A Bertalanffy-Richards Split-Plot Design Model and Analysis

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Abstract

This research presents a class of nonlinear split plot design (SPD) model where the mean function of the SPD model is not linearizable. This was done by fitting intrinsically nonlinear split-plot design (INSPD) model using Bertalanffy-Richards function. Estimated Generalized Least Square (EGLS) technique based on Gauss-Newton with Taylor series expansion by minimizing the model objective function was used for estimating the fitted INSPD model parameters. The variance components for the whole plot and subplot random effects are estimated using Restricted Maximum Likelihood Estimation (REML) and Maximum Likelihood Estimation (MLE) techniques. These techniques are established and paralleled with Ordinary Least Square (OLS) technique for a balanced $3^1 \times 4^2$ replicated mixed Level SPD data from Institute of Agricultural Research, Ahmadu Bello University, Zaria. The adequacy of the estimated INSPD model parameters for the EGLS and OLS are compared using four median adequacy measures. They are resistant coefficient of determination, resistant prediction coefficient of determination, resistant modeling efficiency statistic, and median square error prediction statistic. Also, Akaike's information criterion, corrected Akaike's information criterion, and Bayesian information criterion are used to select the best parameter estimation technique. The results obtained showed that the Bertalanffy-Richards SPD model via EGLS-REML fitted model is a good fit that is adequate, stable and reliable for prediction compared to EGLS-MLE and OLS techniques.

Keywords: Adequacy measures; Bertalanffy-Richards function; Intrinsically nonlinear; Restricted maximum likelihood estimation; Split-plot design

1. Introduction

Split-plot design (SPD) of experiment has since been used in all aspect of agricultural experiments as introduced by Sir R. A. Fishers in 1925 and in the industry too as a linear model (Wang, Kowalski & Vining, 2009; Myers, Montgomery, & Anderson-Cook 2009; Jones & Nachtcheim, 2009; Lu, Anderson-Cook, & Robinson, 2011; Lu & Anderson-Cook, 2012; Lu, Anderson-Cook & Robinson, 2012; Jones & Goos, 2012; Lu & Anderson-Cook, 2014; Anderson & Whitcomb, 2014; Lu, Robinson, & Anderson-Cook, 2014; Anderson, 2016; Kulahci & Menon, 2017; Huameng, Fan & Lei, 2017). However, intrinsically nonlinear SPD (INSPD) modeling has received little attention. This class of model has parameters that are not linearizable. Since the SPD has two sources of random variations, [whole plot error (WPE) and subplot error (SPE)] traditional nonlinear regression will not be suitable because it cannot handle more than one random error variation. If wrongly used the single mean square error (MSE) produced will be a compromise between the WPE and SPE variances (Gumpertz & Rawlings, 1992; Knezevic et al., 2002; Blankenship et al., 2003). Gumpertz & Rawlings (1992) fitted and estimated the parameters of a Weibull unbalanced SPD of experiment for the effect of ozone (O₃) exposure (whole plot [WP] treatment I) on soybean yield at two watering regimes (WP treatment II) on thirty chambers arranged in three randomized blocks (each block has 10 chambers). Two cultivars (SP treatments) are within each chamber where the soybean are grown. Knezevic et al. (2002) and Blankenship et al. (2003) modelled the WP and subplot [SP] effect of three nitrogen rates on "critical period for weed control" (CPWC) in corn yield using Logistic and Gompertz functions. Theoretical presentation on intrinsically nonlinear SPD modelling has been given by Gumpertz, & Pantula (1992), David et al. (2018) and David et al. (2019).

There have been extensive use of the Bertanlanffy-Richards function (BRF) in modeling growth process. For instance Hazarika *et al.* (2020) used the BRF to study growth pattern of the height and width of Indian Bamboo (Bambusa Tulda) and they found the BRF to fit their data well. Similarly, other researchers have applied BFR in modeling the growth of crops, animals, birds and other organisms in terms of length of growth, body size, yield, weight and height (Tariq *et al.*, Bashiru *et al.*, 2020, Lee *et al.*, 2020, and Tekel *et al.*, 2020).

In this research a balanced INSPD modeling is presented. The WP and SP are modeled using a three-parameter Bertanlanffy-Richards function with fixed block effect. The variance covariance matrix, V is estimated using restricted maximum likelihood (REML) technique for estimated generalized least square (EGLS) where results obtained are compared to estimates from maximum likelihood estimation (MLE) for EGLS and ordinary least square (OLS) of the fitted model. All fitted models are assessed for goodness of fit using information criteria and median adequacy measures (MAM) by David *et al.* (2016) and David *et al.* 2020.

2. Materials and Methods

In this section we present the NSPD models and a theoretical structure for estimating the parameters of the models using an iterative Gauss-Newton procedure with Taylor series expansion. The INSPD model which has WPE and SPE are special case of nonlinear model with random effects (also called nonlinear model with **V** that is, WPE and SPE). The formulated model and assumptions are given as follows.

Let

$$Y_{ijk} = \mu + \gamma_i + \alpha_j + w_{ij} + \beta_k + (\alpha\beta)_{jk} + \varepsilon_{ijk}$$
(1)

be the linear SPD model with two factors A and B. The corresponding NSPD model is given as follows.

$$y_{ijk} = f(x_{ijk}, \theta) + w_{ij} + \varepsilon_{ijk}$$
(2)

where, y_{ijk} is the response variable; i = 1, ..., s replicates (*Reps*) or block; j = 1, ..., a levels of the *WP* factor **A**; k = 1, ..., b levels of the *SP* factor **B**; w_{ij} is the *WP* error and ε_{ijk} is the *SP* error; $f(x_{ijk}, \theta)$ is the nonlinear function for the mean describing the relationship of fixed main and interaction effects to the response y_{iik} . The parameters *Reps*, **A** and **B** are assumed fixed.

Assumption 1: it is presumed that the WPE and SPE are random effects. Also, it is assumed that i.i.d. $w_{ij} \sim N(0, \sigma_{w_P}^2)$ and $\varepsilon_{ijk} \sim N(0, \sigma_{s_P}^2)$.

Assumption 2: Let $\hat{\theta}$ be the model parameter estimate of θ which follows an asymptotic normal distribution with mean θ and variance $\sigma^2(\mathbf{F'F})^{-1}$, where \mathbf{F} is the $n \times u$ matrix with elements $(\partial f(x_{ijk}, \theta)/\partial \theta')$ where the columns, u of the matrix is a full rank.

Assumption 3: if the number of parameters in the mean function, $f(x_{ijk}, \theta)$ is p and the number of random effects is r, then the number of measurements in the data set, n, must be at least p + r + l in order to estimate all of the parameters. This implies that $n \ge p + r + l$.

2.1 Split-Plot Model with Bertalanffy-Richards Function as the Mean Curve

The mean curve, $f(x_{ijk}, \theta)$ in equation (2) is substituted with the Bertalanffy-Richards function (BRF). The BRF used for this research is a three-parameter function.

Let $f(x_{ijk}, \theta)$ be a BRF. Therefore,

$$f(x_{ijk}, \theta) = \alpha_{ijk} \times \left(1 - exp(\omega x_{ijk})\right)^{\lambda}$$
(3)

where α_{ijk} is the asymptote and it is tailored as $\alpha_{ijk} = \alpha + Rep_i + A_j + B_k + (AB)_{jk}$. Hence, equation (3) can be rewritten as follows.

$$f(x_{ijk}, \theta) = \left[\alpha + Rep_i + A_j + B_k + (AB)_{jk}\right] \left(1 - exp(\omega x_{ijk})\right)^{\lambda}$$
(4)

The SPD model with the BRF as the mean curve is therefore given as follows.

$$y_{ijkl} = \left[\alpha + Rep_i + A_j + B_k + (AB)_{jk}\right] \left(1 - exp\left(\omega x_{ijk}\right)\right)^{\lambda} + w_{ij} + \varepsilon_{ijk}$$
(5)

where α is the average yield at zero rate or dose, Rep_i is the *i*th replicate or block, A_j is the effect of the *j*th levels of factor *A*, B_k is the effect of the *k*th levels of factor *B*, $(AB)_{jk}$ is the *j*th and *k*th levels interaction effect of the factors *A* and *B* respectively, x_{ijk} is the mean covariate effect in the *i*th replicate at the *j*th factor *A* and *k*th factor *B*, ω and λ are the Weibull scale and shape parameters respectively, w_{ij} is the WP error and ε_{ijk} is *SP* error.

2.2 Method of Estimated Generalized Least Square (EGLS)

When the covariance matrix of y is known then the GLS estimator, $\hat{\theta}_{GLS}$, is found by minimizing the objective function (Gumpertz & Rawlings, 1992; David *et al.*, 2019)

$$\left(y - f(X, \theta)\right)^{t} \mathbf{V}^{-1} \left(y - f(X, \theta)\right)$$
(6)

with respect to θ , where V is a known positive definite (non-singular) covariance matrix which arises from the model

$$y_{ijk} = f(x_{ijk}, \theta) + w_{ij} + \varepsilon_{ijk}$$
(7)

where, $E(w_{ij}) = 0$, $Cov(w_{ij}) = \sigma_w^2 \mathbf{I}_N$, $E(\varepsilon_{ijk}) = 0$ and $Cov(\varepsilon_{ijk}) = \sigma_\varepsilon^2 \mathbf{I}_N$.

Let the V matrix of the observations var(y) be written as

$$\mathbf{V} = \sigma_w^2 \mathbf{I}_N + \sigma_\varepsilon^2 \mathbf{I}_N$$
$$= \sigma^2 \mathbf{I}.$$

By Cholesky decomposition, multiply model (7) by J⁻¹ on both sides yield that

$$\mathbf{J}^{-1}y_{ijk} = \mathbf{J}^{-1}f(x_{ijk},\theta) + \mathbf{J}^{-1}(w_{ij}) + \mathbf{J}^{-1}(\varepsilon_{ijk})$$
(8)

Define $\mathbf{T}_{ijk} = \mathbf{J}^{-1}y_{ijk}$, $\mathbf{M}(x_{ijk}, \theta^*) = \mathbf{J}^{-1}f(x_{ijk}, \theta)$ and $\mathbf{\Omega}_{ijk} = \mathbf{J}^{-1}(w_{ij}) + \mathbf{J}^{-1}(\varepsilon_{ijk})$. Then equation (8) becomes

$$\mathbf{\Gamma}_{ijk} = \mathbf{M}(x_{ijk}, \boldsymbol{\theta}^*) + \mathbf{\Omega}_{ijk}$$
(9)

where, $E(\mathbf{\Omega}_{ijk}) = 0$ and $\mathbf{V}(\mathbf{\Omega}_{ijk}) = \sigma^2 \mathbf{I}$. Thus the GLS model has been transformed to an OLS model. Hence, model (9) is to be solved using the OLS technique as follows.

Taking the summation of both sides of (9) and squaring we have

$$\sum_{i}^{s} \sum_{j}^{a} \sum_{k}^{b} \mathbf{\Omega}_{ijk}^{2} = \sum_{i}^{s} \sum_{j}^{a} \sum_{k}^{b} \left[\mathbf{T}_{ijk} - \mathbf{M}(x_{ijk}, \theta^{*}) \right]^{2}$$

$$\text{Let } L(\theta^{*}) = \sum_{i}^{s} \sum_{j}^{a} \sum_{k}^{b} \mathbf{\Omega}_{ijk}^{2} = \sum_{i}^{s} \sum_{j}^{a} \sum_{k}^{b} \left[\mathbf{T}_{ijk} - \mathbf{M}(x_{ijk}, \theta^{*}) \right]^{2}$$

$$(10)$$

minimize $L(\theta^*)$ w.r.t. θ^* , equate to zero and divide through by -2 we have,

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$$\frac{\partial L(\theta^*)}{\partial \theta_h^*} = \sum_i^s \sum_j^a \sum_k^b \left[\mathbf{T}_{ijk} - \mathbf{M}(x_{ijk}, \theta^*) \right] \times \left[\frac{\partial \mathbf{M}(x_{ijk}, \theta^*)}{\partial \theta_h^*} \right]_{\theta^* = \hat{\theta}^*} = 0$$
(11)

At this point, equation (11) has no closed form hence will be solved iteratively using the Gauss-Newton method with Taylor series expansion of $\mathbf{M}(x_{ijk}, \theta^*)$ at first order (see David *et al.*, 2019). Equation (12) is obtained

$$\eta(\theta^*) = \eta(\theta_0^*) + D_0 \delta \tag{12}$$

where D_0 is the $N \times H$ derivative matrix with elements $\{d_{ijk}\}$ at *h* iterations and this is equivalent to approximating the residuals for the model, that is, $\Omega(\theta^*) = \mathbf{T} - \eta(\theta^*)$ by

$$\mathbf{\Omega}(\theta^*) = \mathbf{T} - \left[\eta(\theta_0^*) + D_0 \delta\right]$$

= $\mathbf{T} - \eta(\theta_0^*) - D_0 \delta$
= $z_0 - D_0 \delta$ (13)

where $z_0 = \mathbf{T} - \eta(\theta_0^*)$ and $\delta = \theta^* - \theta_0^*$.

To achieve numerical stability of the parameter estimates D_0 is decomposed using QR (Q is an orthogonal matrix and R is an inverted or upper triangular matrix) decomposition into the product of an orthogonal matrix and an inverted matrix (Klotz, 2006; David *et al.*, 2019). A point $\hat{\eta}_1 = \eta(\theta_1^*) = \eta(\theta_0^* + \delta_0)$ should now be closer to y than $\eta(\theta_0^*)$, and then move to an improved parameter value $\theta_1^* = \theta_0^* + \delta_0$ and perform another iteration by calculating new residuals $z_1 = \mathbf{T} - \eta(\theta_1^*)$, a new derivative matrix D_0 , and a new increase. This process is reiterated until convergence is achieved, that is, until the increment is so small that there is no useful modification in the elements of the parameter vector (David *et al.*, 2019). A small step in the direction δ_0 is introduced if the new value is not small as projected. A step factor λ is introduced such that $\theta_1^* = \theta_0^* + \lambda \delta_0$ where λ is chosen to ensure that the new residual sum of squares is less than the initial estimate. As suggested by David *et al.* (2019) it is to start with $\lambda = 1$ and halve it until it is satisfied that the new residual sum of squares is less than the initial estimate.

2.3 Variance Component Estimation Via REML

The REML system does not embrace $\hat{\theta}^*$ in the estimation of V. The log-likelihood function is based on vectors in the error space. To obtain these vectors in the error space the linear approximation of the residuals is used $z_0 = D_0 \delta + \varepsilon$. To derive V from the nonlinear functions of y that will not embroil $\hat{\theta}^*$, vectors of the form K^ty are fashioned whereby K is chosen so that K^tD₀ = 0 which falls in the linear approximation to the error space. K is a full rank matrix satisfying K^tD₀ = 0 and smearing maximum likelihood to K^ty, the log likelihood function of K^ty, is

$$\ln L(\mathbf{\Theta}) = -\frac{n}{2} \ln (2\pi) - \frac{1}{2} \ln \left| \mathbf{K}^{\mathsf{t}} \mathbf{V} \mathbf{K} \right| - \frac{1}{2} \left(\mathbf{K}^{\mathsf{t}} y - \mathbf{K}^{\mathsf{t}} f \left(X, \theta \right) \right)^{\mathsf{t}}$$

$$\times \left(\mathbf{K}^{\mathsf{t}} \mathbf{V} \mathbf{K}\right)^{-1} \left(\mathbf{K}^{\mathsf{t}} y - \mathbf{K}^{\mathsf{t}} f\left(X, \theta\right)\right) \tag{14}$$

where $\Theta^t = (\sigma_{WP}^2, \sigma_{SP}^2)^t$, is then approximated by the surface and equation (14) becomes,

$$\ln L(\boldsymbol{\Theta}) = -\frac{n}{2} \ln (2\pi) - \frac{1}{2} \ln \left| \mathbf{K}^{\mathsf{t}} \mathbf{V} \mathbf{K} \right| - \frac{1}{2} \left(\mathbf{K}^{\mathsf{t}} y - \mathbf{K}^{\mathsf{t}} f(x,\theta) \right)^{t} \left(\mathbf{K}^{\mathsf{t}} \mathbf{V} \mathbf{K} \right)^{-1} \left(\mathbf{K}^{\mathsf{t}} y - \mathbf{K}^{\mathsf{t}} f(x,\theta) \right)$$
$$= C - \frac{1}{2} \ln \left| \mathbf{K}^{\mathsf{t}} \mathbf{V} \mathbf{K} \right| - \frac{1}{2} \left(\mathbf{K}^{\mathsf{t}} y - \mathbf{K}^{\mathsf{t}} f(x,\theta) \right)^{t} \left(\mathbf{K}^{\mathsf{t}} y \left(\mathbf{K}^{\mathsf{t}} \mathbf{V} \mathbf{K} \right)^{-1} - \mathbf{K}^{\mathsf{t}} f(x,\theta) \left(\mathbf{K}^{\mathsf{t}} \mathbf{V} \mathbf{K} \right)^{-1} \right)$$
$$= C - \frac{1}{2} \ln \left| \mathbf{K}^{\mathsf{t}} \mathbf{V} \mathbf{K} \right| - \frac{1}{2} \left(\left(\mathbf{K}^{\mathsf{t}} y - \mathbf{K}^{\mathsf{t}} f(x,\theta) \right)^{t} \mathbf{K}^{\mathsf{t}} y \left(\mathbf{K}^{\mathsf{t}} \mathbf{V} \mathbf{K} \right)^{-1} \right)$$
$$+ \frac{1}{2} \left(\left(\mathbf{K}^{\mathsf{t}} y - \mathbf{K}^{\mathsf{t}} f(x,\theta) \right)^{t} \mathbf{K}^{\mathsf{t}} f(x,\theta) \left(\mathbf{K}^{\mathsf{t}} \mathbf{V} \mathbf{K} \right)^{-1} \right)$$
(15)

By matrix algebra on the third and fourth terms of equation (15) respectively by inserting

$$\mathbf{V} = \sigma^{2}\mathbf{I} = K\sum_{i=1}^{2} \sigma_{i}^{2}\mathbf{I}_{i}\mathbf{I}_{i}^{\prime}K^{\prime} \text{ and } \mathbf{V}\mathbf{V}^{-1} = \left(\mathbf{K}\mathbf{V}\mathbf{K}^{\prime}\right)^{-1} = \mathbf{V}\left(\mathbf{K}\left(\mathbf{K}\mathbf{V}\mathbf{K}^{\prime}\right)^{-1}\mathbf{K}^{\prime}\right) = \sigma^{2}\mathbf{I}\left(\mathbf{Q}_{h}\right) = \sigma^{2}\left(\mathbf{Q}_{h}\mathbf{V}_{j}\right).$$

Then differentiate partially the outcome w.r.t σ_i^2 and equate to zero equation (15) becomes

$$\frac{1}{2}(tr(\mathbf{Q}_{h}\mathbf{V}_{i})) = \frac{1}{2}(y^{t}\mathbf{Q}_{h}\mathbf{V}_{i}\mathbf{Q}_{h}y)$$
(16)

Multiply the left hand side of equation (16) by VV^{-1} we have

$$\frac{1}{2} \left(tr \left(\mathbf{Q}_{h} \mathbf{V}_{i} \right) \right) \sigma_{j(h+1)}^{2} \left(\mathbf{Q}_{h} \mathbf{V}_{j} \right) = \frac{1}{2} \left(y' \mathbf{Q}_{h} \mathbf{V}_{i} \mathbf{Q}_{h} y \right)$$
(17)

$$\left\langle tr\left(\hat{\mathbf{Q}}_{(h)}\hat{\mathbf{V}}_{i}\ \hat{\mathbf{Q}}_{(h)}\hat{\mathbf{V}}_{j}\right)\right\rangle \times \left\langle \left(\hat{\sigma}_{j(h+1)}^{2}\right)\right\rangle = \left\langle \left(y^{t}\hat{\mathbf{Q}}_{(h)}\hat{\mathbf{V}}_{i}\ \hat{\mathbf{Q}}_{(h)}y\right)\right\rangle$$
(18)

$$\left\langle \left(\hat{\sigma}_{j(h+1)}^{2} \right) \right\rangle = \left\langle tr \left(\hat{\mathbf{Q}}_{(h)} \hat{\mathbf{V}}_{i} \; \hat{\mathbf{Q}}_{(h)} \hat{\mathbf{V}}_{j} \right) \right\rangle^{-1} \times \left\langle \left(y^{\mathsf{t}} \hat{\mathbf{Q}}_{(h)} \hat{\mathbf{V}}_{i} \; \hat{\mathbf{Q}}_{(h)} y \right) \right\rangle$$
(19)

The solutions to the equations may turn out to be negative when further iteration does not improve the log-likelihood. In such a case, the negative value is changed to zero before the next iteration.

2.4 Median Adequacy Measure (MAM) Statistics

Four proposed Median Adequacy Measure (MAM) statistics for assessing the adequacy of linear SPD models (David *et al.*, 2016) are used for this research to assess the adequacy of the fitted INSPD models. The four statistics used are resistant coefficient of determination (r_r^2) proposed by Kvalseth (1985), resistant prediction coefficient of determination (*Pred-* r_r^2), Resistant Modeling Efficiency (*RMEF*) and Median Square Error Prediction (*MedSEP*). Procedures for calculating the WP and SP respective models residuals are given by Almimi *et al.* (2006) and David *et al.* (2016). These statistics are called resistant due to their ability of withstanding outliers or extreme values and not to increase or decrease unnecessarily when a variable is added or removed from the original model (David *et al.*, 2020). The four statistics are presented as follows.

2.4.1 Resistant Coefficient of Determination (r_r^2)

The statistic to calculate the WP and SP r_r^2 values are as follows:

$$r_{r(wp)}^{2} = 1 - \begin{pmatrix} n \\ M \\ i=1 \\ M \\ M \\ i=1 \\ M \\ i=1 \\ W_{I} \\ W_{I} \\ W_{I} \end{pmatrix}^{2}$$
(20)

$$r_{r(sp)}^{2} = 1 - \begin{pmatrix} {}^{n}_{M}(|\varepsilon_{i}|)_{Sp} \\ {}^{m}_{i=1}(|Y_{i} - \overline{Y}|)_{Sp} \end{pmatrix}^{2}$$
(21)

where M is the median of the absolute values from i = 1 to n and e_i is the fitted models residuals. The statistic (20 and 21) above uses the median instead of the mean in obtaining a coefficient of determination value that is highly resistant to outliers as proposed by Kvalseth (1985), $0 \le r_r^2 \le 1$. However, for nonlinear models the coefficient of determination value can be negative when the fit is worse, that is, $-1 \le r_r^2 \le 1$.

2.4.2 Resistant Prediction Coefficient of Determination (Pred- r_r^2)

The statistic to calculate the WP and SP Pred- r_r^2 values are as follows:

$$_{WP} Pred - r_r^2 = 1 - \left(M_{i=1}^n \left[\frac{(|e_i|)}{(1-h_{ii})} \right]_{WP}^2 M_{i=1}^n \left[\left| Y_{i(WP)} - \overline{Y}_{(WP)} \right| \right]^{-2} \right)$$
(22)

$$_{SP} Pred - r_r^2 = 1 - \left(M_{i=1}^n \left[\frac{(|e_i|)}{(1-h_{ii})} \right]_{SP}^2 M_{i=1}^n \left[\left| Y_{i(SP)} - \overline{Y}_{(SP)} \right| \right]^{-2} \right)$$
(23)

where M is the median of the squared values from i = 1 to n, e_i is the residual, h_{ii} is the hat matrix and $1 \le Pred - r_r^2 \le 1$. However, for nonlinear models the prediction coefficient of determination value can be negative when the fit is worse, that is, $-1 \le Pred - r_r^2 \le 1$.

2.4.3 Resistant Modeling Efficiency (RMEF)

The statistic to calculate the WP and SP RMEF values are as follows:

$$RMEF_{WP} = 1 - \left(\frac{M_{i=1}^{n} \left[\left| Y_{i} - f \left(X_{i} ..., X_{p} \right)_{i} \right| \right]_{WP}}{M_{i=1}^{n} \left(\left| Y_{i} - \overline{Y} \right| \right)_{WP}} \right)^{2}$$
(24)

$$\operatorname{RMEF}_{SP} = 1 - \left(\frac{M_{i=1}^{n} \left[\left| Y_{i} - f\left(X_{i} \dots, X_{p} \right)_{i} \right| \right]_{SP}}{M_{i=1}^{n} \left(\left| Y_{i} - \overline{Y} \right| \right)_{SP}} \right)^{2}$$
(25)

where M is the median of the absolute values from i = 1 to n and $f(X_i,...,X_p)_i$ is the model-predicted values. In a perfect fit RMEF would result in a value equal to one. The upper bound is one and the

(theoretical) lower bound is negative infinity ($-\infty < \text{RMEF} \le 1$).

2.4.4 Median Square Error Prediction (MedSEP)

The statistic to calculate the WP and SP *MedSEP* values are as follows:

$${}_{WP} MedSEP = \left(n\right)_{WP}^{-1} \left(M_{i=1}^{n} \left[\left|Y_{i} - f\left(X_{i}...,X_{p}\right)_{i}\right|\right]_{WP}\right)^{2}$$
(26)

$$_{SP} MedSEP = \left(n\right)_{SP}^{-1} \left(M_{i=1}^{n} \left[\left|Y_{i} - f\left(X_{i}...,X_{p}\right)_{i}\right|\right]_{SP}\right)^{2}$$
(27)

where *M* is the median of the absolute values from i = 1 to *n* and $f(X_i, ..., X_p)_i$ is the model-predicted values. A model with the smallest *MedSEP* value is termed as more adequate.

2.5 Information Criteria Statistics

In this research, Akaike's Information Criteria (AIC), Corrected AIC (AICC) and Bayesian Information Criteria (BIC) are used for testing the goodness of fit of the models and to complement the results obtained from MAM. The statistic for each criterion is given as follows.

$$AIC = 2f(\hat{\theta}) + 2p \tag{28}$$

AICC =
$$2f(\hat{\theta}) + \frac{2np}{n-p-1}$$
 (29)

$$BIC = 2f\left(\hat{\theta}\right) + p\log(s) \tag{30}$$

where f() is the negative of the marginal log-likelihood function, $\hat{\theta}$ is the vector of parameter estimates, p is the number of parameters, n is the number of observations and s is the number of subjects.

2.6 Experimental Data and Analysis Procedure

The data used for this research is a balanced 3¹ x 4² replicated mixed Level SP experimental design data is used. The WP has two factors which are irrigation and rice varieties. The irrigation was administered three different times, 7 days, 14 days and 21 days on four different rice varieties, NERICA 2, NERICA 3, NERICA 4 and NERICA 14. The SP factor is nitrogen fertilizer and it was administered at four different rates, 30kg N ha⁻¹, 60kg N ha⁻¹, 90kg N ha⁻¹ and 120kg N ha⁻¹ on each of the four varieties of rice. The aim of the field trial was to determine irrigation effect on the yield of rice. The research was conducted by Institute of Agricultural Research, Ahmadu Bello University, Zaria, at their experimental field station in Kano State, Nigeria. The procedures for analysis are as follows.

1. Performed a traditional SP experimental design analysis. This was done to see which of the effects are significant because only the significant effects will be included for the main nonlinear model. Another reason is to avoid unnecessary inclusion of factors in the model and to decrease the number of parameter estimates. To achieve this step using SAS software, the Proc Mixed code is used.

- 2. After identifying the significant effects, a reanalysis is performed to obtain the parameter estimates in terms of regression model. The reason is the size of parameters to be estimated will be too large for meaningful nonlinear modeling and as well interpretation of results. At this stage, the main effects, and their significant interaction effects, the WP and SP V are estimated using the MLE and REML methods as implemented in SAS software through Proc Mixed. A total of 11 parameters are estimated including the asymptote, scale and shape parameters. These parameter estimates are used as initial values for the main NSPD models under study.
- 3. The asymptote, shape and scale parameters for each of the nonlinear functions used for remodeling the traditional SPD model where estimated using Proc Nlin code in SAS.
- 4. The 11 parameter estimates are used as initial estimates for the nonlinear models formulated in this research. The SAS Proc Nlmixed code is used at this stage of the research to obtain the results for EGLS. While the Proc Nlin code is used for obtaining the OLS results.
- 5. The residuals obtained from each fitted NSPD models are used to calculate all four median adequacy measures introduced in the research for assessing the adequacy of each fitted models so as to identify which model is a better adequate model.

3. Results and Discussion

Table 1 and Table 2 below present the analysis of variance tables. Table 1 shows that all main effects and two factor interaction effects are significant at 5% significance level since their respective p-values are all less than 5%. However, the three factors interaction effect is not significant because its p-value of 0.1271 is greater than 5% significance level. Based on the outcome of the analysis, the three factor interaction effect is removed and a reanalysis is performed. Table 2 presents the reanalysis which is a regression SPD analysis results. It was adopted to reduce the large treatments combinations from 48 to 11.

Source	DF	Sum of Square	Mean Square	F Value	Pr > F
Rep	1	17.1653420	17.1653420	2.87	0.1184
Ι	2	742.9498466	371.4749233	62.08	<.0001
V	3	118.0203278	39.3401093	6.57	0.0083
I*V	6	113.7322231	18.9553705	3.17	0.0467
WP Error	11	65.8244525	5.9840411		
Ν	3	198.1498628	66.0499543	22.00	<.0001
I*N	6	156.6209531	26.1034922	8.69	<.0001
V*N	9	187.8973217	20.8774802	6.95	<.0001

 Table 1. A 3×4² Split-Plot Design ANOVA Table

I*V*N	18	84.0821159	4.6712287	1.56	0.1271
SP Error	36	108.099063	3.002752		
Total	95	1792.541509			

 Table 2. A 3×4² Regression Analysis with Split-Plot Errors ANOVA Table

Source	DF	Sum of Square	Mean Square	F Value	Pr > F
Rep	1	412.51782	412.5178	26.96	<.0001
Ι	1	342.730368	342.7304	22.4	<.0001
V	1	290.551364	290.5514	18.99	<.0001
I*V	1	0.391008	0.391008	0.03	0.8734
WP Error	1	248.383603	248.3836		
Ν	1	799.986622	799.9866	52.28	<.0001
I*N	1	407.134252	407.1343	26.61	<.0001
V*N	1	27.35356	27.35356	1.79	0.1847
SP Error	88	1346.558516	15.3018		
Total	95	3875.607113			

The results show that all the main effects and interaction effects are significant at 5% significance level except for I*V (Irrigation by variety) and V*N (variety by nitrogen) interaction effects. This is because I*V and V*N respective p-values are greater than 5%. However, these two interaction effects are not plunged for further analysis because their respective main effects (I, V and N) are all significant at 5% level of significance. The covariance components estimates for the WP and SP are obtained based on this final regression analysis with SP errors. The two methods adopted for estimating the covariance components for this research are MLE and REML techniques. Table 3 presents their respective results.

Parameter	MLE	REML
σ_{δ}^2	0	0.01648
$\sigma_{arepsilon}^2$	16.614	15.3018

 Table 3. Covariance Parameter Estimates

The VC estimates presented in table 3 above shows that the WP variance estimate for MLE is zero which is smaller than the estimates from REML (0.01648). However, for the SP variance estimate, the MLE estimate (16.614) is larger than the estimates from REML (15.3018).

Table 4 presents the Bertalanffy-Richards SPD model parameter estimates, standard errors and P-values from the OLS and EGLS-MLE and EGLS-REML.

Parameter	OLS	EGLS	EGLS	Std. Error	Std. Error	Std. Error	P-value a	P-value	P-value c
		(MLE)	(REML)	а	b	с		b	
$lpha_0$	31.9390	29.0865	28.3639	47.3177	6.5597	2.7898	0.5013	<.0001	<.0001
α_1	2.0587	0.9095	0.3935	3.2736	0.5781	0.6278	0.5309	0.119	0.5322
α_{2}	-1.3165	-0.7443	-0.7994	2.6220	1.1689	1.5459	0.6168	0.5258	0.6063
α_3	0.1809	0.05905	0.2146	0.2865	0.03983	0.07851	0.5293	0.1415	0.0075
$lpha_4$	-0.1208	-0.01086	-0.03419	0.2145	0.06536	0.08182	0.5746	0.8684	0.677
α_5	-0.01252	-0.00379	-0.01289	0.01955	0.002291	0.004147	0.5236	0.1014	0.002
α_6	0.04049	0.01641	0.02241	0.06339	0.008079	0.008382	0.5245	0.045	0.008
ω	-251E-17	-0.03399	-0.3503	0	0.1464	0.1287	<.0001	0.8169	0.007
λ	0.02946	0.08134	15.3236	0.04714	0.1574	13.4821	0.5335	0.6065	0.2585
$\hat{\sigma}_{\delta}^2$	13.4165	5.1112	49.363	0.1378	3.7457	15.5941	<.0001	0.1756	0.002
$\hat{\sigma}_arepsilon^2$	1.4504	6.0407	5.6774	0.04987	1.0725	0.7883	<.0001	<.0001	<.000

Table 4: Bertalanffy-Richards Split-Plot Design Model Parameter Estimates

Letters a, b and c represents OLS, EGLS (MLE) and EGLS (REML) respectively. Bold values imply significance at 5%.

It is seen from table 4 that the parameter estimates obtained from OLS estimation technique and EGLS via MLE and REML estimation techniques are quite similar except for the shape and whole plot variance parameter estimates. However, the model mean estimates, 31.9390, 29.0865 and 28.3639 respectively from the three techniques, OLS, EGLS via MLE and EGLS via REML are not much different from each other but their respective p-values of 0.5013, 0.0001 and 0.0001 shows that only the OLS mean estimate is not significant at 5% significance level. However, the replicate parameter estimates of 2.0587, 0.9095 and 0.3935 with p-values of 0.5309, 0.119 and 0.5322 for OLS and EGLS via MLE and REML respectively are not significant at 5% significance level. Similarly, the variety parameter estimates of -1.3165, -0.7443 and -0.7994 with p-values of 0.6168, 0.5258 and 0.6063 for OLS and EGLS via MLE and REML respectively are not significant at 5% significance level. However, for nitrogen fertilizer effect parameter estimates of 0.1809, 0.05905 and 0.2146 with p-values of 0.5295, 0.1415 and 0.0075 for OLS and EGLS via MLE and REML respectively are REML respectively shows that only EGLS via REML estimate is significant at 5% significance level.

Also, I*V interaction parameter estimates from OLS (-0.1208) and EGLS via MLE (-0.01086) and REML (-0.03419) are not significant because their p-values of 0.5746, 0.8684 and 0.677 are all greater than 5% significance level. However, I*N interaction parameter estimates of -0.01252, -0.00379 and -0.01289 with p-values of 0.5236, 0.1014 and 0.0025 from OLS and EGLS via MLE and REML respectively indicates a significant estimate from EGLS via REML only at 5% significance level. Also, V*N interaction effect parameter estimates of 0.04049, 0.01641 and 0.02241 with p-values of 0.5245, 0.045 and 0.0088 from OLS and EGLS via MLE and REML respectively shows that only the OLS

estimate is not significant at 5% significance level.

The OLS estimates for scale parameter (ω) of -251E-17 is smaller compared to the EGLS estimates via MLE (-0.03399) and REML (-0.3503). Their respective p-values of 0.0001, 0.8169 and 0.0077 indicate that the EGLS via MLE scale parameter estimate is not significant since its p-value is greater than 5% significance level. However, the shape parameter (λ) estimates from OLS (0.02946) which is smaller than that of the estimates from EGLS via MLE (0.08134) and REML (15.3236) but their respective p-values of 0.5335, 0.6065 and 0.2585 implies that the shape parameter estimates are not significant at 5% significance level.

The final whole plot variance component ($\hat{\sigma}_{\delta}^2$) parameter estimate of 49.363 from EGLS via REML is larger than the OLS estimate of 13.4165 and EGLS via MLE estimate of 5.1112. However, the OLS and EGLS via REML estimates are both significant because their p-value of 0.0001 and 0.0021 are less than 5% significance level. But, the EGLS via MLE p-value of 0.1756 is not significant at 5% significance level. While the split-plot variance component estimate ($\hat{\sigma}_{\varepsilon}^2$) from OLS (1.4504) is also smallest compared to the EGLS via MLE (6.0407) and REML (5.6774) estimates. However, their p-values of 0.0001 respectively indicate a significant split-plot variance component parameter estimate at 5% level of significance.

Generally, the standard errors for each of the estimates from the OLS, EGLS-MLE, and EGLS-REML in Table 4 shows that the EGLS via MLE and REML produced similar standard errors compared to the OLS technique parameter estimates standard errors. Conversely, for the model scale parameter and whole plot variance component parameter estimates where the EGL-REML technique produced the largest values compared to the EGLS-MLE and OLS as well. This gives a pre-confirmation that either the EGLS via MLE or REML estimates for Bertanlaffy-Richards SPD model are estimated adequately with better stability. Hence, one of EGLS via MLE or REML techniques is more efficient than the OLS technique. The OLS, EGLS-MLE and EGLS-REML estimated fitted models for the BRSPD model are presented as follows.

$$y_{ijkl} = [31.939 + 2.0587 Rep - 1.3165V + 0.1809N - 0.1208IV - 0.01252IN + 0.04049VN] \\ \times (1 - exp (-251E-17I))^{0.02946}$$
(35)
$$y_{ijkl} = [29.0865 + 0.9095 Rep - 0.7443V + 0.05905N - 0.01086IV - 0.00379IN + 0.01641VN] \\ \times (1 - exp (-0.03399I))^{0.08134}$$
(36)
$$y_{ijkl} = [28.3639 + 0.3935 Rep - 0.7994V + 0.2146N - 0.03419IV - 0.01289IN + 0.02241VN]$$

$$\times (1 - exp(-0.03399I))^{15.3236}$$
(37)

Table 5 below shows that the r_r^2 , *Pred*- r_r^2 , *RMEF* and *MedSEP* values for the OLS, EGLS-MLE and EGLS-REML estimated fitted BRSPD Models are similar for the WP and SP sub models. However,

it can be seen that the EGLS-REML have the largest r_r^2 values of 99.99979% and 83.91%, *Pred-r_r*² values of 99.999758% and 75.5%, and *RMEF* values of 99.9997% and the smallest *MedSEP* values of 2.76E-12 and 0.027643 for the WP and SP sub models respectively. This implies that the EGLS-REML estimated fitted BRSPD model has a larger proportion of variability explained in the data, better prediction power, more efficient and better error prediction strength for the WP and SP sub models by their respective factors, I, V and N. However, the WP sub design model have larger r_r^2 , *Pred-r_r^2* and *RMEF* values compared to the SP sub design model and the *MedSEP* values for the WP sub design model is smaller compared to the SP sub design model for all the OLS, EGLS-MLE and EGLS-REML estimated fitted BRSPD model.

	r_r^2		$Pred - r_r^2$		RMEF		MedSEP	
	WP	SP	WP	SP	WP	SP	WP	SP
OLS	0.9934546	0.7286645	0.99259238	0.586442	0.999665	0.779233	2.59E-05	0.078609
MLE	0.999686	0.7776782	0.99964469	0.661147	0.992581	0.73505	5.97E-08	0.052775
REML	0.9999979	0.8390977	0.99999758	0.75476	0.999997	0.840852	2.76E-12	0.027643

Table 5. Median Adequacy Measures Results

However, Table 6 below presents the goodness of fit results for the fitted models and it showed that EGLS-REML produced the lowest AIC, AICC and BIC values of 483.7, 486.8 and 473.8 respectively. This implies that the EGLS-REML estimation technique produces reliable and stable estimates compared to EGLS-MLE and OLS parameters estimates.

Method	AIC	AICC	BIC
OLS	496.4	499.5	524.6
MLE	487.5	490.6	477.6
REML	483.7	486.8	473.8

Table 6. Model Goodness of Fit Test Results

4. Conclusion

Based on the research results from the analysis on a balanced $3^1 \ge 4^2$ replicated mixed Level SP experimental design data, it was observed that the fitted BRSPD model is a good fit for the EGLS-REML estimated model. This is because all the four MAM for assessing the adequacy of the fitted model produced larger r_r^2 , *Pred-r_r*² and *RMEF* values and smaller *MedSEP* values for the WP and SP sub models and as well smaller AIC, AICC and BIC values compared to the EGLS-MLE and OLS estimated models respectively. Also, all the respective OLS, EGLS-MLE and EGLS-REML estimated fitted INSPD models for the WP sub models produced better adequacy measure values compared to the SP sub models. However, the OLS, EGLS-MLE and EGLS-REML respective parameter estimates

standard errors showed that the EGLS-REML parameter estimates are quite stable and reliable because of its comparable small standard errors values with that of EGLS-MLE and OLS standard errors estimates. Also, seven out of the eleven parameter estimates for the EGLS-REML were significant at 5% significance level compared to OLS fitted model with only three significant parameters and none for EGLS-MLE. Therefore, it can be concluded that the EGLS-REML fitted model is a good fit that is adequate, stable and reliable for prediction.

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6. References

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