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FULL LENGTH RESEARCH PAPER

Modified Inverse Polynomial and Ordinary Polynomial as a Response Surface Model: A case study of Nitrogen, Phosphate and Potassium levels on the yield of maize.

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ABSTRACT

A statistical modelling method is presented for yield of maize with fertilizer response using response surface methodology. It was shown that careful consideration of the class of response surface model (RSM). using domain knowledge, give models which are of order two magnitude as good as the more conventional polynomial models. This study shows that the modified inverse polynomial performs better in studying the response of the yield of maize as against the ordinary polynomial.

Keywords: *Modified inverse polynomial. ordinary polynomial. response surface model. Maize.*

INTRODUCTION

Response surface model (RSM) is a technique whereby a simulated performance is modelled using statistical fitting techniques (Box and Draper. 1987; Box *et al*., 1978). The measurement and simulation can be expensive or time consuming to carry out. RSMs then effectively replace the measurement (or simulation) and can then be used to investigate very rapidly trade-off between conflicting performance criteria and or for optimization tasks (Box *et al*., 1978). RSMs have recently received attention for modelling the performance of agronomic trial (Nelder. 1962).

The simplest RSMs are just ordinary regression models that assume that responses and performance can be related linearly by. essentially. two terms: a systematic component and the random error term. The elements of the error term are assumed to be independent with the same normal distribution. The parameters are estimated using the method of least square i.e. by minimizing the sum of squares of the difference between responses and their expected values.
If $X = (x_1, \ldots, x_p)$ are the independent variables or factors. we can consider an experimental design region R (design space). then. the model is.

$$Y = Y(x) = f(x, \theta) + \varepsilon \qquad \ldots\ldots (1)$$

Where $\theta = (\theta 1, \ldots, \theta_p)$ we determine $\hat{\theta}$ an estimate of θ, so that the estimated model is

$$\hat{Y} = \hat{Y}(x) = f(x, \hat{\theta})$$

In RSMs Y is called the response and $\hat{Y}$ the fitted surface. It concentrates on the shape of Y (or $\hat{Y}$). A proposed model is the general quadratic model.

$$Y = \theta_o + \sum_{i}^{3} \theta_i x_i + \sum \theta_{ii} x_{ii}^2 + \sum_{ij}^{3} \theta_{ij} x_i x_j + \varepsilon \quad \ldots\ldots (2)$$

i=1,2,3 and j= 1,2,3

where ε is the error component, with normal distribution with $\mu = 0$ and finite variance σ^2.
The objective of this study is to compare the modified inverse polynomials and the ordinary polynomial as a RSM in terms of the deviance and coefficient of determination for the effect of Nitrogen, Phosphorous and Potassium on the yield of maize.

MATERIALS AND METHODS

The mean yield of maize for two years was obtained from the trial conducted at the Institute for Agricultural Research Farm, Samaru (11^0 11' N, 07^0 38' E and 686m altitude). The treatment of the trials comprises of the treatment combination of three levels each of Nitrogen, Phosphorous and Potassium. The trial consists of 3^3 factorial experiment. The experiment was conducted in a Randomized complete block design with two replications. In the earlier result shown by Salihu (2004), the yield of maize had the highest growth parameter at maximum Nitrogen, Phosphorous and Potassium fertilizer rate of 150: 75: 75 kg ha^{-1} and that the yield component and grain were attained at 120:60:60 kg ha^{-1}. Based on his result, he deducted that the crop performed best at 120:60:60 kg ha^{-1} and that application of the fertilizer beyond 120:60:60 kg ha-^{1} gave no advantage.

Modified Inverse Polynomials (MIP)

To make a RSM model we use a fraction of the total runs or treatment combination to make a RSM model and the other data (i e. data which were not used in the model making process) to check how good the predicted responses from the RSM are. The usual approach to modelling the responses would be to try fitting the data by an ordinary polynomial such as the one in equation (2).

Fitting this model to a particular data then yields estimates of the coefficients θ. Model checking should be carried out to test the validity of the model (Box *et al.*, 1978). This type of model can often give apparently adequate methods within the region of initial investigation. Ordinary polynomials do, however, have serious drawback that the response can become negative (which may be unphysical) and the responses will always extrapolate to plus or minus infinity (which again may be unphysical).

Consideration of the properties of the yield of an agronomic trial which can not be negative, this would imply that although a simple polynomial may appear adequate it would be better to investigate other model classes. Inverse polynomial model, first introduced by Nelder. (Nelder, 1962), have advantage over ordinary polynomial models: the responses are bound and asymptotic as well as being non-negative for positive θ. Note that the coefficients must be positive otherwise singularities would appear in the response. They can also be estimated using the GLM frame work with a software package such as Genstat.

The simplest form of the inverse linear polynomial is

$$x / f = \theta_0 + \theta_1 x \qquad \text{with } x > 0 \qquad \ldots\ldots (4)$$

Where f is the expected value of the response variable, θ's are the parameters to be estimated and X is the input variable. This RSM will have θ_1^{-1} as an asymptote and θ_0^{-1} is the gradient of the response curve at the origin. For the yield of maize we use an inverse quadratic polynomial,

$$x_1 x_2 x_3 / f = \theta_o + \theta_1 x_1 + \theta_2 x_2 + \theta_3 x_3 + \theta_{11} x_1^2 + \theta_{22} x_2^2 + \theta_{33} x_3^2 + \theta_{12} x_1 x_2 + + \theta_{13} x_1 x_3 + \theta_{23} x_2 x_3 + \varepsilon \quad \ldots\ldots (5)$$

where our independent variable X are the fertilizer component.

The above model equation (5) differ from equation (2) in the sense that the structure of the dependent variable of the two equations differs.

Model fitting

If the parameters in the model are linear and the errors satisfy the required statistical conditions, the least square regression approach may be used. In a 3 dimensional quadratic model, suppose we take observations $Y_1, \ldots, Y_n$ at $(x_{11}, x_{21}\ x_{31}), \ldots, (x_{1n}, x_{2n}, x_{3n})$ respectively. The least square analysis would seek to minimize

$$\sum \varepsilon^2 = \sum_{i=1}^{n} \{ Y_i - f[(x_{1i}, x_{2i}, x_{3i}), \theta] \}^2$$

The solution can be expressed in the matrix notation as

$$\theta = (X^T X)^{-1} X^T Y$$

where

$$\hat{\theta} = (\hat{\theta}_0, \hat{\theta}_1, \hat{\theta}_2, \hat{\theta}_{11}, \hat{\theta}_{22}, \hat{\theta}_{12})^T$$

$Y = (Y_1, \ldots\ldots, Y_n)$, and,

$$X = \begin{pmatrix} 1 & X_{11} & X_{21} & X^2_{11} & X^2_{21} & X_{11}X_{21} \\ 1 & X_{12} & X_{22} & X^2_{12} & X^2_{22} & X_{12}X_{22} \\ \vdots & \vdots & \vdots & \vdots & \vdots & \vdots & \vdots \\ 1 & X_{1n} & X_{2n} & X^2_{1n} & X^2_{2n} & X_{1n}X_{2n} \end{pmatrix}$$

The matrix X^TX can be written conveniently in term of the "moments about the origin" of the X values:

-

$$M_{10} = X_1 = {}^1/_n \sum X_{1i}$$

$$M_{01} = X_2 = {}^1/_n \sum X_{2i}$$

$$M_{20} = {}^1/_n \sum X^2_{1i}$$

$$M_{02} = {}^1/_n \sum X^2_{2i}$$

$$M_{11} = {}^1/_n \sum X_{1i} X_{2i}$$

Thus

$$X^TX = n \begin{pmatrix} 1 & M_{10} & M_{01} & M_{20} & M_{02} & M_{11} \\ M_{10} & M_{20} & M_{11} & M_{30} & M_{12} & M_{21} \\ M_{01} & M_{11} & M_{02} & M_{21} & M_{03} & M_{12} \\ M_{20} & M_{30} & M_{21} & M_{40} & M_{22} & M_{31} \\ M_{02} & M_{12} & M_{03} & M_{22} & M_{04} & M_{13} \\ M_{11} & M_{21} & M_{12} & M_{31} & M_{13} & M_{22} \end{pmatrix}$$

$$= n M$$

Where M is the moment matrix and X^TX is the information matrix. The theory tells that the covariance matrix of the parameter estimates is given by

$\mathrm{Cov}(\hat{\theta}) = \sigma^2 (X^TX)^{-1} = \sigma^2 {}^1/_n M^{-1}$, where σ^2 is the variance.

RESULTS AND MODIFIED INVERSE POLYNOMIAL

We have a total of 27 runs formed by taking a full factorial experiment design of the three input variables at three levels. The method chosen to compare the different techniques involves using only the information available to make our models. We can then check how well the models fit by comparing all the 27 points of the actual results with 27 points predicted from our models. An interpolation test can be carried out since all the predicted values would lie within the range of the data used to make the model.

If f_i is the value of the response at the i^{th} run (out of a total of N runs) and $\hat{f}_i$ is the value predicted by our model then we can use the deviance as a test of the model's predictive power.

$$\text{Deviance} = \sum (f_i - f^{\wedge}_i)^2$$

Where f_i is an observed value and that $f^{\wedge}_i$ is a fitted value

Dividing this by the degree of freedom and taking the square root gives a prediction standard deviation for the model of f. The assumption of normal error distribution is considered in fitting the inverse polynomial that justifies the expression for deviance.
For the ordinary polynomial (2) the overall test gave a deviance of 4993.94 with the coefficient of determination, R^2 = 59.3%. This shows how badly this model predicted when extrapolated. The fitting of a quadratic inverse polynomial (5) gave a model over 174 times as good (with a deviance equal to 28.73) and coefficient of determination, R^2 = 94%. There is, however, a problem with these models, in that, in the quadratic response model six of the fitted regression coefficients turn out to be negative, while, in the quadratic inverse polynomial only the main effect regression coefficients are negative.
Non-linear model classes were considered to improve the accuracy of the model. This is time consuming and difficult but it is possible to modify it to the bilinear inverse polynomial that gives excellent result as well as preserving the essential physical characteristics,

$$f^{-1} = \alpha_0 + \alpha_1 / x_1^{\theta} + \alpha_2 / x_2^{\theta} + \alpha_3 / x_3^{\theta} + \ldots + \alpha_{12} / x_1^{\theta} x_2^{\theta} + \ldots$$

as proposed by (Zahid and Nelder, 2007) for testing the extrapolation fit a value of θ = 0.67 was quickly established. This model gave a deviance of (1.97×10^{-8}); this is more than thousands times as good as the ordinary polynomial.

The scatter plot, observed and fitted plot for the models were shown in Fig. 1- 4.

CONCLUSION

It has been shown that the modified bilinear polynomial is an excellent model for the yield of maize. This type of model is useful in other fields where the response is asymptotic and goes through the origin (Salawu, 2007). It is noted that taking into account any physical knowledge known about a system could pay dividends when making a statistical model.

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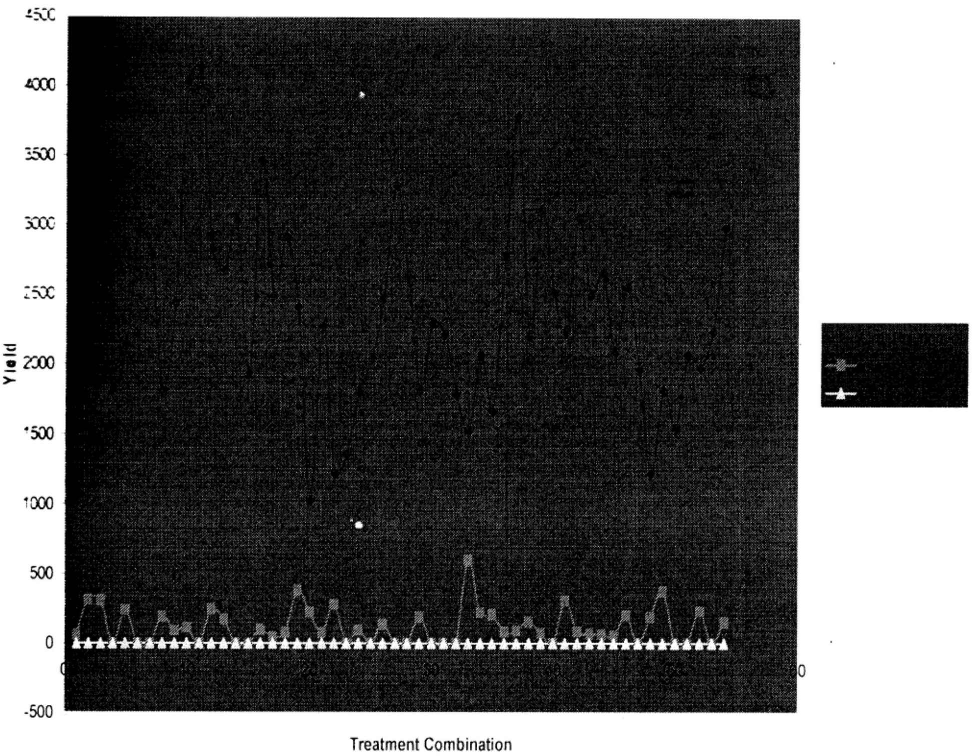

FIG: 1

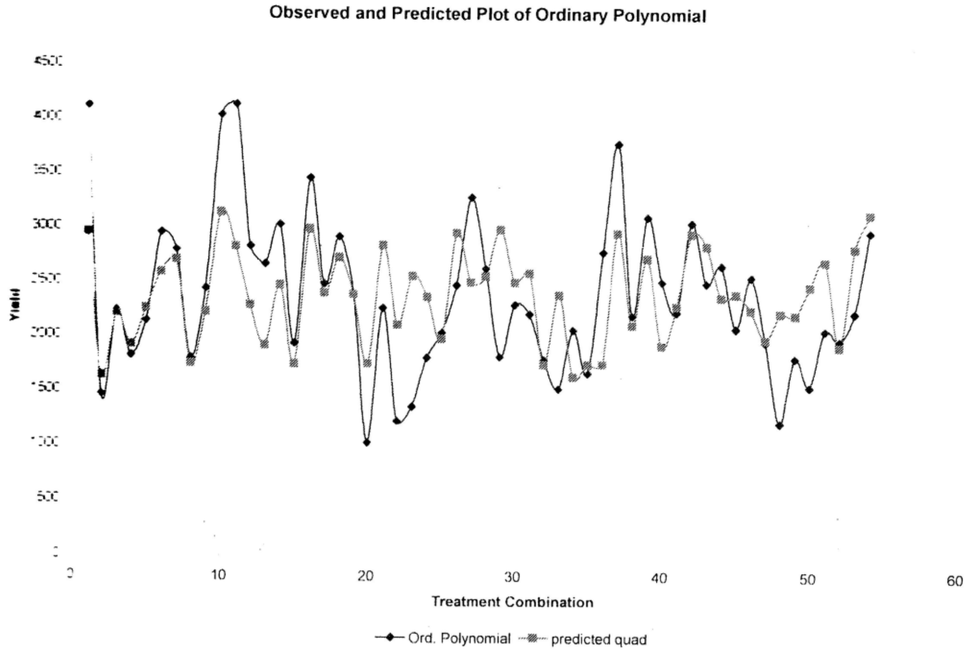
Observed and Predicted Plot of Ordinary Polynomial
Yield
10
20
30
40
50
60
Treatment Combination
Ord. Polynomial
predicted quad

FIG. 2.

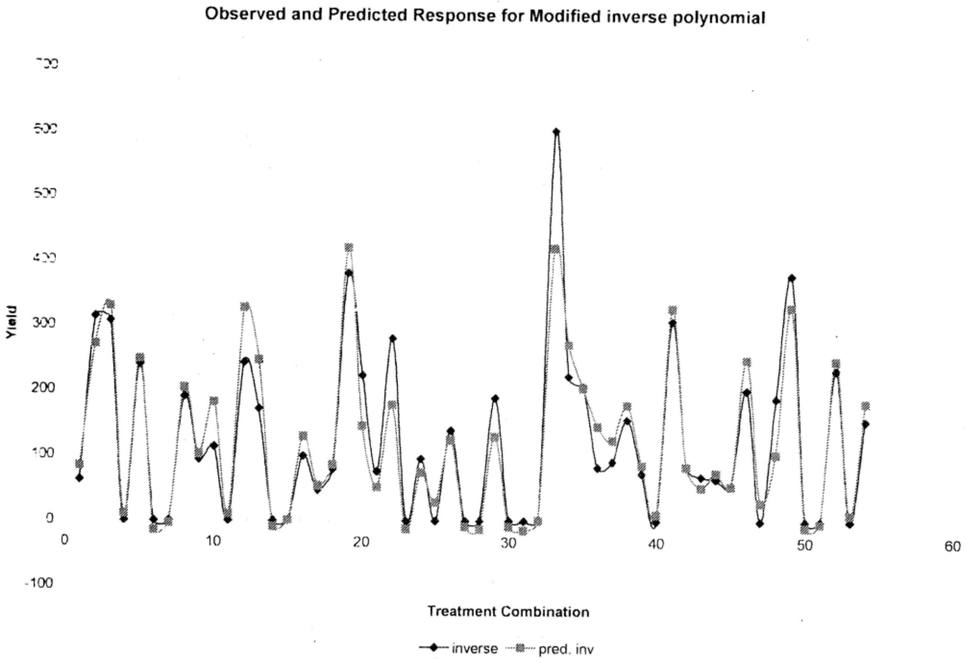
Observed and Predicted Response for Modified inverse polynomial
Yield
300
200
100
0
-100
0
10
20
30
40
50
60
Treatment Combination
inverse
pred. inv

FIG: 3

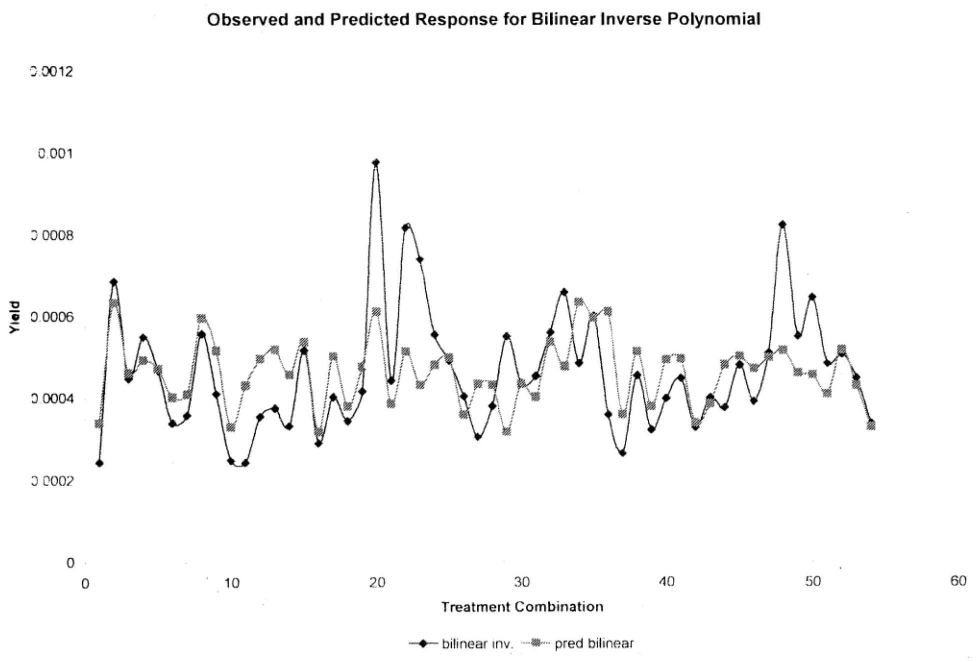
Observed and Predicted Response for Bilinear Inverse Polynomial
Yield
0.0012
0.001
0.0008
0.0006
0.0004
0.0002
0
0
10
20
30
40
50
60
Treatment Combination
bilinear inv.
pred bilinear

FIG: 4