$ and the vector of Papadakis estimators is

$$\underset{t\times 1}{\hat{\alpha}^p} = m^{-1} \{TY - \frac{1}{2} \hat{\beta} TN(I - m^{-1}T'T)Y\} , \qquad (2.3.4)$$

where $\hat{\alpha}^p = (\hat{\alpha}_1^p, \hat{\alpha}_2^p, \ldots, \hat{\alpha}_t^p)'$. The estimator $\hat{\beta}$ can also be expressed in matrix notation as a ratio of quadratic forms:

$$\hat{\beta} = \frac{2Y'(I-m^{-1}T'T)N(I-m^{-1}T'T)Y}{Y'(I-m^{-1}T'T)N^2(I-m^{-1}T'T)Y} . \qquad (2.3.5)$$

The maximum likelihood estimator in matrix notation is

$$\hat{\alpha}^w = m^{-1}\{TY - \frac{\hat{\rho}}{1+\hat{\rho}^2}(TNY - TNT'\hat{\alpha}^w)\} .$$

This implies

$$\hat{\alpha}^w = m^{-1}\{(I - m^{-1}\hat{\gamma}TNT')^{-1}(TY - \hat{\gamma}TNY)\}$$

$$= (TV^{-1}T')^{-1}TV^{-1}Y , \qquad (2.3.6)$$

where

$$\hat{\alpha}^w = (\hat{\alpha}_1^w, \hat{\alpha}_2^w, \ldots, \hat{\alpha}_t^w)' ,$$

$$\hat{\gamma} = \hat{\rho}/(1+\hat{\rho}^2) ,$$

$$V^{-1} = I - \hat{\gamma}N .$$

Note that $TT' = mI$. Equation (2.3.6) is equivalent to (23) of Wilkinson et al. (1983), as pointed out by discussants to the latter, and also to (5.34) of Ripley (1981).

It is well known that

$$(I - A)^{-1} = I + A + A^2 + A^3 + \ldots \qquad (2.3.7)$$

if and only if all the eigenvalues of the matrix A are smaller than one in absolute value. We can thus apply the above expansion to $\hat{\alpha}^w$ if all the eigenvalues of $m^{-1}\hat{\gamma}TNT'$ are less than one in absolute value. The matrix TNT' is of basic importance in these sorts of analyses because its $(s,w)^{th}$ element is the number of times treatment s appears adjacent to treatment w in the design. We shall later need and define matrices of the form $TN^{(\nu)}T'$ to express more distant spatial relationship. For Type II(a) designs with $c = 2$,

$$m^{-1}\hat{\gamma}TNT' = \underset{(m+1) \times (m+1)}{\begin{bmatrix} a & b & b & \cdots & b \\ b & a & b & \cdots & b \\ b & b & a & \cdots & b \\ \vdots & \vdots & \vdots & \ddots & \vdots \\ b & b & b & \cdots & a \end{bmatrix}} \qquad (2.3.8)$$

where $a = 0$, $b = 2m^{-1}\hat{\gamma}$, and has the two distinct eigenvalues (Rao, 1973, p. 67)

1. $a - b = -2m^{-1}\hat{\gamma}$,

2. $a + mb = 2\hat{\gamma}$.

Both eigenvalues here are less then one in absolute value which guarantees the convergence of the corresponding expansion. Expanding gives

$$\begin{aligned} \hat{\alpha}^{W} &= m^{-1}\{(I + m^{-1}\hat{\gamma}TNT' + m^{-2}\hat{\gamma}^{2}TNT'TNT' + \cdots)(TY - \hat{\gamma}TNY)\} \\ &= m^{-1}\{TY - \hat{\gamma}TNY + m^{-1}\hat{\gamma}TNT'TY - m^{-1}\hat{\gamma}^{2}TNT'T + \cdots\} \\ &= m^{-1}\{TY-\hat{\gamma}TN(I-m^{-1}T'T)Y-m^{-1}\hat{\gamma}^{2}TNT'TN(I-m^{-1}T'T)Y \\ &\qquad - m^{-2}\hat{\gamma}^{3}TNT'TNT'TN(I-m^{-1}T'T)Y - \cdots\}. \qquad (2.3.9) \end{aligned}$$

Because $E(\hat{\beta}/2) \doteq \gamma$, we see that the Papadakis estimator picks the zero and first order terms in $\hat{\gamma}N$ from the autoregressive process, while ignoring the higher order terms. Note also the repetitive application of the Papadakis correction term with higher and higher power of $m^{-1}\hat{\gamma}TNT'$ in the full expansion.

Bartlett (1978) suggested that the Papadakis procedure should be an iterative one, i.e., the corrected yields $y_i^* = y_i - m^{-1} \sum_{[i]=s} y_i$ should be changed in the j^{th} iteration to $y_i^{*(j)} = y_i - \hat{\alpha}_s^{p(j-1)}$ to give

$$\hat{\alpha}^{p(j)} = m^{-1}\{TY - \frac{1}{2}\,\hat{\beta}TN(Y - T'\hat{\alpha}^{p(j-1)})\} \qquad (2.3.10)$$

where $\hat{\alpha}^{p(0)} = m^{-1}T'Y$ so that $\hat{\alpha}^{p(1)}$ is (2.3.4). Martin (1982) showed that indeed this procedure converges to the maximum likelihood estimator for Type II(a) designs, for $\hat{\beta}$ fixed. Convergence occurs because the Papadakis expression (2.3.4) consists of a truncated portion of a convergent expansion (2.3.9) of the maximum likelihood estimator (2.3.6).

Some useful neighbor balanced designs suggested by Williams (1952) are given in Appendix 1.

2.4 An Exact Solution

In fact, for Type II(a) designs, iterative use of the approximate Papadakis formula is unnecessary. The $(I-m^{-1}\hat{\gamma}TNT')$ matrix has a form similar to (2.3.8) where, for example, for type II(a) designs with c = 2,

$$a = 1, \qquad b = -2m^{-1}\hat{\gamma} \,. \tag{2.4.1}$$

This allows it to be inverted as a patterned matrix (Rao, 1973, p. 67). In general, the inverse of such a pattern matrix (see Rao, 1973, p. 67) is

$$\underset{n\times n}{\begin{bmatrix} a' & b' & b' & \cdots & b' \\ b' & a' & b' & \cdots & b' \\ b' & b' & a' & \cdots & b' \\ \vdots & \vdots & \vdots & \ddots & \vdots \\ b' & b' & b' & \cdots & a' \end{bmatrix}} , \tag{2.4.2}$$

where

$$\begin{aligned} a' &= \frac{a+(n-2)b}{[a+(n-1)b][a-b]} \,, \\ b' &= \frac{-b}{[a+(n-1)b][a-b]} \,. \end{aligned} \tag{2.4.3}$$

This provides the exact solution to 2.3.6.

$$\hat{\alpha}^{W} = \frac{1-2\hat{\gamma}(m-1)/m}{m[1-2\hat{\gamma}][1+2\hat{\gamma}/m]} \; \{I + \frac{1}{m-2(m-1)\hat{\gamma}} \hat{\gamma} TNT'\}\{TY-\hat{\gamma} TNY\} . \qquad (2.4.4)$$

Substitution of this in Equation (2.1.5) provides a single equation to solve for $\hat{\rho}$, e.g., via the Newton-Raphson method. The solution is then used in (2.4.4). (The existence of this explicit solution method seems not to have been noted by previous authors.)

3. ONE DIMENSION, TWO-SIDED ERROR STRUCTURE

3.1 The Simultaneous Autoregressive Model

If we apply the one-sided error structure approach of Section 2 to the two dimensional case, geometrical imbalance occurs. This can be rectified by a two-sided error structure assumption, as we shall discuss in Section 4. Once this point is appreciated, it is then natural to return to the one-dimensional case and consider the consequences of a two-sided error structure assumption. We thus assume (following Besag, 1974, simultaneous autoregressive model, p. 201) that

$$y_i = \alpha_s + x_i \quad i = 1,\ldots,n \quad s = 1,\ldots,t \tag{3.1.1}$$

where, now,

$$x_i = \rho(x_{i-1} + x_{i+1}) + \varepsilon_i \tag{3.1.2}$$

with $\varepsilon \sim N(0, I\sigma^2)$. The likelihood function is (Besag, 1974, p. 201, Equation 4.13 taking $\mu = 0$),

$$(2\pi\sigma^2)^{-n/2}|B|\exp\{-(2\sigma^2)^{-1}(X'B'BX)\}, \tag{3.1.3}$$

where

$$\begin{aligned} B &= I - \rho N , \\ X &= Y - T'\alpha, \end{aligned} \tag{3.1.4}$$

and N, T, Y and α are defined as before. The maximum likelihood estimator for α is

$$\hat{\alpha} = (TV^{-1}T')^{-1}TV^{-1}Y, \tag{3.1.5}$$

where

$$V^{-1} = (I - \hat{\rho}N)^2 . \tag{3.1.6}$$

Note that, since $TT' = mI$, (3.1.5) can be rewritten as

$$\hat{\alpha} = m^{-1}\{[I-m^{-1}T(2\hat{\rho}N-\hat{\rho}^2N^2)T']^{-1}T[I-(2\hat{\rho}N-\hat{\rho}^2N^2)]Y\} \tag{3.1.7}$$

and since

$$N^2 = N^{(2)} + 2I, \tag{3.1.8}$$

where $N^{(2)}$ is the "lag two" neighbor-specification matrix whose i^{th} row contains 1 in positions j for which plot j is adjacent but one to plot i and zeroes otherwise. An alternative form is

$$\hat{\alpha} = m^{-1}\left\{\left[I-m^{-1}T\left(\frac{2\hat{\rho}}{1+2\hat{\rho}^2} N - \frac{\hat{\rho}^2}{1+2\hat{\rho}^2} N^{(2)}\right)T'\right]^{-1} T\right.$$

$$\left.\left[I - \left(\frac{2\hat{\rho}}{1+2\hat{\rho}^2} N - \frac{\hat{\rho}^2}{1+2\hat{\rho}^2} N^{(2)}\right)\right] Y\right\}. \qquad (3.1.9)$$

3.2 The Modified Papadakis Estimator

The expansion of the inverse matrix $[I-m^{-1}T(2\hat{\rho}N-\hat{\rho}^2N^2)T']^{-1}$ in (3.1.7) converges if and only if all the eigenvalues of $m^{-1}T(2\hat{\rho}N-\hat{\rho}^2N^2)T'$ are less then one in absolute value. For example, for designs of Type III (Williams, 1952) which are obtained by imposing simultaneously two conditions on the design:

(i) That each treatment should occur equally often adjacent to every other treatment.

(ii) That each treatment should occur equally often adjacent but one to every other treatment.

For example, the design

$$(1,2,3,4)\ (2,1,3,4)\ (1,3,2,4) \tag{3.2.1}$$

has each treatment occurring twice adjacent to every other treatment, and twice adjacent but one to every other treatment assuming the design is circular, that is the final 4 is adjacent to the initial 1. The matrix $m^{-1}T(2\hat{\rho}N-\hat{\rho}^2N^2)T'$ is of form (2.3.8) with

$$a = -2\hat{\rho}^2, \quad b = (4\hat{\rho}-2\hat{\rho}^2)/m\ . \tag{3.2.2}$$

Again, such a matrix has two distinct eigenvalues that can be found explicitly. For Type III designs, they are:

$$\begin{aligned} &\text{(i)} \quad a + mb = -4\hat{\rho}^2 + 4\hat{\rho}, \\ &\text{(ii)} \quad a - b = -2\hat{\rho}^2 - (4\hat{\rho}-\hat{\rho}^2)/m\ . \end{aligned} \tag{3.2.3}$$

It is easy to check that if $\hat{\rho}$ satisfies

$$(1-2^{\frac{1}{2}})/2 < \hat{\rho} < \{[1+m(m-1)/2]^{\frac{1}{2}} - 1\}/(m-1)\ , \tag{3.2.4}$$

then both eigenvalues are between -1 and 1, so that the expansion converges. Expanding (3.1.7) gives

$$\hat{\alpha} = m^{-1}\{TY-T(2\hat{\rho}N-\hat{\rho}^2N^2)(I-m^{-1}T'T)Y$$

$$- m^{-1}T(2\hat{\rho}N-\hat{\rho}^2N^2)T'T(2\hat{\rho}N-\hat{\rho}^2N^2)(I-m^{-1}T'T)Y - \cdots\}. \qquad (3.2.5)$$

We now define the "modified Papadakis estimator" as the terms of zero and first order in $Q = 2\hat{\rho}N-\hat{\rho}^2N^2$ in (3.2.5), namely

$$\hat{\alpha}^{MP} = m^{-1}\{TY-T(2\hat{\rho}N-\hat{\rho}^2N^2)(I-m^{-1}T'T)Y\} . \qquad (3.2.6)$$

In fact, because $T(I-m^{-1}T'T) = 0$ we can simply replace N^2 by $N^{(2)}$ in (3.2.6) to get

$$\hat{\alpha}^{MP} = m^{-1}\{TY-T(2\hat{\rho}N-\hat{\rho}^2N^{(2)})(I-m^{-1}T'T)Y\}. \qquad (3.2.7)$$

This form suggests that we should correct the mean not only by the effect of the nearest neighboring plots but also by the effect of the "lag two" neighboring plots with appropriate coefficients, as shown in Table 1 .

		i-2	i-1	i	i+1	i+2		
		x	•		•	x		

Table 1. Pattern of residual correction to treatment averages for the one dimention "two sided" error structure.

This estimator, (3.2.7), if applied iteratively in designs for which the matrix expansion is valid, converges for fixed β to the maximum likelihood estimator (3.1.7). In the j^{th} iteration,

$$\hat{\alpha}^{MP(j)} = m^{-1}\{TY - T(2\hat{\beta}N - \hat{\beta}^2 N^{(2)})(Y - T'\hat{\alpha}^{MP(j-1)})\} \tag{3.2.8}$$

where $\hat{\alpha}^{MP(0)}$ is $m^{-1}TY$; thus $\hat{\alpha}^{MP(1)}$ is (3.2.7).

3.3 An Exact Solution

In fact, we do not need to iterate our modified Papadakis estimator for Type III designs because an explicit solution can be obtained (below), but it does provide an appropriate parallel to the ordinary Papadakis estimator, for the present case. For Type III designs with $c = 2$, $TV^{-1}T'$ has the same form as (2.3.8) with

$$a = m(1+2\hat{\beta}^2), \quad b = 2(2\hat{\beta}-\hat{\beta}^2). \tag{3.3.1}$$

Using (2.4.2) and (2.4.3), (3.1.5) becomes

$$\hat{\alpha} = m^{-1} \frac{1 - \dfrac{2(m-1)(2\hat{\rho}-\hat{\rho}^2)}{m(1+2\hat{\rho}^2)}}{(1+2\hat{\rho}^2)\left[1 - \dfrac{2(2\hat{\rho}-\hat{\rho}^2)}{(1+2\hat{\rho}^2)}\right]\left[1 + \dfrac{2(2\hat{\rho}-\hat{\rho}^2)}{m(1+2\hat{\rho}^2)}\right]} \times$$

$$\left\{\left[I + \frac{2\hat{\rho}-\hat{\rho}^2}{m(1+2\hat{\rho}^2)-2(m-1)\hat{\rho}(2-\hat{\rho})} TNT'\right]\right.$$

$$\left. \times\ T[I-(2\hat{\rho}N-\hat{\rho}^2N^2)]Y\right\}. \tag{3.3.2}$$

Note that $TN^{(2)}T'$ is a t by t matrix whose $(s,w)^{th}$ element is the number of times treatment s appears adjacent but one to treatment w in the design.

3.4 Maximum Likelihood Estimator for ρ

The maximum likelihood equation for ρ is obtained in several stages. We first find the maximum likelihood estimator for σ^2,

$$\hat{\sigma}^2 = \frac{(Y-T'\hat{\alpha})'(I-\hat{\rho}N)^2(Y-T'\hat{\alpha})}{n}, \tag{3.4.1}$$

then we differentiate the logarithm of Equation (3.1.3) with respect to ρ and set the result equal to zero to give

$$-\frac{n}{2}\,\frac{(Y-T'\hat{\alpha})'(-2N+2\hat{\rho}N^2)(Y-T'\hat{\alpha})}{(Y-T'\hat{\alpha})'(I-2\hat{\rho}N+\hat{\rho}^2N^2)(Y-T'\hat{\alpha})}+\frac{[\partial|I-\rho N|/\partial\rho]_{\rho=\hat{\rho}}}{|I-\hat{\rho}N|}=0. \qquad (3.4.2)$$

The second term on the left hand side of (3.4.2) has an interesting, continued fraction form. First of all the term is $-2n$ times the $(i,i+1)$ element of $(I-\hat{\rho}N)^{-1}$. This is easy to observe using the fact that the derivative of determinant of a matrix is the sum of the determinants of the original matrix differentiated column by column. Here

$$\frac{\partial}{\partial\rho}\begin{vmatrix} 1 & -\rho & 0 & \cdots & 0 & 0 & -\rho \\ -\rho & 1 & -\rho & \cdots & 0 & 0 & 0 \\ 0 & -\rho & 1 & \cdots & 0 & 0 & 0 \\ \vdots & \vdots & \vdots & \ddots & \vdots & \vdots & \vdots \\ 0 & 0 & 0 & \cdots & 1 & -\rho & 0 \\ 0 & 0 & 0 & \cdots & -\rho & 1 & -\rho \\ -\rho & 0 & 0 & \cdots & 0 & -\rho & 1 \end{vmatrix} =$$

$$
= \begin{vmatrix}
0 & -\rho & 0 & \cdots & 0 & 0 & -\rho \\
-1 & 1 & -\rho & \cdots & 0 & 0 & 0 \\
0 & \rho & 1 & \cdots & 0 & 0 & 0 \\
\vdots & \vdots & \vdots & \ddots & \vdots & \vdots & \vdots \\
0 & 0 & 0 & \cdots & 1 & -\rho & 0 \\
0 & 0 & 0 & \cdots & -\rho & 1 & -\rho \\
-1 & 0 & 0 & \cdots & 0 & -\rho & 1
\end{vmatrix}
$$

$$
+ \begin{vmatrix}
1 & -1 & 0 & \cdots & 0 & 0 & -\rho \\
-\rho & 0 & -\rho & \cdots & 0 & 0 & 0 \\
0 & -1 & 1 & \cdots & 0 & 0 & 0 \\
\vdots & \vdots & \vdots & \ddots & \vdots & \vdots & \vdots \\
0 & 0 & 0 & \cdots & 1 & -\rho & 0 \\
0 & 0 & 0 & \cdots & -\rho & 1 & -\rho \\
-\rho & 0 & 0 & \cdots & 0 & -\rho & 1
\end{vmatrix}
$$

$$
+ \begin{vmatrix}
1 & -\rho & 0 & \cdots & 0 & 0 & -\rho \\
-\rho & 1 & -1 & \cdots & 0 & 0 & 0 \\
0 & -\rho & 0 & \cdots & 0 & 0 & 0 \\
\vdots & \vdots & \vdots & \ddots & \vdots & \vdots & \vdots \\
0 & 0 & 0 & \cdots & 1 & -\rho & 0 \\
0 & 0 & 0 & \cdots & -\rho & 1 & -\rho \\
-\rho & 0 & 0 & \cdots & 0 & -\rho & 1
\end{vmatrix} + \cdots
$$

$$\cdots + \begin{vmatrix} 1 & -\rho & 0 & \cdots & 0 & 0 & -1 \\ -\rho & 1 & -\rho & \cdots & 0 & 0 & 0 \\ 0 & -\rho & 1 & \cdots & 0 & 0 & 0 \\ \vdots & \vdots & \vdots & \ddots & \vdots & \vdots & \vdots \\ 0 & 0 & 0 & \cdots & 1 & -\rho & 0 \\ 0 & 0 & 0 & \cdots & -\rho & 1 & -1 \\ -\rho & 0 & 0 & \cdots & 0 & -\rho & 0 \end{vmatrix} . \qquad (3.4.3)$$

Thus, the sum of these determinants is $-2n$ times the co-factor of the $(i,i+1)$ element in $I-\rho N$ and

$$\frac{[\partial|I-\rho N|/\partial\rho]_{\rho=\hat{\rho}}}{|I-\hat{\rho}N|} \qquad (3.4.4)$$

is $-2n$ times the $(i,i+1)$ element of $(I-\hat{\rho}N)^{-1}$. Now

$$(I-\hat{\rho}N)^{-1} = \begin{bmatrix} a & b & c & d & \cdots & e & d & c & b \\ b & a & b & c & \cdots & f & e & d & c \\ c & b & a & b & \cdots & g & f & e & d \\ d & c & b & a & \cdots & j & g & f & e \\ \vdots & \vdots & \vdots & \vdots & \ddots & \vdots & \vdots & \vdots & \vdots \\ e & f & g & h & \cdots & a & b & c & d \\ d & e & f & g & \cdots & b & a & b & c \\ c & d & e & f & \cdots & c & b & a & b \\ b & c & d & e & \cdots & d & c & b & a \end{bmatrix} . \qquad (3.4.5)$$

For n odd, the $(i,i+1)$ element of $(I-\hat{\rho}N)^{-1}$ takes a form which we illustrate for $n = 11$:

$$\cfrac{-\hat{\rho}}{\cfrac{\hat{\rho}^2}{1-\cfrac{\hat{\rho}^2}{1-\cfrac{\hat{\rho}^2}{1-\cfrac{\hat{\rho}^2}{1-\hat{\rho}}}}}+2\hat{\rho}^2-1} \, . \tag{3.4.6}$$

In general, there are $\frac{1}{2}(n-3)$ "$\hat{\rho}^2$ terms" in the continued fraction. For n even, we illustrate for $n = 12$, for which the required expression is

$$\cfrac{-\hat{\rho}}{\cfrac{\hat{\rho}^2}{1-\cfrac{\hat{\rho}^2}{1-\cfrac{\hat{\rho}^2}{1-\cfrac{\hat{\rho}^2}{1-2\hat{\rho}^2}}}}+2\hat{\rho}^2-1} \, . \tag{3.4.7}$$

In general, there are $\frac{1}{2}(n-4)$ "$\hat{\rho}^2$ terms" in the continued fraction, not counting the final $\hat{\rho}^2$ in the denominator $1-2\hat{\rho}^2$. Thus, an explicit solution is obtained by substituting the $\hat{\alpha}$ in Equation (3.3.4) into Equation (3.4.2), solving for $\hat{\rho}$, for example, using the Newton-Raphson method, and then obtaining $\hat{\alpha}$ from (3.3.4) once $\hat{\rho}$ is found. From the practical point of view, however, examination of the likelihood over an interval of ρ, using the solution for $\hat{\alpha}$ in terms of $\hat{\rho}$ is easier than solving explicitly for $\hat{\rho}$.

(Note that if all $\hat{\rho}^2$ values in the continued fractions are replaced by zeros, we obtain $\hat{\rho}$, which thus provides an approximate solution.)

3.5 Least Squares Solution for ρ

The least squares solution for ρ is the $\hat{\rho}$ that minimizes the weighted residual sum of squares. This turns out to be

$$\hat{\rho}^{LS} = \frac{(Y-T'\hat{\alpha}^{LS})'N(Y-T'\hat{\alpha}^{LS})}{(Y-T'\hat{\alpha}^{LS})'N^2(Y-T'\hat{\alpha}^{LS})}, \qquad (3.5.1)$$

which is similar to (2.3.5) with $m^{-1}TY$, the vector of treatment averages, replaced by the least squares estimator of α. The latter is of form identical to $\hat{\alpha}$, the maximum likelihood solution, but with the least squares $\hat{\rho}$ inserted.

4. TWO DIMENSIONS, "ONE-SIDED" ERROR STRUCTURE

The natural extension of the one dimension, first order, one-sided autoregressive model to two dimensions is to consider the model

$$y_{ij} = \alpha_s + x_{ij} \quad i = 1,\ldots,c \quad j = 1,\ldots,r$$
$$s = 1,\ldots t, \qquad (4.1)$$

where

$$x_{ij} = \rho(x_{i-1,j} + x_{i,j-1}) + \varepsilon_{ij}, \qquad (4.2)$$

and $\varepsilon \sim N(0, I\sigma^2)$. Let $cr = n$, the total number of observations. The likelihood function is

$$(2\pi\sigma^2)^{-n/2} \exp\{-(2\sigma^2)^{-1} \sum_{j=1}^{r} \sum_{i=1}^{c} [x_{ij} - \rho(x_{i-1,j} + x_{i,j-1})]^2\} =$$

$$= \cdots = (2\pi\sigma^2)^{-n/2} \exp\{-(2\sigma^2)^{-1}[(1+2\rho^2) \sum_{j=1}^{r} \sum_{i=1}^{c} x_{i,j}^2$$

$$- 2\rho \sum_{j=1}^{r} \sum_{i=1}^{c} x_{i,j}\, x_{i,j-1} - 2\rho \sum_{j=1}^{r} \sum_{i=1}^{c} x_{i,j}\, x_{i-1,j}$$

$$+ 2\rho^2 \sum_{j=1}^{r} \sum_{i=1}^{c} x_{i-1,j}\, x_{i,j-1} + \sum_{i=1}^{c} x_{i,r}^2 + \sum_{j=1}^{r} x_{c,j}^2$$

$$+ \rho^2 \sum_{i=1}^{c-1} x_{i,r}^2 + \rho^2 \sum_{j=1}^{r-1} x_{c,j} + \rho^2 \sum_{i=1}^{c} x_{i,o}^2$$

$$+ \rho^2 \sum_{j=1}^{r} x_{o,j}^2]\} . \tag{4.3}$$

To obtain the maximum likelihood estimator for α_s we first replace the x_{ij}'s in (4.3) by $Y_{ij} - \alpha_s$. The appropriate Jacobian is the identity matrix. The maximum likelihood estimator is:

$$\hat{\alpha}_s = \ell^{-1}\Big\{\sum_{[i,j]=s} Y_{ij} - \frac{\hat{\beta}}{1+2\hat{\beta}^2} \sum_{[i\pm 1]=s} \sum_{[j\pm 1]=s} (Y_{ij} - \hat{\alpha}_s)$$

$$+ \frac{\hat{\beta}^2}{1+2\hat{\beta}^2} \sum_{[i-1]=s} \sum_{[j+1]=s} (Y_{ij} - \hat{\alpha}_s)$$

$$+ \frac{\hat{\beta}^2}{1+2\hat{\beta}^2} \sum_{[i+1]=s} \sum_{[j-1]=s} (Y_{ij} - \hat{\alpha}_s)\Big\} , \tag{4.4}$$

where ℓ is the number of times treatment s was applied, i.e., the maximum likelihood estimator $\hat{\alpha}_s$ will correct the average of all the yields from the plots receiving treatment s , by the residual effects of the neighboring plots (i-1,j), (i+1,j), (i,j-1), (i,j+1) with coefficient $-\hat{\beta}/[\ell(1+2\hat{\beta}^2)]$ (plots marked with • in Table 2);

and by those of plots (i-1,j+1) and (i+1,j-1) with coefficient $\hat{\rho}^2/[\ell(1+2\hat{\rho}^2)]$ (plots marked with x); however plots (i-1,j-1) and (i+1,j+1) are ignored. Equation (4.4) can be rewritten in matrix form as

$$\hat{\alpha} = \ell^{-1}\left\{\left[I - \ell^{-1}T\left(\frac{\hat{\rho}}{1+2\hat{\rho}^2}N - \frac{\hat{\rho}^2}{1+2\hat{\rho}^2}N^{(12)}\right)T'\right]^{-1} \times T\left[I - \left(\frac{\hat{\rho}}{1+2\hat{\rho}^2}N - \frac{\hat{\rho}^2}{1+2\hat{\rho}^2}N^{(12)}\right)\right]Y\right\} \qquad (4.5)$$

where T, N, Y, α defined as before and $N^{(12)}$ is the n by n "semi diagonal neighboring" matrix symbolized by x in Table 2.

	i-1	i	i+1
j-1		•	x
j	•		•
j+1	x	•	

Table 2. Pattern of residuals corrections to treatment averages for the two-dimensions "one-sided" error structure.

If it were thought reasonable that plots $(i-1,j-1)$, $(i-1,j+1)$, $(i+1,j-1)$, $(i+1,j+1)$ should have the same influence on plot (i,j), this "one-sided" extension would not be appropriate. However, one blocking factor could be time or influences such as prevailing wind direction or slope of the ground may make a 'one-sided' or 'semi-one-sided' model appropriate in some contexts. Because of its similarity to the work of Section 5, but with a redefinition of the $N^{(12)}$ matrix, we do not deal further with this case here.

5. TWO DIMENSIONS, "TWO-SIDED" ERROR STRUCTURE

5.1 The Simultaneous Autoregressive Model

Consider a lattice consisting of a finite set of sites, each site having associated with it a univariate random variable. To quote Besag (1974, p. 192): "In most ecological applications, the sites will represent points or regions in the Euclidean plane and will often be subject to a rigid lattice structure. For example, Cochran (1936) discussed the incidence of spotted wilt over a rectangular array of tomato plants. The disease is transmitted by insects and, after an initial period of time, we should expect to observe clusters of infected plants." We assume the model:

$$y_{ij} = \alpha_s + x_{ij}, \quad i = 1,2,\dots,c \quad j = 1,2,\dots,r,$$
$$s = 1,2,\dots,t, \tag{5.1.1}$$

where

$$x_{ij} = \rho(x_{i-1,j} + x_{i+1,j} + x_{i,j-1} + x_{i,j+1}) + \varepsilon_{ij}. \tag{5.1.2}$$

We assume that $\varepsilon \sim N(0, I\sigma^2)$, where $\varepsilon = (\varepsilon_{11}, \varepsilon_{21}, \varepsilon_{31}, \ldots, \varepsilon_{c1}, \varepsilon_{12}, \ldots, \varepsilon_{cr})$. If we set $n = rc$, the likelihood function is

$$(2\pi\sigma^2)^{-n/2}\exp\{-(2\sigma^2)^{-1}\sum_{j=1}^{r}\sum_{i=1}^{c}[x_{ij}-\rho(x_{i-1,j}+x_{i+1,j}+x_{i,j-1}+x_{i,j+1})]^2\}$$

$$\doteq (2\pi\sigma^2)^{-n/2}\exp\{-(2\sigma^2)^{-1}[(1+4\rho^2)\sum_{i=2}^{c-1}\sum_{j=2}^{r-1}x_{ij}^2$$

$$+ 2\rho^2\sum_{i=2}^{c-1}\sum_{j=2}^{r-1}x_{i-1,j}x_{i+1,j} + 2\rho^2\sum_{i=2}^{c-1}\sum_{j=2}^{r-1}x_{i,j-1}x_{i,j+1}$$

$$+ 4\rho^2\sum_{i=2}^{c-1}\sum_{j=2}^{r-1}x_{i,j}x_{i+1,j+1} + 4\rho^2\sum_{i=2}^{c-1}\sum_{j=2}^{r-1}x_{i,j+1}x_{i+1,j}$$

$$- 4\rho\sum_{l=2}^{c-1}\sum_{j=2}^{r-1}x_{ij}x_{i+1,j} - 4\rho\sum_{i=2}^{c-1}\sum_{j=2}^{r-1}x_{i,j}x_{i,j+1}]\}. \qquad (5.1.3)$$

The maximum likelihood estimator of α_s is

$$\hat{\alpha}_s = \ell^{-1}\left\{\sum_{[i,j]=s} y_{ij} - \frac{2\hat{\rho}}{1+4\hat{\rho}^2}\sum_{[i\pm 1]=s}\sum_{[j\pm 1]=s}(y_{ij}-\hat{\alpha}_{ij})\right.$$

$$+ \frac{2\hat{\rho}^2}{1+4\hat{\rho}^2}\sum_{[i\mp 1]=s}\sum_{[j\pm 1]=s}(y_{ij}-\hat{\alpha}_{ij})$$

$$\left.+ \frac{\hat{\rho}^2}{1+4\hat{\rho}^2}\sum_{[i\pm 2]=s}\sum_{[j\pm 2]=s}(y_{ij}-\hat{\alpha}_{ij})\right\}, \qquad (5.1.4)$$

where ℓ is the number of times treatment s was applied. Here, the average of all the plots receiving treatment s will be corrected for the residual effects of the neighboring plots (i-1,j), (i+1,j), (i,j-1), (i,j+1) with coefficient $-2\hat{\rho}/[\ell(1+4\hat{\rho}^2)]$ (shown as $\cdot$ in Table 3); for those of plots (i-1,j-1), (i-1,j+1), (i+1,j-1), (i+1,j+1) with coefficient $2\hat{\rho}^2/[\ell(1+4\hat{\rho}^2)]$ (shown as x); and for those of plots (i-2,j), (i+2,j), (i,j-2), (i,j+2) with coefficient $\hat{\rho}^2/[\ell(1+4\hat{\rho}^2)]$ (shown as *) .

	i-2	i-1	i	i+1	i+2
j-2			*		
j-1		x	•	x	
j	*	•		•	*
j+1		x	•	x	
j+2			*		

Table 3. Pattern of residuals corrections to treatment averages for the two-dimensional, "two-sided" error structure.

We now recast Equation (5.1.4) into matrix form. The likelihood function and the maximum likelihood estimator for α are exactly the forms of Equations (3.1.3) and (3.1.5), but with redefined N and T. For example, for the 5×5 knight's move Latin square given by

$$
\begin{array}{ccccc}
1 & 2 & 3 & 4 & 5 \\
4 & 5 & 1 & 2 & 3 \\
2 & 3 & 4 & 5 & 1 \\
5 & 1 & 2 & 3 & 4 \\
3 & 4 & 5 & 1 & 2
\end{array}
\qquad (5.1.5)
$$

we have

$$
\underset{5\times 25}{T} = \left[\begin{array}{*{25}{c}}
1&0&0&0&0&0&0&1&0&0&0&0&0&0&1&0&1&0&0&0&0&0&0&1&0 \\
0&1&0&0&0&0&0&0&1&0&1&0&0&0&0&0&0&1&0&0&0&0&0&0&1 \\
0&0&1&0&0&0&0&0&0&1&0&1&0&0&0&0&0&0&1&0&1&0&0&0&0 \\
0&0&0&1&0&1&0&0&0&0&0&0&1&0&0&0&0&0&0&1&0&1&0&0&0 \\
0&0&0&0&1&0&1&0&0&0&0&0&0&1&0&1&0&0&0&0&0&0&1&0&0
\end{array}\right]
\qquad (5.1.6)
$$

The n by n neighbor-specification matrix N is now different from that of Chapters 2 and 3. Here

$$
\underset{25\times 25}{N} = \underset{5\times 5}{N_c^*} \circledast \underset{5\times 5}{I_r} + \underset{5\times 5}{I_c} \circledast \underset{5\times 5}{N_r^*} \qquad (5.1.7)
$$

where

$$\underset{5\times 5}{N_r^*} = \underset{5\times 5}{N_c^*} = \begin{bmatrix} 0 & 1 & 0 & 0 & 1 \\ 1 & 0 & 1 & 0 & 0 \\ 0 & 1 & 0 & 1 & 0 \\ 0 & 0 & 1 & 0 & 1 \\ 1 & 0 & 0 & 1 & 0 \end{bmatrix} \qquad (5.1.8)$$

and $\circledast$ is the Kronecker product. In general, N_r^* and N_c^* are the r by r and c by c neighbor-specification matrices for rows and columns respectively. We can write

$$N^2 = N^{(2)} + 2N^{(12)} + 4I \qquad (5.1.9)$$

where, with a slight change of notation from the one-dimensional case, which offers no "diagonal plots", $N^{(12)}$ is the "diagonal neighbor-specification" matrix, symbolized by x in Table 3, and $N^{(2)}$ is the "lag two" neighbor-specification matrix, symbolized by * in Table 3. The • symbolizes N. Then,

$$V^{-1} = (I-\beta N)^2 = (1+4\beta^2)I - 2\beta N + 2\beta^2 N^{(12)} + \beta^2 N^{(2)}. \qquad (5.1.10)$$

We thus obtain, from (3.1.5) and (5.1.10),

$$\hat{\alpha} = \ell^{-1}\left\{\left[I - \ell^{-1}T\left(\frac{2\hat{\rho}}{1+4\hat{\rho}^2}N - \frac{2\hat{\rho}^2}{1+4\hat{\rho}^2}N^{(12)} - \frac{\hat{\rho}^2}{1+4\hat{\rho}^2}N^{(2)}\right)T'\right]^{-1} T\right.$$

$$\left.\times \left[I - \left(\frac{2\hat{\rho}}{1+4\hat{\rho}^2}N - \frac{2\hat{\rho}^2}{1+4\hat{\rho}^2}N^{(12)} - \frac{\hat{\rho}^2}{1+4\hat{\rho}^2}N^{(2)}\right)\right] Y\right\}, \quad (5.1.11)$$

which is identical to (5.1.4).

5.2 The Modified Papadakis Estimator

The maximum likelihood estimator can be expanded if and only if all the eigenvalues of $\ell^{-1}T(2\hat{\rho}N-\hat{\rho}^2N^2)T'$ are smaller than one in absolute value. For example, for two dimensional designs derived by making a row by row cyclic permutation mt times of the Type III designs of Williams (1952, p. 159), $\ell^{-1}T(2\hat{\rho}N-\hat{\rho}^2N^2)T'$ is a pattern matrix of the form of (2.3.8) with

$$a = -8\hat{\rho}^2, \qquad b = 8(\hat{\rho}-\hat{\rho}^2)/m, \quad (5.2.1)$$

with the two distinct eigenvalues

$$\text{(i)} \quad a + mb = -8\hat{\rho}^2 + 8(\hat{\rho}-\hat{\rho}^2) ,$$
$$\text{(ii)} \quad a - b = -8\hat{\rho}^2 - 8(\hat{\rho}-\hat{\rho}^2)/m . \qquad (5.2.2)$$

If $\hat{\beta}$ satisfies

$$(1-2^{\frac{1}{2}})/4 < \hat{\beta} < [\{1+m(m-1)/2\}^{\frac{1}{2}}-1]/\{2(m-1)\}, \qquad (5.2.3)$$

the expansion is valid and takes the form

$$\hat{\alpha} = \ell^{-1}\{TY-T(2\hat{\beta}N-\hat{\beta}^2N^2)(I-\ell^{-1}T'T)Y$$
$$- \ell^{-1}T(2\hat{\beta}N-\hat{\beta}^2N^2)T'T(2\hat{\beta}N-\hat{\beta}^2N^2)(I-\ell^{-1}T'T)Y - \cdots \}. \qquad (5.2.4)$$

Deletion of all terms in $\hat{\beta}$ whose powers exceed one gives an estimator of the Papadakis type for the two dimensional case

$$\ell^{-1}\{TY - 2\hat{\beta}TN(I-\ell^{-1}T'T)Y\} \qquad (5.2.5)$$

which may be compared with (2.3.4). If we retain terms of order zero and one in $Q = 2\hat{\beta}N - \hat{\beta}^2N^2$, so that corrections for diagonal and "lag two" plots are included, we can define a "modified Papadakis estimator":

$$\ell^{-1}\{TY - T(2\hat{\beta}N - \hat{\beta}^2N^2)(I - \ell^{-1}T'T)Y\} \qquad (5.2.6)$$

and we achieve the same phenomena as in the one dimensional case of reproducing the term $\ell^{-1}T(2\hat{\beta}N-\hat{\beta}^2N^2)T'$ again and again. If Bartlett's (1978) suggestion of iterating is followed for the "modified Papadakis estimator" (5.2.6), convergence to the maximum likelihood estimator occurs, for $\hat{\beta}$ fixed, for designs for which the matrix expansion is valid. Because $T(I-m^{-1}T'T)=0$, we can also write this "modified Papadakis estimator" in the form

$$\ell^{-1}\{TY-T(2\hat{\beta}N-2\hat{\beta}^2N^{(12)}-\hat{\beta}^2N^{(2)})(I-\ell^{-1}T'T)Y\} \qquad (5.2.7)$$

which directly reflects the pattern of Table 3.

5.3 An Exact Solution

Iteration is not actually needed for designs of the type described above, however. As in the one-dimensional case, we can again get an explicit solution for cyclically permuted (t times, or mt times, with appropriate bordering treatments, different for the two cases) Type III designs without resorting to the Papadakis estimator, by using pattern results to invert the matrix $TV^{-1}T'$ that has the form of (2.3.8) with

$$a = m^2(m+1)(1+8\hat{\rho}^2),$$

$$b = -m(m+1)(8\hat{\rho}-8\hat{\rho}^2). \tag{5.3.1}$$

For example, the solution for Type III designs cyclically permuted mt times is

$$\frac{1}{m^2(m+1)(1+8\hat{\rho}^2)} \frac{1-\dfrac{(m-1)(8\hat{\rho}-8\hat{\rho}^2)}{m(1+8\hat{\rho}^2)}}{\left[1-\dfrac{8\hat{\rho}-8\hat{\rho}^2}{1+8\hat{\rho}^2}\right]\left[1+\dfrac{8\hat{\rho}-8\hat{\rho}^2}{m(1+8\hat{\rho}^2)}\right]}$$

(5.3.2)

$$\times\left\{\left[I+\frac{2\hat{\rho}-2\hat{\rho}^2}{m(m+1)[m(1+8\hat{\rho}^2)-(m-1)(8\hat{\rho}-8\hat{\rho}^2)]}TNT'\right]T\left[I-(2\hat{\rho}N-\hat{\rho}^2N^2)\right]Y\right\}.$$

Note that $TN^{(12)}T'$ is a t by t matrix whose $(s,w)^{th}$ element is the number of times treatment s appears on the diagonal of treatment w in the design, and $TN^{(2)}T'$ is a t by t matrix whose (s,w) element is the number of times treatment s appears adjacent but one to treatment w in the design.

5.4 Maximum Likelihood Estimator for ρ

The maximum likelihood equation for $\hat{\rho}$ is obtained as in section (3.4)(pp. 32-35) with symbols appropriately redefined for two dimensions. We now need $-4n$ times the $(i,i+1)$ element of $B^{-1} = (I-\hat{\rho}N)^{-1}$. Because of the form of B, B^{-1} will have a special form. The first column of B^{-1}, b_1, say, consists of a small subset containing q, say, elements which recur throughout B^{-1}. The n equations $Bb_1 = (1,0,0,...,0)'$ reduce to q equations $B^*b^* = (1,0,0,...,0)'$ where B^* is $q \times q$ and both b^* and the right-hand-side are $q \times 1$ vectors. The element we want is then $(B^*)^{-1}_{j1}$ where j is the position of the required element in b^*, this position being our arbitrary choice. The value of q is

$$q = \sum_{i=1}^{RU} i\,, \qquad (5.4.1)$$

where

$$RU = RU\{\tfrac{1}{2}(n^{\frac{1}{2}} + 1)\}, \qquad (5.4.2)$$

and $RU(\theta)$ means "round up θ to the next integer if it is not already an integer". A specific example for such a procedure is given in Appendix 2. As before, we now solve iteratively for $\hat{\rho}$ in Equation (5.1.11), or (5.3.2).

The least squares solution for ρ is similar to (3.5.1) with ℓ replacing m, and with N appropriately redefined.

6. SIMULATION STUDY

A simulation study to compare the different estimators described in Chapters 2, 3, and 5 was conducted both for one and two dimensions.

6.1 <u>One Dimension</u>

In one dimension, four estimation procedures were compared:

(i) The maximum likelihood estimator for the simultaneous autoregressive model (Section 3.1).

(ii) The modified Papadakis estimator (Section 3.2).

(iii) The maximum likelihood estimator for the first order autoregressive model (Section 2.1).

(iv) The Papadakis estimator (section 2.2).

The design assumed was the Type III design

$$(1,2,3,4)(2,1,3,4)(1,3,2,4). \qquad (6.1.1)$$

The observations were generated as follows:

(1) The model assumed was

$$Y = T'\alpha + X, \tag{6.1.2}$$

where

$$X = \rho N X + \varepsilon \ ,$$

so $\varepsilon = (I - \rho N)X \Longrightarrow X = (I - \rho N)^{-1}\varepsilon$.

(2) Using generated normal random variables with zero mean and three different standard deviations (0.01, 0.1, 1) X was found for fixed ρ .

(3) On the X was superimposed a treatment effect as required by the design (6.1.1) to get the observations Y .

(4) The above scheme was used to construct twenty data sets for various combinations of ρ and σ .

The four different estimation procedures were then applied to all 20 data sets.

In Table 4, the maximum likelihood estimator for ρ is given as well as the weighted residuals sum of squares for the different models and methods. Note that, for the modified Papadakis estimator, $\hat{\rho}$ was derived from the likelihood function of the simultaneous autoregressive model with the modified Papadakis estimator for α inserted; this explains the difference in the $\hat{\rho}$ for the maximum likelihood estimator and the $\hat{\rho}$ for the modified Papadakis estimator. The weighted residuals sum of squares was calculated as

$$(Y - T'\hat{\alpha})'V(Y - T'\hat{\alpha}) \qquad (6.1.3)$$

where

(1) $V^{-1} = (I - \hat{\rho}N)^2$ for the estimator from the simultaneous autoregressive model.

(2) $V^{-1} = (I - \hat{\rho}N)^2$ for the modified Papadakis estimator.

(3) $V^{-1} = I - \hat{\gamma}N$ for the estimation from the first order autoregressive model.

(4) $V^{-1} = I - \frac{1}{2}\hat{\beta}N$ for the Papadakis estimator.

We observe, from Table 4, that overall the simultaneous autoregressive model does better, as might be expected. Only for certain ρ values, as tabulated, do the other methods provide close estimates of $\hat{\rho}$. The weighted residual sum of squares is smallest for the simultaneous autoregressive model everywhere except for simulation 7, and 19 where the modified Papadakis estimator is slightly better.

Table 4. Values of the Maximum Likelihood Estimator of ρ and of Weighted Residual Sums of Squares Values for Different Models and Methods and for Various True Values of ρ and σ in One Dimension.

Model →			Simultaneous Autoregressive		Modified Papadakis		Autoregressive Model		Papadakis	
Simulation No.	ρ	σ	$\hat{\rho}$	WRSS	$\hat{\rho}$	WRSS	$\hat{\rho}$	WRSS	$\frac{1}{2}\hat{\beta}$	WRSS
1	.95	.01	.851	.087	.271	.303	.351	.350	.487	.276
2	.85	.01	.761	.078	.261	.110	.491	.104	.332	.118
3	.75	.01	.711	.082	.261	.111	.741	.101	.432	.125
4	.65	.01	.641	.087	.371	.343	.861	.267	.512	.240
5	.55	.01	.601	.089	.391	1.78	.861	1.5	.532	.98
6	.45	.01	.691	.099	.341	.164	.731	.138	.476	.142
7	-.95	.01	-.969	.030	-.979	.029	-.399	2.6	-.614	1.7
8	-.85	.01	-.899	.037	-.909	.038	-.409	.316	-.682	.171

Table 4. (Continued)

Model → Simulation No.	ρ	σ	Simultaneous Autoregressive $\hat{\beta}$	Simultaneous Autoregressive WRSS	Modified Papadakis $\hat{\beta}$	Modified Papadakis WRSS	Autoregressive Model $\hat{\beta}$	Autoregressive Model WRSS	Papadakis $\frac{1}{2}\hat{\beta}$	Papadakis WRSS
9	-.75	.01	-.769	.045	-.779	.049	-.569	.138	-.650	.060
10	-.65	.01	-.629	.042	-.649	.068	-.829	.190	-.572	.078
11	.95	.1	.941	.158	.331	2.709	.421	3.602	.835	1.179
12	.95	.1	.951	.362	.331	9.471	.541	11.399	.813	4.507
13	.85	.1	.841	.175	.321	.537	.521	.623	.660	.368
14	.75	.1	.831	.182	.291	.453	.501	.486	.561	.375
15	.55	.1	.611	.187	.401	1.849	.891	1.738	.545	.903
16	.55	.1	.641	.904	.391	2.645	.891	2.403	.541	1.5

Table 4. (Continued)

Model → Simulation No.	ρ	σ	Simultaneous Autoregressive $\hat{\rho}$	WRSS	Modified Papadakis $\hat{\rho}$	WRSS	Autoregressive Model $\hat{\rho}$	WRSS	Papadakis $\frac{1}{2}\hat{\beta}$	WRSS
17	.55	.1	.591	.127	.411	4.069	.891	4.071	.545	1.939
18	.55	1	.591	9.309	.391	593.9	-.199	34.813	.536	308.84
19	-.95	1	-.969	4.459	-.979	4.151	-.439	496.26	-.886	109.69
20	-.85	1	-.729	17.86	-.749	20.41	-.819	24.177	-.467	27.25

6.2 Two Dimensions

For two dimensions, three estimators were compared

(i) The maximum likelihood estimator from the simultaneous autoregressive model (Section 5.1).

(ii) The modified Papadakis estimator (Section 5.2).

(iii) The extension of the Papadakis estimator into two dimensions (Section 5.2).

The design used was (6.1.1) row by row cyclically permuted 12 times. Thirteen different data sets were generated in a manner similar to that described for the one dimensional case. Table 5 is constructed in the same manner as was Table 4 for the one dimensional case, with the obvious extension into two dimensions.

Table 5 shows the same characteristics for two dimensions that Table 4 showed for one dimension except that the comparison flatters the simultaneous autoregressive model even more. Note that the data in Table 5 involves 144 observations, compared with the 12 used in Table 4.

Table 5. Values of the Maximum Likelihood Estimator of ρ and of Weighted Sums of Squares Values for Different Models and Methods and for Various True Values of ρ and σ^2 in Two Dimensions.

Model →			Simultaneous Autoregressive		Modified Papadakis		Papadakis	
Simulation No.	ρ	σ	$\hat{\rho}$	WRSS	$\hat{\rho}$	WRSS	$\frac{1}{4}\hat{\beta}$	WRSS
1	.95	.1	.941	1.574	.811	5.260	.965	1.688
2	.85	.1	.821	1.521	.671	2.690	.340	3.503
3	.75	.1	.731	1.509	.441	1.570	.225	2.615
4	.65	.1	.641	1.515	.461	1.664	.210	8.533
5	.55	.1	.551	1.559	.551	2.061	-.004	52.920
6	.45	.1	.451	1.560	.441	1.759	.026	10.760
7	-.95	.1	-.949	1.954	-.909	3.330	-.017	59.930
8	-.85	.1	-.839	1.923	-.779	2.447	.014	8.550

Table 5. (Continued)

Model → Simulation No.	ρ	σ	Simultaneous Autoregressive $\hat{\rho}$	WRSS	Modified Papadakis $\hat{\rho}$	WRSS	Papadakis $\frac{1}{4}\hat{\beta}$	WRSS
9	-.75	.1	-.739	1.886	-.699	2.10	.025	5.03
10	-.65	.1	-.649	1.897	-.639	2.027	.040	9.335
11	-.55	.1	-.529	1.894	-.539	1.908	.018	51.391
12	.45	.1	-.449	1.841	-.439	1.796	.018	18.598
13	.95	1	-.941	160.13	.941	167.39	-2.37	13.533

7. REMARK

Expansion of the MLE equations for any given model set-up may or may not be valid. If it is, the "zero and first order" terms provide an appropriate Papadakis-type estimator for the problem studied, and iteration on this estimator converges to the MLE. Thus the point made by Wilkinson et al. (1983) that the iterated Papadakis estimator will provide a positively biased treatment F-ratio is puzzling. A possible explanation is that the Papadakis-type estimators used by Wilkinson et al. (1983) may not be the appropriate Papadakis-type estimator provided by the first term in a valid matrix expansion under the model assumed. Alternatively, such an expansion may not be valid. These issues appear to need further exploration.

Appendix 1. Some Useful One and Two Dimensional Neighbor Balanced Designs Reproduced from Williams 1952 and Freeman 1979. (See Section 2.3)

One Dimension: Type II(a) Designs with c = 2 (Williams 1952).

In Type II(a) designs, each treatment occurs n times and equally often, c times, say, next to every other treatment.

m = 4 (1,2,3,4,5)(3,4,1,5,2)(4,5,3,1,2)(3,1,4,2,5)

m = 5 (1,2,3,4,5,6)(2,5,3,6,4,1)(5,3,1,6,4,2)(5,1,6,3,2,4)
(3,1,4,5,6,2)

m = 6 (1,2,3,4,5,6,7)(5,3,6,4,7,2,1)(4,2,5,1,6,3,7)
(1,3,5,4,7,6,2)(5,6,4,3,2,7,1)(6,2,4,1,5,7,3)

m = 7 (1,2,3,4,5,6,7,8)(6,4,2,5,1,3,8,7)(5,3,6,2,7,4,8,1)
(7,3,4,1,6,5,8,2)(6,3,7,4,8,1,2,5)
(3,2,4,5,8,6,7,1)(6,4,1,3,8,2,7,5)

One Dimension: Type III Designs with c = 2 (Williams 1952).

Type III designs satisfy the condition of Type II(a) designs; also each treatment occurs equally often adjacent but one to every other treatment.

m = 2 (1,2,3)(1,2,3)

m = 3 (1,2,3,4,)(2,1,3,4)(1,3,2,4)

m = 4 (1,2,3,4,5)(2,4,1,5,3)(1,4,5,3,2)(5,1,2,4,3)

Two Dimensions: Complete Latin Squares (Freeman 1979).

Complete Latin squares are designed such that any two treatments occur next to each other once in a row and once in a column. (Note that the designs are not assumed to be torus designs.)

$$m = 4 \quad \begin{array}{cccc} 1 & 2 & 3 & 4 \\ 3 & 1 & 4 & 2 \\ 2 & 4 & 1 & 3 \\ 4 & 3 & 2 & 1 \end{array}$$

$m = 6$

1	2	3	4	5	6
3	1	5	2	6	4
2	4	1	6	3	5
5	3	6	1	4	2
4	6	2	5	1	3
6	5	4	3	2	1

$m = 8$

1	2	3	4	5	6	7	8
2	7	1	8	3	5	4	6
3	1	5	7	6	8	2	4
4	8	7	5	2	1	6	3
5	3	6	2	8	4	1	7
6	5	8	1	4	7	3	2
7	4	2	6	1	3	8	5
8	6	4	3	7	2	5	1

Appendix 2. An Example of the Derivation of the Maximum Likelihood Estimator for ρ. (See Section 5.4)

Consider the 5 by 5 Latin square:

1	2	3	4	5
2	3	4	5	1
3	4	5	1	2
4	5	1	2	3
5	1	2	3	4

$$\underset{25\times 25}{B^{-1}} = (I-\hat{\rho}N)^{-1} = \left[\begin{array}{c|c|c|c|c} R & S & T & T & S \\ \hline S & R & S & T & T \\ \hline T & S & R & S & T \\ \hline T & T & S & R & S \\ \hline S & T & T & S & R \end{array}\right]$$

where

$$R = \begin{bmatrix} a & b & c & c & b \\ b & a & b & c & c \\ c & b & a & b & c \\ c & c & b & a & b \\ b & c & c & b & a \end{bmatrix}$$

$$S = \begin{bmatrix} b & d & e & e & d \\ d & b & d & e & e \\ e & d & b & d & e \\ e & e & d & b & d \\ d & e & e & d & b \end{bmatrix}$$

$$T = \begin{bmatrix} c & e & f & f & e \\ e & c & e & f & f \\ f & e & c & e & f \\ f & f & e & c & e \\ e & f & f & e & c \end{bmatrix}$$

The 25 equations $Bb_1 = (1,0,0,\ldots,0)'$ now reduce to $q = 6$ equations $\underset{6\times 6}{B^*}\underset{6\times 6}{b^*} = (1,0,0,0,0,0)'$ where

$$\underset{6\times 6}{B^*} = \begin{bmatrix} 1 & -4\hat{\rho} & 0 & 0 & 0 & 0 \\ -\hat{\rho} & 1 & -\hat{\rho} & -\hat{\rho} & 0 & 0 \\ 0 & -\hat{\rho} & 1-\hat{\rho} & 0 & -2\hat{\rho} & 0 \\ 0 & -2\hat{\rho} & 0 & 1 & -2\hat{\rho} & 0 \\ 0 & 0 & -\hat{\rho} & -\hat{\rho} & 1-\hat{\rho} & -\hat{\rho} \\ 0 & 0 & 0 & 0 & -2\hat{\rho} & 1-2\hat{\rho} \end{bmatrix}$$

and $b^* = (a,b,c,d,e,f)'$. We need only to solve for the portion of the solution involving element b of b^*.

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Field trials when observations are correlated with those in neighboring or nearby plots in one and two dimensions are analyzed using simultaneous autoregressive models. The relationships between the maximum likelihood solutions and the corresponding well-known Papadakis estimators are clarified and it is shown that the maximum likelihood solutions are, for specific types of designs, easier to obtain directly then by iterating on the Papadakis estimator as has been suggested. A simulation study compares the different models and methods for one and two dimensions.

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