

## **A Comparison of Estimation Methods for Field Trial Data in the Presence of Spatial Trends**

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(Received : August, 1996)

### **SUMMARY**

In this paper we compare a number of different methods of estimating treatment effects from field trial data collected sequentially from experimental units arranged in strips which contain spatial trends. The methods of analysis compared are completely randomized design analysis, incomplete block design analysis based on blocks of differing sizes, two forms of nearest neighbor analysis, and methods of estimating treatment effects based on models having polynomial approximations for trend of varying degrees.

*Keywords* : Incomplete blocks, Nearest neighbor analysis, Polynomial approximation.

### *1. Introduction*

The presence of strong local gradients in field trial experiments is well documented, e.g., see Papadakis [11], Bartlett [1] and Wilkinson, *et al* [15] for references concerning this problem. For example, Weibe [14] conducted a uniformity field trial at the agricultural research experiment station located in Aberdeen, Idaho. In this uniformity trial, Federation wheat was planted in each of 1500 plots arranged in 12 series of 125 plots each. It was observed in each of the 12 series that plot yields varied substantially but seemed to vary systematically around a relatively "smooth" trend. In a true field trial experiment, trends such as those observed in the Weibe uniformity trial can cause great difficulty in trying to estimate treatment effects, particularly when the differences among treatments are small compared to the magnitude of the trend.

Traditionally, blocking has been used by experimenters as a means to account for trends such as present in the data described above. However, even the use of relatively small blocks in fields may only be partially successful in accounting for trend. This may occur because the trend is dependent on

environmental factors and thus not be predictable prior to the experiment or there may be significant trends even within small blocks.

As an alternative to accounting for trends by blocking in a field trial experiment, different methods of analyzing data in the presence of trends have been proposed. One set of methods which have received a good deal of attention in the literature over the years are called nearest neighbor (NN) methods. These forms of analysis are related closely to techniques which have been derived for analyzing nonstationary time series data. In particular, NN methods of analysis essentially consist of applying a differencing operator to an ordered set of field trial data. The purpose of differencing is to reduce the influence that "smooth" spatial trends may have on the observed field trial data so that treatment effects may be more efficiently estimated.

In this paper we compare several different methods of estimating treatment effects in the presence of trend via simulation studies. In particular methods of estimating treatment effects based on blocking are compared to several types of NN analysis as well as methods of analysis which estimate treatment effects based on models that include polynomial approximations for trend.

## 2. Notation and Background

All methods considered in this paper for analyzing data obtained from a field trial experiment are based on the mixed linear model whose general form is

$$Y = X\beta + U\theta + \epsilon \quad (2.1)$$

where  $Y$  is a vector of observations,  $\beta$  is a vector of fixed parameter effects,  $X$  is a matrix of known constants, determined from the experimental design for the fixed effects,  $\theta$  is a vector of random effects,  $U$  is a matrix of known constants determined from the experimental design for random effects and  $\epsilon$  is the usual random error or residual term. We assume throughout that

$$E\begin{pmatrix} \theta \\ \epsilon \end{pmatrix} = \begin{bmatrix} 0 \\ 0 \end{bmatrix} \quad \text{and} \quad \text{Var}\begin{pmatrix} \theta \\ \epsilon \end{pmatrix} = \begin{bmatrix} W & 0 \\ 0 & V \end{bmatrix} \quad (2.2)$$

where  $W = \text{Var}(\theta)$  and  $V = \text{Var}(\epsilon)$ . So  $E(Y) = X\beta$  and  $\text{Var}(Y) = UWU' + V$ . We assume there is interest in estimating both the random and the fixed effects in the model when both are present.

For fixed effects, attention is usually focussed on the estimation of estimable functions of the form  $l'\beta$ . For the model given in (2.1) the general least square (GLS) solution for  $\beta$  is

$$\hat{\beta} = (X' [\text{Var}(Y)]^{-1} X)^{-1} X' [\text{Var}(Y)]^{-1} Y \quad (2.3)$$

where  $A^{-}$  denotes a generalized inverse for a given matrix  $A$ . So  $l' \hat{\beta}$  is the best linear unbiased estimator (BLUE) for  $l' \beta$ . We note that when  $\text{Var}(Y) = \sigma^2 I_n$ , the expression given in (2.3) reduces to the usual ordinary least squares estimator for  $\beta$ .

For models with random effects, it is often of interest to estimate various linear combinations of the variance components. A number of methods are available for estimating variance components. Two of the most widely used and when appropriate the ones used in this paper are maximum likelihood (ML) and the restricted maximum likelihood (REML) procedures described in Harville [7].

Instead of estimating the fixed effects and variance components of a mixed model separately, in recent years there has been interest in estimating predictable functions of the form  $l' \beta + m' \theta$  where  $l' \beta$  is an estimable function. Such predictable functions can be estimated from the mixed model generalization of (2.3) derived by Henderson [8] and Harville [6] are given by

$$\begin{bmatrix} \hat{\beta} \\ \hat{\theta} \end{bmatrix} = \begin{bmatrix} X' W^{-1} X & X' V^{-1} U \\ U' V^{-1} X & U' V^{-1} U + W^{-1} \end{bmatrix} \begin{bmatrix} X' V^{-1} Y \\ U' V^{-1} Y \end{bmatrix} \quad (2.4)$$

Henderson calls the estimator  $l' \hat{\beta} + m' \hat{\theta}$  derived from these equations for  $l' \beta + m' \theta$  the best linear unbiased predictor (BLUP) for  $l' \beta + m' \theta$ . We shall adopt this terminology in this paper.

In more recent years, it has been suggested that in certain types of field trial experiments where the number of treatments is fairly large (more than 20, say), it may be more efficient to assume the treatment effects are random and to estimate them using BLUP analysis. This latter approach is contrary to the traditional assumption in field experiments that treatment effects are fixed and are typically estimated by obtaining BLUE's. It has been found that in experiments which are unbalanced and the distribution of treatment effects fairly symmetric, BLUP estimators for treatment effects can be more efficient than the traditional BLUE's. For more discussion of this topic, the reader is referred to Copas [3].

### 3. NN Analysis Methods

As mentioned in the introduction, in field trial experiments, it is not uncommon for spatial trends to exist. The presence of such trends can cause substantial difficulty in trying to estimate the true effects of the treatments being

investigated. This is particularly true when the magnitude of the trends are large when compared to the magnitude of the differences in the effects of the treatments being studied.

To handle situations such as this, several different methods of NN analysis have been proposed for usage. Papadakis [11] appears to have been the first to propose NN analysis as a means of analyzing field trial data in the presence of trends. But in recent years, other forms of NN analysis have been proposed, e.g., see Bartlett [1], Wilkinson *et al* [15], Besag and Kempton [2] and Gleeson and Cullis [5] to name several. However, all of the different forms of NN analysis proposed share the same general approach. Following Stroup and Mulitze [13], let

$$Y = X\beta + S + \epsilon \quad (3.1)$$

where  $Y$  is an  $n \times 1$  vector of observations,  $X$  is a matrix of constants describing the design for fixed effects, including the treatment effects,  $\beta$  is the vector of fixed effects,  $S$  is a "smooth" trend vector, and  $\epsilon$  is the vector of random error or residual terms. We assume  $\text{Var}(\epsilon) = \sigma^2 I_n$ . We also assume throughout that there is no interaction between the trend and the fixed effects.

The basic idea behind NN analysis is to apply a differencing operator to each side of model (3.1) to reduce the magnitude of the effects of the "smooth" trend. To demonstrate this process with a simple example, suppose we assume that  $t$  treatments under study are being applied sequentially to experimental units occurring in a single strip. For this example the vector  $\beta$  in (3.1) can be replaced by the  $t \times 1$  vector  $t$  of treatment effects. If we let  $Y' = (y_1, \dots, y_n)$  denote the ordered vector of observations obtained, then NN analysis involves taking differences  $d_1 = y_1 - y_2, d_2 = y_2 - y_3, \dots, d_{n-1} = y_{n-1} - y_n$  between successive or adjacent pairs of observations in  $Y$  and analyzing the differenced observations. This process is equivalent to applying the differencing matrix

$$D = \begin{bmatrix} 1 & -1 & 0 & 0 & \dots & 0 \\ 0 & 1 & -1 & 0 & \dots & 0 \\ \vdots & \vdots & \vdots & \vdots & & \vdots \\ 0 & 0 & 0 & 0 & \dots & 1 & -1 \end{bmatrix}$$

to both sides of model (3.1) to obtain

$$d = DY = DXt + DS + D\epsilon = Zt + (F + \delta) \quad (3.2)$$

where  $Z = DX, F = DS$ , and  $\delta = D\epsilon$ . If differencing has been successful, then the effects of the smooth trend will have been reduced and  $F = DS$  can

essentially be considered as part of a new residual vector for the vector  $\mathbf{d}$  of differenced observations. The amount of variability contributed to the residual vector  $F + \delta$  by  $F$  is often approximated by  $\text{Var}(F) = \sigma_f^2 I_{n-1}$ ; hence  $\text{Var}(\mathbf{d}) = \text{Var}(F) + \text{Var}(\delta) = \sigma_f^2 I_{n-1} + \sigma^2 DD'$ .

If needed, to try and further reduce the effects of trend in the model, one could again take differences between the successive components of  $\mathbf{d}$ . However, experience and simulation studies have shown that in field trial experiments second and higher order differencing does not generally reduce the effects of trend and in fact usually results in a loss of efficiency for estimating treatment effects. The reader is referred to Wilkinson, *et al* [15] for a further discussion of the effects of higher order differencing on trend and efficiency. Based on first differences, the GLS solution for the treatment effects is

$$\hat{\mathbf{t}} = (\mathbf{Z}' [\text{Var}(\mathbf{d})]^{-1} \mathbf{Z})^{-1} \mathbf{Z}' [\text{Var}(\mathbf{d})]^{-1} \mathbf{d} \quad (3.3)$$

The above analysis is based on the assumption that the treatment effects are fixed and hence  $l' \hat{\mathbf{t}}$  is the BLUE for any estimable function of the form  $l' \mathbf{t}$ .

As mentioned previously, an alternative method to obtaining estimates for treatment effects in a field trial experiment can be used if it is assumed that the treatment effects are random. In particular, BLUP estimates for the treatment effects can be obtained. In addition, one can find NN analysis BLUP's (NNABLUP's) for treatment effects when trend is present as described in Stroup and Multize [13]. In the example described above, we assume  $\mathbf{t}$  is a vector of random treatment effects, such that  $E(\mathbf{t}) = 0$  and  $\text{Var}(\mathbf{t}) = G$ . Typically,  $G = \sigma_t^2 I_t$ . Thus, for the example, a nearest neighbor mixed model is

$$Y = U\mathbf{t} + S + \epsilon \quad (3.4)$$

where  $U$  replaces  $X$  in (3.1). Applying the difference matrix  $D$  to both sides of (3.4) gives

$$\mathbf{d} = D\mathbf{Y} = DU\mathbf{t} + DS + D\epsilon = \mathbf{Z}\mathbf{t} + F + \delta \quad (3.5)$$

where  $\mathbf{Z} = DU$ . Once again, the residual vector for the differenced observations consists of  $F + \delta$  and the variance of this residual vector is  $R = \sigma_f^2 I_n + \sigma^2 DD'$ . The BLUP for  $\mathbf{t}$  can now be obtained from (2.4) to be

$$\hat{\mathbf{t}} = (\mathbf{Z}' R^{-1} \mathbf{Z} + W^{-1})^{-1} \mathbf{Z}' R^{-1} \mathbf{d} \quad (3.6)$$

The covariance matrices  $W$  and  $R$  depend on the variance components  $\sigma_t^2$ ,  $\sigma_f^2$  and  $\sigma^2$  for treatment, "smooth" trend and random error, respectively. These variance components can be estimated using iterative maximum likelihood methods such as described in Harville [7] and demonstrated for examples such as described above in Stroup and Mulitze [13].

#### 4. The Simulation Study

The primary purpose of this study was to compare a number of different methods for analyzing field trial data in the presence of trend. The methods of analysis compared were completely randomized design analysis, incomplete intrablock analysis using blocks of size 3, 4 and 6, NNBLUE analysis, NNBLUP analysis and the estimation of treatment effects using models of the form

$$Y_i = t_p + \beta_1 i + \beta_2 i^2 + \dots + \beta_p i^p + \epsilon_i, i = 1, \dots, n \quad (4.1)$$

where  $p$  ranges in value from one to three. In (4.1),  $t_p$  is the effect of treatment  $p$  which is applied to the  $i$ th experimental unit in a sequence of  $n$  experimental units and the remaining terms in the model represent a polynomial approximation for the trend of degree  $p$ ,  $p = 1, 2, 3$ . It is assumed throughout that the plots are equally spaced and the polynomial approximation is a function of the order in which the observations are obtained.

To compare these methods of estimating treatment effects in the presence of trend various sequences of 36 observations were selected from Weibe uniformity trial mentioned above. These sequence of 36 observations were used to simulate typical trend which might occur in a field. Twelve random treatment effects were generated from a normal distribution having a mean of zero and a standard deviation of 60. This particular distribution was selected because of its symmetry (which seems to favour BLUP analysis, e.g., Copas [3] and because the magnitude in the differences between the treatment effects generated tended to be smaller than the magnitude of the variation in the various sequences of 36 observations caused by trend thus causing estimates for treatment effects to be influenced by the trend. Each of the twelve generated treatment effects were then added to three of the observations in a given sequence according to each of two experimental designs. Both designs were constructed so that they could be viewed as block designs with blocks of differing sizes and also have additional desirable properties. In particular the first design, denoted by D1, was constructed so that the sum and sum of squares of the position numbers of the experimental units (1 through 36) to which each treatment was assigned were as equal as possible. This assignment of treatments to experimental units essentially had the effect of making the estimates for differences in treatment

effects obtained from the design as close to being orthogonal to the linear and quadratic polynomial terms in model (4.1) as possible. Such designs are sometimes called *nearly linear or quadratic trend free designs*. The second design, denoted by D2, was constructed so that when considering it as a block design with 9 blocks of size 4 (each set of 4 successive observations was a block), it was the dual of a balanced incomplete block design having 12 blocks of size 3. Such an incomplete block design is optimal for estimating treatment effects under most optimality criteria, e.g., see Shah and Sinha [12]. The order of treatments in blocks for D2 was also arranged so that no treatment occurred next to any other treatment in the sequence more than once. Designs having this latter property are sometimes called *nearly neighbor balanced* and have been shown to be efficient when NN methods of analysis are used for estimating treatment effects, e.g., see Wilkinson, *et al* [15]. Each method of analysis described above was then used to estimate the treatment effects. When implementing BLUP analysis, to cut down on the amount of computation required, the true value of  $\sigma_t^2$  was assumed known and the value of  $\sigma_f^2$  was estimated for each sequence of 36 observations selected from the original Weibe [14] data. This latter estimate was obtained by differencing successively the original observations in each sequence and then using the variance of these differenced observations as the estimate of  $\sigma_f^2$ . Also, in the initial simulations, estimation procedure for treatment effects were compared for  $\sigma^2 > 0$  and  $\sigma^2 = 0$ . In all cases, all measures of goodness for estimating treatment effects described below were essentially the same for  $\sigma^2 > 0$  and  $\sigma^2 = 0$ . These results are analogous to those found in Stroup and Muiltze [13]. Hence, because the inclusion of  $\sigma^2 > 0$  in the model substantially increases the computation required for estimating treatment effects and because it contributes nothing of value to the estimation process, only models with  $\sigma^2 = 0$  were subsequently considered and only the results for  $R = \sigma_f^2 I_{n-1}$  are presented here.

For each sequence-design-method of analysis combination, three measures of analysis efficiency were computed. These were the mean squared deviations between the true values of the spanning set of estimable treatment differences  $t_i - t_1, i = 2, \dots, 12$  and their estimated value  $\hat{t}_i - \hat{t}_1$  derived from the data, the correlation between the actual and the estimated treatment effects and the rank correlation between the true and estimated treatment effects. The above procedure was carried out for each 20 different sequences of 36 observations derived from the Weibe data and for each such sequence-design combination, 500 different set of 12 treatment effects were generated. The averages for the mean squared deviations and correlation coefficients were then computed for

each of the 40 different design-sequence combinations. SAS IML was used for all computations. Results typical of those obtained in the study are given in Tables 1 and 2 in the Appendix. Plots of the various sequences of 36 observations selected from the original Weibull data and used to simulate field trend for the tables given are also given in Figures 1 and 2 in the Appendix. In Tables 1 and 2, column one corresponds to the various methods used to analyze the data generated for the various design-sequence combinations, columns two, three and four give the average measures of goodness of estimation computed for design D1 under the different methods of data analysis being compared and columns five, six and seven give the average measures of goodness of estimation computed for design D2 under the different methods of data analysis being compared. The following shorthand notation is also used in the tables:

crd = complete randomized design analysis.

nnablue = nearest neighbor best linear unbiased estimator analysis.

nnablup = nearest neighbor best linear unbiased predictor analysis.

block size k = incomplete block analysis based on blocks of size k for k = 3, 4, 6.

linear (quadratic, cubic) = analysis of treatment effects based on a model including a linear (quadratic, cubic) approximation for trend.

Rank Correlation = the average correlation between the ranks of the true treatment effects and the ranks of the estimated treatment effects.

Correlation = the average correlation between the true treatment effects and the estimated treatment effects.

MSE = the average of the mean squared deviations between the true values of the spanning set of estimable treatment differences  $t_i - t_1$  for  $i = 2, \dots, 12$  and their estimated values.

The actual assignment of treatments to plots under designs D1 and D2 is given in the Appendix.

In evaluating the results of the study, the following general observations seemed clear:

1. As found in Stroup and Mulitze [13], initial simulations indicated that the model assuming  $\sigma^2 > 0$ , i.e.,  $R = I_n \sigma_r^2 + DD' \sigma^2$ , was no better for estimating treatment effects according to the measures of goodness described above than the model assuming  $\sigma^2 = 0$ , i.e.,  $R = I_n \sigma_r^2$ .



Because of these findings and because the assumption  $\sigma^2 > 0$  adds to the computational complexity of the simulation study but seemed to contribute nothing to the estimation procedures being compared, the only results presented here are for the case  $\sigma^2 = 0$ .

2. In design D1, the average correlation coefficients were almost always higher for the NNBLUE's than for the NNBLUP's whereas for design D2, the NNBLUP's slightly out performed the NNBLUE's in terms of average correlation coefficients. However, for both designs, the differences in average correlation coefficients for NNBLUE analysis and NNBLUP analysis was usually small. In both designs D1 and D2, the average mean squared deviations between estimable functions of the term  $t_i - t_j$ ,  $i = 2, \dots, 12$  and their estimates were almost always smaller for the NNBLUP's than the NNBLUE's, but again the differences tended to be relatively small. These findings are slightly different than those given in Stroup and Multize [13] who found that NNBLUP's tended to be better than NNBLUE's. However, these small differences may be due to differences in how the data for the two simulation studies were generated as well as differences in the two types of experiments being considered. The studies done in Stroup and Multize [13] involved larger number of unequally replicated treatments while the study conducted here involved smaller numbers of equally replicated treatments.
3. Smaller block sizes tended to do worse than medium block sizes in both designs. In the initial simulations, blocks of size 2 were also considered but proved so bad as to be excluded from the study after several runs. Blocks of size 4 and 6 tended to be best for this particular simulation study. The fact that small blocks do not do a very adequate job of accounting for trend is somewhat surprising. However, it may be that the usage of larger numbers of small blocks requires the usage of too many degrees of freedom for the estimation of block effects to account for trend at the expense of efficiently estimating treatment effects.
4. For design D1, the one constructed so as to be close to orthogonal to linear and quadratic trends, the polynomial models consistently estimated treatment effects better than either blocking or the NN methods of analysis under all measures of goodness.
5. In design D2, the polynomial models consistently had higher average correlation coefficients than the NN methods of analysis but were only slightly better under the mean squared deviation measure of goodness. The best of the incomplete block methods of analysis tended to slightly out perform the polynomial models in D2 under all measures of goodness but the worst of the incomplete block methods tended to

- perform significantly worse than the polynomial models under all measures.
6. For both designs D1 and D2, in most data sets, there were only small differences (less than .02) in the average correlation coefficients for models containing differing degrees of polynomial approximations for trend. Thus, the estimation of treatment effects under such polynomial models appear fairly robust against the wrong degree of polynomial approximation being included though some loss of efficiency does occur.
  7. With regard to designs D1 and D2, D1 consistently out performed D2 under the polynomial models and the completely randomized design model whereas design D2 out performed D1 under both the block and the NN methods of analysis. These latter results are perhaps not surprising since D1 was constructed to be nearly orthogonal to polynomial trends of degrees one and two where as D2 was constructed so as to be an optimal block design with nearest neighbor properties. This latter property for D2 has been shown to make NN procedures more efficient.
  8. Neither design D1 nor D2 seemed to consistently out perform the other over all sequences of observation's considered.

### 5. Conclusions

Based on the results of the simulation studies performed here, it appears that NNBLUE analysis has a tendency to be as good as NNBLUP analysis though the differences are usually small. Therefore, because NNBLUE's are computationally simpler to find than NNBLUP's, the former method of NN analysis may be preferable to the latter when estimating treatment effects in the presence of trend. This finding is in conflict with that determined in Stroup and Miltze [13] but may be due to differences in the studies conducted.

Blocking can be an effective means of accounting for trend as indicated by the results obtained in the study for design D2. However, one must be careful to select the correct block size in a field trial experiment. Selection of the wrong block size can be disastrous as indicated by some of the rather large differences in average correlation coefficients derived from intrablock analyses based on blocks of different sizes. The selection of proper block size prior to conducting a field trial experiment may be difficult and thus appears to be a major problem when using blocking to account for trend.

Estimation of treatment effects based on models containing polynomial approximations for trend tend to be generally as or more efficient than either

NN analyses or incomplete block analysis. This result seems to be fairly robust even against inclusion of an incorrect polynomial approximation for trend in model (4.1) as changing the degree of the approximating polynomial slightly does not seem to have large effects on the measures of estimation efficiency considered here.

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**APPENDIX****Designs Used in the Simulation Study**

D1 = { 1, 2, 3, 4, 5, 6, 7, 8, 9, 10, 11, 12, 6, 11, 5, 10, 4, 12, 9, 3, 8, 2, 7, 1, 12, 7, 8, 9, 10, 11, 1, 2, 3, 4, 5, 6 }

D1 is nearly linear and quadratic trend free.

D2 = { 4, 2, 3, 1, 5, 10, 7, 4, 12, 6, 3, 5, 7, 9, 12, 2, 1, 6, 8, 7, 11, 10, 1, 12, 8, 3, 10, 9, 11, 6, 4, 9, 2, 5, 8, 11 }

When considering successive sets of four plots in D2 as blocks, the resulting incomplete block design is the dual of a balanced incomplete block design. Design D2 is also nearly neighbor balanced with no treatment adjacent to any other treatment more than once in the sequence.

Table 1 : Data Set 32

Model	Design Matrix Number 1			Design Matrix Number 2		
	Rank Correlation	Correlation	MSE	Rank Correlation	Correlation	MSE
crd	0.79526	0.84761	1618	0.71234	0.74524	5220
nnablue	0.74590	0.80240	4450	0.74401	0.76306	2420
nnablup	0.74508	0.79903	2491	0.74379	0.76805	1683
block size 3	0.64983	0.70433	11463	0.65839	0.70717	3086
block size 4	0.73239	0.78927	1961	0.77697	0.81845	2730
block size 6	0.84014	0.88764	1004	0.79852	0.84306	1853
linear	0.79466	0.84764	1668	0.83000	0.86612	1955
quad.	0.80283	0.85525	1505	0.81664	0.85755	2386
cubic	0.80554	0.85650	1957	0.80941	0.85023	2660

Data Set 32

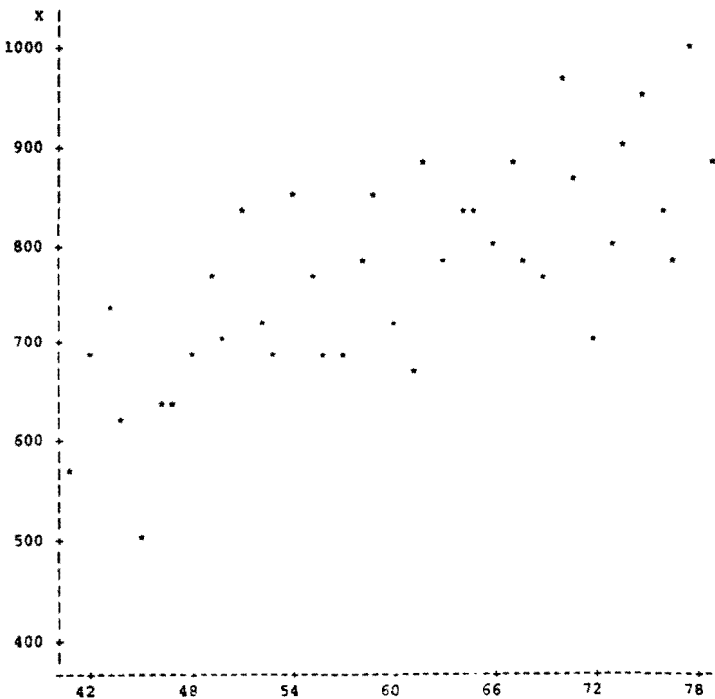
Plot of  $X \cdot I$ . Symbol used is '\*'

Fig. 1

Table 2 : Data Set 72

Model	Design Matrix Number 1			Design Matrix Number 2		
	Rank Correlation	Correlation	MSE	Rank Correlation	Correlation	MSE
crd	0.92994	0.96151	433	0.87912	0.91968	1634
nnablue	0.94540	0.97361	242	0.92761	0.95947	742
nnablup	0.94294	0.97151	356	0.92888	0.96085	635
block size 3	0.89316	0.93255	660	0.85376	0.89686	1143
block size 4	0.92117	0.95510	516	0.94771	0.97500	440
block size 6	0.93642	0.96563	287	0.95719	0.98065	186
linear	0.93041	0.96149	419	0.92206	0.95523	730
quad.	0.93283	0.96400	226	0.94913	0.97483	411
cubic	0.93533	0.96579	216	0.94785	0.97281	480

Data Set 72 Plot of X\*I. Symbol used is '\*'. \*

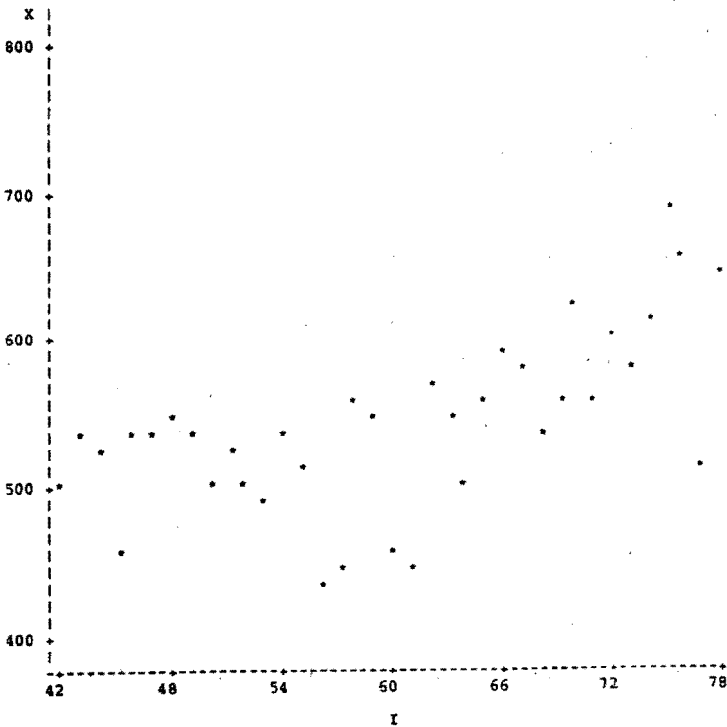


Fig. 2