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On the Use of Spatial Information in the Analysis of Field Experiments*

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I feel very honoured for being chosen as Session's President and invited to deliver technical address during 48th session of the Indian Society of Agricultural Statistics. I am very grateful to the society for giving me this opportunity. My association with the society started some thirty three years ago when I was a student in the Indian Agricultural Statistics Research Institute (IASRI), and since then I have been associated with Agricultural Statistics, more or less continuously. The subject which I have chosen has developed in the last twenty years and is concerned with the analysis of field experiments. This is one of the main areas of interest to the members of the Society. Going through the back issues of the Society Journal I could find only one paper devoted to this topic and that too in the latest issue. Through this address, I would like to draw attention of the members of the Society and of Agricultural Statisticians to involve more deeply in studying the properties of new methods of analysis of field experiments which are reported to be 100 to 200 percent more efficient than the conventional methods of analysis.

Introduction

Sir R.A. Fisher introduced three fundamental principles of design and analysis of experiments viz. randomization, replication and local control. Local control reduces the error thus making estimates more precise; replicatious enable us to estimate the error and increase precision of the estimates; randomization neutralises the effect of spatial correlation thus giving unbiased estimates of treatment contrasts and validating the analysis of variance. The main advantages of the above are that the analysis is easy and is not based on any model. Time to time it has been felt that when blocks are too large there may be a considerable variability in fertility levels within each block. Yates introduced incomplete blocks and lattice designs so as to reduce the block size thus increasing the precision. Usually fertility levels are slowly changing over space and thus they are likely to be highly correlated among neighbouring plots. In

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early stages of field trials the spatial information had been used by introducing check plot i.e., having a standard treatment regularly placed in the field trials, thus making it possible to adjust treatment yields through the yields of check plots. This technique is still in use in many places in the selection stages of variety trials. If the fertility trend is present then location of the plot can also be used as a covariate to adjust such trends. Systematic designs (Cox, [7]) were also considered to eliminate the effect of such trends.

Classical method of analysis completely ignores the information regarding the relative position of each treatment in the block. In a very early attempt Papadakis [27] adjusted the plot values by the analysis of covariance when covariates were residuals from neighbouring plots. In the subsequent sections I shall describe some important methods for using spatial information, and about the experience of using these methods in analysing data from field experiments.

Papadakis Method

Usually the fertility levels of neighbouring plots are highly correlated. This information is ignored by the usual analysis of variance and effect of such correlations is neutralised by randomization. Papadakis [27], using residuals from the neighbouring plots as covariate, adjusted estimates of treatment contrasts and obtained adjusted standard errors. He reported substantial reduction in error variance. Subsequently Pearce and Moore [32] and Pearce [31] reported substantial gain in efficiencies due to the use of Papadakis method. As the covariate used itself is a random variable, and thus violating the assumptions of analysis of covariance (ANCOVA), the method was not much discussed in the literature till 1969. However, after introduction of spatial models by Whittle [35], Besag [3] and others, it was possible to base Papadakis method on sound theoretical footings. This was done by Atkinson [1] and Bartlett [2], and then followed by many others. Once a theoretical model has been developed for Papadakis method it has been possible to compare the efficiency of this method with the conventional method of analysis for different values of parameters of the model. It has also been possible to fit theoretical models to the data by using efficient methods, such as generalised least squares (GLS) and the maximum likelihood (ML), and compare efficiencies. In some cases it has also been possible to compare efficiencies of different methods from uniformity trial data.

Papadakis Method and Auto-Regressive Error Structure

Atkinson [1] showed that the properties of Papadakis estimator are very close to those of ML estimators when applied to plots arranged in a row and underlying error structure is the first order auto-regressive, AR(1), process. When observations are independent then using this method does not lead to a

great increase in variance of the estimators, whereas failure to take into account of the error structure leads to a considerable loss of precision.

Papadakis method does not assume any error structure. However, Bartlett [2] considered the model as,

$$\mathbf{Y} = \mathbf{X}\ \theta + \epsilon\,, \tag{1}$$

where $\mathbf{Y}$ is the observation vector, $\mathbf{X}$ the design matrix with r-fold replication, θ a $(p \times 1)$ vector of treatment parameters and ϵ is the error vector with zero mean and variance $k\ \mathbf{B}^{-1}$, where $\mathbf{B} = \mathbf{I} - \beta\,\mathbf{N}$ and $N_{rs} = 1$ if r and s are nearest neighbours (NN) and zero otherwise. This variance structure arises from the conditional version of the model,

$$E(Y_r \mid \text{all other plot values}) = \beta\,(Y_{r-1} + Y_{r+1}) \tag{2}$$

$$V(Y_r \mid \text{all other values}) = k\,.$$

Under the assumption of normality of ϵ_r the ML estimator of θ is,

$$\theta^{ML} = (\mathbf{X}'\mathbf{B}\mathbf{X})^{-1}\,\mathbf{X}'\,\mathbf{B}\mathbf{Y}\,, \tag{3}$$

with variance $k(\mathbf{X}'\,\mathbf{B}\mathbf{X})^{-1}$. Equation (3) can be written as

$$\theta^{ML} = \left[\mathbf{X}'\,\mathbf{Y} - \beta\,\mathbf{X}'\,\mathbf{N}\,(\mathbf{Y} - \mathbf{X}\,\theta^{ML})\right] / r, \tag{4}$$

where r is the number of replications of each treatment. Let $\theta^{0} = \mathbf{X}'\ \mathbf{Y}/r$ be the ordinary least squares (OLS) estimator of θ. Then Papadakis estimator is given by

$$\theta^{P} = \left[\mathbf{X}'\,\mathbf{Y} - \alpha_1\,\mathbf{X}'\,\mathbf{N}\,(\mathbf{Y} - \mathbf{X}\,\theta^{o})\right],$$

where α_1 is the crude approximation of β. Therefore, Papadakis method can be considered as a first approximation towards obtaining the ML estimator based on the spatial model (2). In ML method β is to be estimated by numerical procedures., while Papadakis only considered the first approximation based on ANCOVA. Bartlett also generalised the model to two dimensions and studied the efficiencies for different values of the parameters. He concluded that the gain is substantial when number of treatments is large as the blocks are not effective to remove the heterogeneity within block. Iteration of the analysis, i.e. ML estimate, generally increases the efficiency. Kempton and Howes [18], based on the extensive data analysis, reported substantial gain by Papadakis analysis over simple randomized block analysis, and it was almost as efficient as row-column lattice squares.

Error in Variable Model

Bartlett's [2] paper generated considerable interest in the papadakis estimator and other models were proposed to take into account the correlation among neighbouring plots. Besag [4] proposed error in variable model,

$$\mathbf{Y} = \mathbf{X}\theta + \eta + \xi, \tag{5}$$

where η reflects local fluctuation in soil fertility and ξ corresponds to intrinsic plot-to-plot variability, independent of η. ML estimates can be employed for different assumptions about η. Besag and Kempton [5] assumed that the first differences $\eta_i - \eta_{i+1}$ are uncorrelated random variables with zero mean and constant variance. The components of ξ have zero mean and constant variance and are uncorrelated among themselves and with the components of η. Parameters can be estimated by ML method based on the differences $Y_i - Y_{i+1}$ of plot yields on ith and (i+1)th position. The greatest advantage of this model is that it avoids estimation of β and gives good results in many analyses.

Wilkinson et al [36] considered a similar model as (5), assuming η to represent a smooth trend in local fertility. Here the assumption of smoothness of trend means that the variation in residual trend components, after local linear detrending, $\eta'_i = \eta_i - \bar{\eta}_{Ni}$ where $\bar{\eta}_{Ni}$ denotes the average trend components of the neighbouring plots, is small relative to the local errors. Based on this model they suggested a moving block analogue of the classical fixed block analysis. They have also described the results of extensive Monte-Carlo randomization studies of the Papadakis method of uniformity trial data. Their results showed that while a non-iterated Papadakis analysis is reasonably valid under randomization, iteration leads to an upward bias in F-ratio. They suggested use of designs which are partially NN balanced. Their method of analysis removes the defects of Papadakis method thus giving approximately unbiased results. However, in the discussion of the paper, it is pointed out that there is no difference between this analysis and Papadakis iterated analysis, except for the estimation of the coefficient β.

Patterson [28] assumed that components of η in (5) follow an AR(1) correlation structure and called it exponential variance (EV) model. Patterson and Hunter [29] fitted EV model to 166 variety trials and showed that variance of pairwise difference between yields of two plots separated by d – 1 other plots is of the form,

$$2\sigma^2(1 - \lambda\rho^d),$$

where $\sigma^2 = 0.21\,(t/ha)^2$, $\lambda = 0.71$, $\rho = 0.94$.

Williams [38] proposed a linear variance (LV) model which is equivalent

to the first difference model of Besag and Kempton [5] in which,

$$\text{Var}(Y_i - Y_j) = k|i-j| + 2k', \quad i \neq j,$$

where Y_i and Y_j are the yields of plots $|i-j|$ distance apart. Analysing 166 trials data of Patterson and Hunter [29], by using WLS method and LV error structure, he obtained an average efficiency of 179% in comparison to RBD analysis, where measure of efficiency is the ratio of error variances. Average efficiency of incomplete block analysis in comparison to RBD analysis was 143%. This shows that the analysis based on the first difference is about 20 per cent more efficient than that based on incomplete blocks.

Gleeson and Cullis [15] considered a generalization of the first difference model of Besag and Kempton [5] in which trend effects η of (5) were modelled by ARIMA process. Cullis and Gleeson [9] in a study of over 1,000 variety trials demonstrated that use of their method resulted in a reduction of 42% in variances of varietal yield differences compared with RBD analysis, whereas incomplete block analysis resulted in a reduction of 33%.

Cullis and Gleeson [10] carried out two dimensional analysis of data from 24 uniformity trials on different crops. The mean efficiency of block analysis in comparison to completely randomized analysis (without blocks) were : rows 113%; columns 130%; rows and columns 158%. The two-dimensional neighbour analysis was, however, much more effective and gave a mean efficiency of 278%.

Katyal [17] analysed uniformity trial data on wheat for different plot sizes and shapes. He also considered analysis of different designs such as RBD and Incomplete blocks by Papadakis and Wilkinson methods. With 20 plots per block of RBD the coefficient of variation, C.V., of Papadakis method was 50% and that of Wilkinson method was 26% in comparison to conventional RBD analysis. However, when compared to incomplete blocks of size five, the C.V. of Papadakis method was 81% and that of Wilkinson method was 43%.

Another approach based on random field has been described by Zimmerman and Harville [39]. A. good description of these models has been given in a book by Cressie [8].

Comparison of Different Methods Under Randomization Framework

Most of the spatial methods proposed, except that of Papadakis, are model based and use ML or GLS method for estimation of parameters. The estimates of variances are based on asymptotic expressions. Now for an experimenter it is important to know to what extent these asymptotic variances reflect the accuracy of experiment in hand, under randomization. This was discussed by Besag in Wilkinson et al [36] and also reported in Besag and Kempton [5].

Some more results on these lines are given by Zimmerman and Harville [39]. To answer this question Besag and Kempton [5] imposed 20 randomizations of RBD on five sets of uniformity trial (UT) data. They then calculated average empirical variance (Emp) and average predicated variance (Pre) of all pair-wise treatment differences, and averaged them over all 20 randomizations.

$$\text{Emp} = \sum_{\substack{k=1 \\ k \neq l}}^{p} \sum_{l=1}^{p} (\hat{\tau}_k - \hat{\tau}_l)^2 / p(p-1)$$

$$\text{Pre} = \sum_{\substack{k=1 \\ k \neq l}}^{p} \sum_{l=1}^{p} \text{Estimated variance } (\hat{\tau}_k - \hat{\tau}_l)/p(p-1).$$

In the above estimate treatment effect $\hat{\tau}_k$ and variance-$\left(\hat{\tau}_k - \hat{\tau}_l\right)$ are calculated by using formulae for respective methods. In UT data only one treatment is used and thus treatment differences are zero. A small value of Emp reflects high accuracy. In randomization framework Emp and Pre should be approximately equal over all randomization and hence should be approximately equal for a sample of 20 randomizations. The important methods, included for this study, were RBD, Papadakis, iterated Papadakis, Wilkinson's and first difference. For RBD Emp and Pre were almost same as expected. On the average Emp for Papadakis method was about half of RBD and there was a close agreement between Emp and Pre. Further iteration of Papadakis generally reduced Emp to one-third of RBD but Pre was usually considerably smaller than Emp showing an over optimistic estimate of accuracy. For Wilkinson's and first difference methods the Emp were very close to that of iterated Papadakis method but there was a close agreement between Emp and Pre, showing validity of estimates of error under randomization for Wilkinson's and first difference methods. Thus it can be concluded that any method for fertility adjustment will lead to substantial increase in precision over RBD analysis. For a proper choice of method one can also obtain fairly accurate estimates of standard error under randomization.

Model for Competition Effects

In the preceding sections use of correlation structure among the neighbouring plots for estimating the contrasts among treatments efficiently has been discussed. However, the neighbouring responses may compete with each other and it may be more appropriate to model them as,

$$\mathbf{Y} = \mathbf{X}\theta + \beta \mathbf{N}\mathbf{Y} + \mathbf{Z}, \tag{6}$$

where θ may contain block and treatment parameters, **N** the neighbourhood

matrix and in a row arrangement it may have off-diagonal elements (i–1, i+1) as 1/2, and β being the competition coefficient. It may be of interest to make inference about β and if β is non-zero then estimate parameter θ after taking into account for β . The model can be written as,

$$\mathbf{Y} = \mathbf{G}^{-1}\mathbf{X}\theta + \mathbf{G}^{-1}\mathbf{Z}$$

where $\mathbf{G} = (\mathbf{I} - \beta\mathbf{N})$ and the ML method can be used to make inference about parameters. For further details see Besag and Kempton [5].

Such competition models have been used for the analysis of inter- crop experiments. The yield of crop has been modelled taking into account arrangements of rows of different crops and proportion of each crop. Once the model is fitted it is possible to find the optimum proportion and row arrangement (Reddy, [33]).

Models for Interference from Neighbouring Treatments

In some situations the yield may also be affected by treatments applied to the neighbouring plots. It may happen with treatments like irrigation or spraying. In fertiliser experiments treatments may leach to the plants of neighbouring plots. Pearce [30] described such model as,

$$\mathbf{Y} = \mathbf{B}\eta + \mathbf{T}\tau + \mathbf{R}\mathbf{T}\phi + \mathbf{Z}, \qquad (7)$$

where η is the block effect with incidence matrix $\mathbf{B}$, τ is direct treatment effect with incidence matrix $\mathbf{T}$, and ϕ is remote treatment effect with $\mathbf{R}$ as neighbour incidence matrix. No special problem arises in estimation of the parameters of this model as it is linear in parameters and if the errors can be assumed to be independent and have constant variance then the OLS method can be used. However, Draper and Guttman [11] use a special case where $\phi_k = \lambda\tau_k$, λ being the coefficient of interference. Thus,

$$\mathbf{Y} = \mathbf{B}\eta + \mathbf{H}\tau + \mathbf{Z},$$

where $\mathbf{H} = (\mathbf{I} + \lambda\mathbf{R})\mathbf{T}$. Now the model is non-linear in τ and λ. OLS can be carried out iteratively to estimate parameters. Significance of ϕ and λ can be tested and adjusted estimates of treatment parameters τ can be obtained.

Experimental Designs for Spatially Correlated Observations

In the conventional analysis of data from field experiments under randomization the relative position of each treatment within block is ignored and the analysis depends upon the information of whether or not treatments occur together in the same block. However, under the spatially correlated structure and GLS estimation procedure, the relative position of treatment in

a block is important and is used in the analysis. Thus it may be useful to investigate optimum designs under different error structures and calculate gain in efficiency over RBD. The important papers in this area are : Williams [37], Kiefer [19], Kiefer and Wynn [21], Cheng [6], Martin [24][25], Gill and Shukla [13][14], Kunert [22][23], Russell and Eccleston [34], Morgan and Chakravarti [26] and Grondona and Cressie [16].

Optimality criterion used here is that of universal optimality, proposed by Kiefer [20], which uses the information matrix of $\hat{\tau}$, denoted by $\mathbf{C}(\hat{\tau}, \mathbf{X}, \Sigma)$, where $\hat{\tau}$ is the least squares estimates of treatment parameters τ, $\mathbf{X}$ being the design matrix and Σ being the variance-covariance matrix of the errors. Let α be the vector of all linearly independent estimable functions of τ, then universal optimality minimises (i) generalised variance of $\hat{\alpha}$ (D-optimality), (ii) average variance of components of $\hat{\alpha}$ (A–optimality), (iii) maximum variance of components of $\hat{\alpha}$ (E-optimality). Sufficient conditions for universal optimality, as given by Kiefer [20], are (i) $\mathbf{C}(\hat{\tau}, \mathbf{X}, \Sigma)$ is completely symmetric, and (ii) trace $\mathbf{C}(\hat{\tau}, \mathbf{X}, \Sigma)$ is maximum. Williams [37] obtained designs for error structure of AR(1) and AR(2) processes, using ML estimates and criterion being simplicity in analysis. For AR(1) process the designs are balanced for nearest neighbourhood, NN, i.e. each treatment occurs with every other treatment as NN equal number of times, and for AR(2) process the designs are balanced for second neighbour in addition to being balanced for NN. Kiefer [19] showed that such designs are asymptotically optimal for AR(1) and AR(2) processes, respectively. Kiefer and Wynn [21] obtained designs for MA(1) error structure.

Gill and Shukla [13] studied the efficiency of NN balanced block design (NNBD) for AR(1) error structure. It has been found that NNBD are approximately optimum under AR(1) and MA(1) error structures. In incomplete block designs they should be BIBD in addition to NNBD.

The efficiency of the optimum designs with GLS analysis over conventional RBD with OLS analysis has been studied, by comparing the average variance of elementary treatment contrasts. The reduction in variance by GLS analysis is substantial in comparison to OLS analysis, particularly when correlation is high and block size is large. However, this should be noted here that in such a situation incomplete block will normally be used and efficiency of GLS analysis will be modest in comparison to OLS analysis. This result has been confirmed by extensive simulation studies.

It may also be of considerable interest to compare the efficiency of optimum designs with RBD when GLS analysis is used in both the cases with AR(1) error structure. Simulation results based on uniformity trial data showed that there is a considerable advantage of using NNBD as far as generalised variance

of treatment contrasts (D-optimality) and balance of variance of treatment contrasts (E-optimality) are concerned. However, average variance of treatment contrasts (A-optimality) is not much affected by the choice of designs. This result is consistent with the theoretical results. For more results on comparison of efficiencies see Grondona and Cressie [16].

Optimum designs have also been obtained in case of two-dimensions (row-column) by Gill and Shukla [14] and Martin [25]. For optimum designs in other correlated situations see Gill [12].

Main features of optimal designs are NN balance and balance for number of times treatment occurs in the beginning (or end) of the block. Number of blocks required for satisfying these constraints is excessively high and in some cases such designs do not exist at all.

SUMMARY

In 1978 Bartlett, after studying the theoretical properties of Papadakis method, concluded that this technique is available for randomized blocks as a possible ancillary device for improving the accuracy of treatment comparisons. Since then many other model based methods, to remove the fertility trend in one or two dimensions, have been proposed. The usefulness of these methods have been demonstrated by analysing vast amount of experimental and uniformity trial data, and by Monte-Carlo studies. Gain in efficiencies of order of 100% have been reported by using Papadakis method over randomized block analysis. By using other model based methods gain in efficiencies of 100% to 200% have been reported. Even when efficient incomplete block designs were used instead of randomized blocks gain in efficiency by using spatial analysis over incomplete block analysis was of the order of 30%. Of course, actual gain will depend upon plot, block sizes and shapes, actual correlation structure and model used. From all these studies it is almost certain that spatial analysis of data will result in modest to substantial gain in efficiencies. Of course many problems still remain to be resolved such as the choice of model, method of estimation of parameters and desirability of adopting NN balanced designs. Main advantages of randomized block analysis is its simplicity and robustness. But, I think, that there is enough evidence available now to justify the use of new techniques, along with the conventional method of analysis, atleast on the exploratory basis, so as to examine in individual cases how much can be gained or lost on efficiency and robustness. This has become very important today when very fast computational power is available very cheaply almost everywhere.

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