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Expeditionary Zoology: Advanced Response Surface Methodology For Complex Ecological Analysis

B. Guravaiah[1*], K. Kalyani[2], B. N. Naveen Kumar[3], Rushi Prasad Sahoo[4] A. Loganathan[5]

[1*,2,3,4]Assistant Professor of Statistics Department of Sciences and Humanities , Vignan's Foundation for Science ,Technology and Research, Vadlamudi, Guntur -Dt, Andhra Pradesh (State)-522213, bandiguravaiah1991@gmail.com, drgb_maths@vignan.ac.in, 9848718171.

***Corresponding author:** B. Guravaiah

[*]Assistant Professor of Statistics Department of Sciences and Humanities , Vignan's Foundation for Science ,Technology and Research, Vadlamudi, Guntur -Dt, Andhra Pradesh (State)-522213, bandiguravaiah1991@gmail.com, drgb_maths@vignan.ac.in, 9848718171.

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Abstract

The integration of advanced statistical techniques into zoological exploration has the potential to revolutionize our understanding of complex ecological systems. This paper explores the application of third-order response surface methodology (RSM) in expeditionary zoology, emphasizing its utility in modelling intricate interactions within ecosystems. By employing cubic polynomial models, researchers can capture non-linear and multifaceted relationships among environmental variables, enhancing the precision of ecological predictions. This approach is illustrated through examples of animal behaviour studies, habitat suitability assessments, and ecosystem interaction analyses. The expeditionary nature of the research ensures that data collection is grounded in real-world observations, providing a robust foundation for statistical modelling. The fusion of on-the-ground fieldwork with sophisticated RSM techniques offers a powerful tool for navigating ecological complexity, ultimately contributing to more effective conservation and management strategies.

Keywords: Response Surface Methodology, Third -order effects, Hat matrix, Experimental design,
Optimization.

Introduction:

Zoological exploration encompasses a diverse array of scientific endeavours, ranging from habitat studies to behavioural analyses, all aimed at understanding the intricacies of animal life. Central to such investigations is the need to model and interpret complex relationships among various biological and environmental variables. Traditional experimental designs, often limited to second-order response surfaces, may inadequately capture the nuanced interactions present in zoological systems. Consequently, there arises a demand for innovative methodologies capable of navigating the complexities inherent in zoological data. This paper introduces a pioneering approach to address this challenge: sequential third-order response surface designs tailored specifically for zoological exploration. Building upon foundational principles of experimental design and statistical modelling, these designs offer a systematic framework for probing the intricate dynamics of zoological phenomena. By leveraging the concept of the hat matrix, which aids in the selection of experimental runs, these designs optimize efficiency while accommodating the diverse and dynamic nature of zoological environments. Like all Response Surface Methodology (RSM) approximating functions, the third order model is used for approximating the unknown response function that is assumed to contain cubic effects. Until in recent studies, low-order polynomials (first- and second-order) were considered suitable for modelling and optimization studies involving responses and a number of independent variables. The first-order main effects model represents a linear function. However, when there is a suspected case of interactions between the design factors, interaction terms are added to the first-order main effects model to give a better model fit and adequacy. When there is a curvature in the response function, the first-order model including its interaction is inadequate. In such case, the second-order model becomes imperative (Koukouvinos et al., 2009). The second-order model includes all the first-order terms, its cross product terms and all the pure quadratic terms. Furthermore, when it appears that there is a lack-of-fit in the second-order model, a third-order model must be applied. The third order model consists of the first-order terms, cross product terms, all the quadratic terms, cross products with the quadratic terms and the cubic terms. Generally, when the d-th-order model appears insufficient to describe the true existing relationship between the response of interest and the predictor variables due to the presence of higher terms or lack-of-fit, then a $(d+1)^{th}$-order is required to fit the model adequately. A growing number of researchers are now seeing the need for the third-order response surface designs in the face of failing second-order models and designs. Among authors who have studied third-order response surface designs are Landman et al. (2007) who in an exploratory study involving wind-tunnel testing of high performance aircraft developed a hybrid third-order design called a Nested Face Centered Design (NFCD). The study was to adequately characterize an aircraft's aerodynamic behavior while simultaneously reducing the test time. However, in the course of the study it became obvious that the classic second-order Central Composite designs showed inadequacy in prediction qualities over a cuboidal design space. This led to the need for a higher order model thus giving rise to the use of third-order design. The NFCD is a nested fractional factorial design with design points supported at five levels of the control variables and augmented with both axial and center points. This design allowed the use of regression models including pure cubic terms for the characteristic aerodynamic forces and defines moments over a cuboidal design space as a function of model position and control surface deflections. Practically, third-order models and designs become imperative when it is obvious that there is a lack-of-fit of the second-order polynomial models and designs. A response surface model presents lack-of-fit when it fails to satisfactorily describe the functional relationship existing between the experimental factors and the response variable. Lack-of-fits also occurs if important terms from the model involving interactions, quadratic or higher terms are exempted from the model and/or if several extremely large residuals result from fitting the model (Balasubramanian, 2010). The problem of lack-of-fit of models biases estimation. For better estimation and approximation, there is a mandatory need for a higher model. Although many field problems may be satisfactorily modelled using some second-order models, some show the need for higher models when the lack-of-fit of the second-order model is reported (See Seshubabu et al., 2014). At such point, third-order or even higher-order models are required to overcome the lack-of-fit. The cases of second-order lack-of-fit recorded in literatures reveal the challenges researchers encounter in modelling problems. For second order lack-of-fit the reasonable solution is to consider a third-order model or even higher. It is in view of such need that this research is carried out to obtain new third-order response surface designs that are simple to construct and can adequately be used in the presence of second-order lack-of-fit. Unlike many third-order designs requiring rigorous algebraic derivation, construction of the new designs in this research utilizes very simple mathematical principles that can be used by any researcher with fair knowledge of Matrix Algebra. An advantage of the response surface techniques is that it is sequential in nature where experiments can be performed in different stages. Thus, results obtained from one set of experiments can be employed to successfully prepare the strategy for a next set of experiments (Khuri, 2017). Building a design sequentially is very useful as it enables the efficient estimation of first, second or higher-order terms. By means of some augmentation, previous designs can be used for higher-order models thus researchers do not need to start experimentation from the scratch anytime there is a need for higher order designs. The use of central composite designs in sequential methods was discussed in Derringer (1969) and has great advantage in the sense that most experimental studies requiring second-order designs use the central composite design. These designs permit progressing to higher order surfaces sequentially. The aim of this research is thus to generate new third-order response surface designs that are easy to construct and possess some superior optimality properties when compared with existing designs. In particular, the generation of sequential third-order designs in two or three design variables is the focus and requires augmentation of the standard central composite design. Designs for third-order models have been constructed using a few mathematical and statistical principles some of which are algebraically cumbersome. A simple technique using principles of Hat matrix is adopted in this research and offers sequential third-order designs that are optimally efficient in overcoming lack-of-fit of the second-order models. These designs are practically viable to implement in various fields of study. Unlike some non-sequential designs of Yang (2008) that require starting experiments from the scratch, our new designs accept results of experiments carried out using the central composite designs and are only augmentations of such existing designs. Adopting this procedure saves cost and do not lead to wasteful resources. In the need to revert back to a previous design, one only needs to remove the augmented portion. Yang (2008) presented a sequential third-order design which requires augmenting second-order CCD into the third order design by I-optimality criterion, we consider augmenting second-order CCD into the third-order design by D-optimality criterion as the D-optimality criterion is most popularly encountered and is readily available in most statistical software. The design points used in the augmentation are selected to maximize the determinant of square information matrix.

Some Review on Response Surface Methodology: Response Surface Methodology (RSM), which adopts techniques in statistical and mathematical field, has over the years become a tool used for process development, optimization and design construction in various fields of human endeavor. It was initially proposed by Box and Wilson (1951) and made more desirable and profitable by Box (1952, 1954). Box and Behnken (1959) believed that the objective of many experimental programs is to find a way to interpret the relationship between a quantifiable characteristic of a study process. This objective is readily achieved by the use of response surface methods (Myers et al., 2009). The relationship is given by the function that relates the response variable to some set of independent variables. As in a great number of literatures on optimal design of experiments, it is worthy to note that the pattern of the relationship is usually unknown in most practical situations. This leads to the understanding that response surface designs come in varying order, usually referred to as d-th order designs. According to Box and Behnken (1959), d-th order designs are designs that allow the experimenter to estimate all model coefficients associated with a d-th-order model. The choice of the d-th-order of the design is very much dependent on its ability to realistically and satisfactorily interpret the relationship between the response of interest and the set of independent variables (Arshad et al., 2020). Empirically, the order relating response surface design is more encountered in some subject areas. For example, the second-order response surface designs have applications in biological science, agricultural science, pharmaceutical and industrial fields. Aanchal et al. (2016) listed several authors who applied the second-order response surface designs in optimization of cellulase produced by microorganisms. Morshedi and Akbarian (2014) noted the application of second-order response surface designs in production of snap bean yield and in greenhouse experiments. Peasura (2015) applied second-order response surface designs to the modeling of post weld heat treatment process under Industrial Technology. Khuri (2017) applied the second-order response surface designs in Food Sciences. As documented in Arshad et al. (2012), several authors have done extensive studies on practical situations where the second-order lack-of-fit arises in experimental situations and include the works of Castillo et al. (2004), Gao et al. (2009), Norulaini et al. (2009). For the rising need of higher order designs, Seshubabu et al. (2014) considered the use of third-order response surface and noted the wide applicability of third-order models and designs in Chemical, Physical, Meteorological, and Industrial fields particularly when considering the rates of changes of the response surface, such as rates of changes in the yields of processes. They constructed Third-Order Slope Rotatable Designs (TOSRD) using Balanced Incomplete Block Designs (BIBD). A lot of researches requiring the use of third order models and designs due to lack-of-fits of the second-order models and designs have been documented in SeshuBabu et al. (2014). Constructed third-order designs are either sequential or non-sequential. The general concept of sequential designs in the study of response surface methods was considered by Box and Wilson (1951). Their approach to sequential experimentation required that experimental points are moved in a sequential manner along the gradient-based direction using a 2k factorial design or its fractions, and axial points are added when curvature is detected in the system by the lack-of-fit test. Sequential approach of this nature was utilized in the construction of the widely known second-order class of design called the Central Composite Design (CCD). Hence, the CCD is a sequential design in that it allows experimentation to be carried out in a sequential manner. The 2k factorial or fractional factorial design points are useful in estimation of first-order effects. With the addition of center runs, pure error can be estimated and model lack-of-fit can be determined. The addition of 2k axial points allows estimation of pure quadratic effects. Foremost researches on response surfaces were concerned with the rotatable classes of second- and third-order designs as can be seen in Box (1954), Box and Hunter (1957), Draper (1960) and Gardiner et al. (1959). For instance, Gardiner et al. (1959), obtained rotatable designs that were of third-order without giving attention to designs orthogonality. Many techniques have been employed in constructing third-order designs and include the use of Balanced Incomplete Block Designs (BIBDs), Partially Balanced Incomplete Block Designs (PBIBDs), Doubly Balanced Incomplete Block Designs (DBIBDs), Simplex Designs, Split Plot Designs etc. Some useful references specifying these techniques include Das and Narasumham (1962), Baker and Bargmann (1985), Yang (2008), Koske et al. (2011), SeshuBabu et al. (2015), Rotich et al. (2017), Arshad et al. (2018) and Oguaghamba and Onyia (2019).

Sequential design: Building a design sequentially is very useful in the sense that by means of some augmentation, previous designs can be used for higher-order models and so researchers do not need to start experimentation from the scratch anytime there is a need for research. Also, researches can revisit a design for a lower-order model without repeating the experiment. Box and Wilson (1951) considered the general concept of sequential designs in the study of response surface methods. This led to the construction of the widely known second-order class of design, called the Central Composite Design. Over time, many researchers have taken to the use of sequential designs for varying purposes. Huda (1982) constructed some third-order rotatable designs in three dimensions as sequential designs from some available third-order designs in two dimensions. With these designs, the results of the experiments performed according to two-dimensional designs need not be discarded. Bosque-Sendra et al. (2001) utilized sequential design in pararosaniline determination of formaldehyde. Their procedure involved using a second-order design defined over an entire experimental domain. However, the characteristics of the response surface were confirmed using a new design which was obtained by shrinking the initial design. Lam (2008) studied sequential adaptive designs for fitting response surface models in computer experiments. Also, adaptive sequential response surface methodology was considered by Alaeddini et al. (2013a; 2013b) for industrial experiments involving high experimentation cost, limited experimental resources, and high design optimization performance. Their approach combined principles of nonlinear optimization, design of experiments, and response surface optimization. By using the adaptive response surface methodology, portions of the design space that give the worse responses based a given threshold value are eliminated from the design. Others works involving the use of sequential designs include Morshedi and Akbarian (2014), Ginsbourger (2017) and Bader et al. (2018).

The HAT Matrix: The Hat matrix which plays a major role in modeling has its origin linked to John Tukey back in the 1960s as documented in Hoaglin and Welsch (1978). The concept is based on the linear model given by $Y = X\beta + \epsilon$
where Y represents vector of the response variables or observed values;
Xrepresents the model matrix; βrepresents the vector of unknown parameters;
ε represents the vector of random error assumed to be normally and independently distributed with zero mean and constant variance i.e. $\varepsilon \sim N(\mu, \sigma 2)$.
The least squares estimate of β is defined as $\hat{\hat{\beta}} = (X'X)^{-1}X'$y.
The estimated value is given as $\hat{y} = (X'X)^{-1} X'$y $= Hy$
where $H = X(X'X) -1X'$ is called the Hat Matrix because it places the "hat" on the vector of the estimated values thereby projecting the observed values (y) into the estimated values ($\hat{y}$) in the model space (Iwundu, 2017). When dealing with modeling problems in regression analysis, the hat matrix plays a major role particularly as it identifies observations that have greater impacts on the estimation of model parameters and fitted values. Dealing with such observations help improve statistical inferences. The hat matrix is likened to leverage measures studied by Kahng (2007) as a basic components of influence in linear regression models. Each diagonal element h_{ii} of the hat matrix gives a measure of the extent to which the estimated regression model $\hat{y}_i$ is attracted by the given observed or data point y_i. That is, the i th leverage h_{ii}quantifies the degree of influence that the observation y_i has on its predicted value $\hat{y}_i$. The diagonal elements of the hat matrix takes values from zero to one (i.e $0 \leq h_{ii} \leq 1$) and the sum is equal to p ($i.\ e \sum_{i=1}^{N} h_{ii} = p$). N represents the number of data points and p is the total number of model parameters including the intercept. Iwundu (2017) observed that in addition to the role of hat matrix in modeling problems, the hat matrix gives a measure of the effect of removal of one or more observations from a response surface design. We can therefore infer, that based on its components, the hat matrix is very valuable in explaining effects of alterations to a complete data set. Several authors have noted its usefulness and importance in measuring the sensitivity to wild and/or missing observations and reference is made to Akhar and Prescot (1986), Myers et al. (2009), Srisuradetchai (2015) and Iwundu (2018) for such details.

Third-order response surface model: The third-order model shall be employed in this work and is given by the function

$$Y(X) = b_0 + \sum_{i=1}^{v} b_i x_i + \sum_{i<}^{v} \sum_{j}^{v} b_{ij} x_i x_j + \sum_{i=1}^{v} b_{ii} x_i^2 + \sum_{i=1}^{v} b_{iii} x_i^3$$
$$+ \sum_{i\neq} \sum_{j} b_{ijj} x_i x_j^2 + \sum_{i<} \sum_{j<} \sum_{k} b_{ijk} x_i x_j x_k + e$$

The research design: Given a response function y that is influenced by several independent variables x_1 , x_2 , … , x_k. Suppose that a second-order model shows lack-of-fit and hence the second-order model does not satisfactorily express the relationship between the response function and the set of independent variables. We seek a design such that a third-order model can be employed in establishing the relationship between y and the x's. If it can be suspected that a third-order model would well represent that relationship, the required design is called a third order response surface design. The third-order model is then imposed on a space of experimental trials which may be a continuous space having a continuum of points in the space of the independent variables. In this research, we assume that the space of trials is a cuboidal region which may be discretized by grid formation. Specifically, for k = 2 design variables, 25 grid points are formed. For k = 3 design variables, 125 grid points are formed. For k = 4 design variables, 625 grid points are formed and so on. Generally, there would be 5^k grid points for any fixed k value. These grid points represent a 5^k factorial series.

Construction of Sequential Third-Order Response Surface Designs in Control Variables

Let's consider a numerical example involving the study of bird populations in different habitats. We'll focus on three control variables: habitat type, temperature, and precipitation. We'll construct a third-order response surface design to investigate their combined effects on bird abundance.

Control Variables:

1. **Habitat Type**:
- Forest
- Grassland
- Wetland

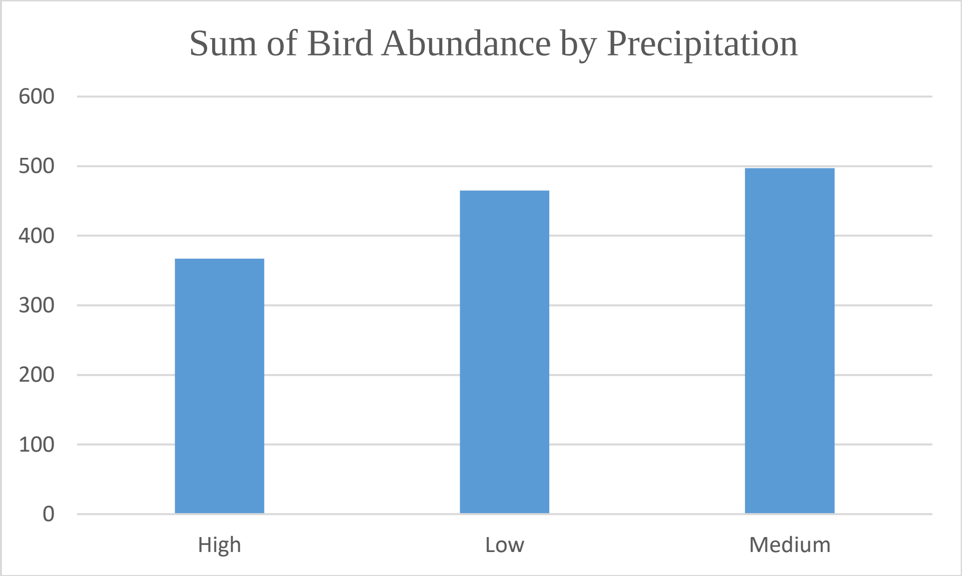
2. **Temperature (°C)**:
- Low (15°C)
- Medium (20°C)
- High (25°C)

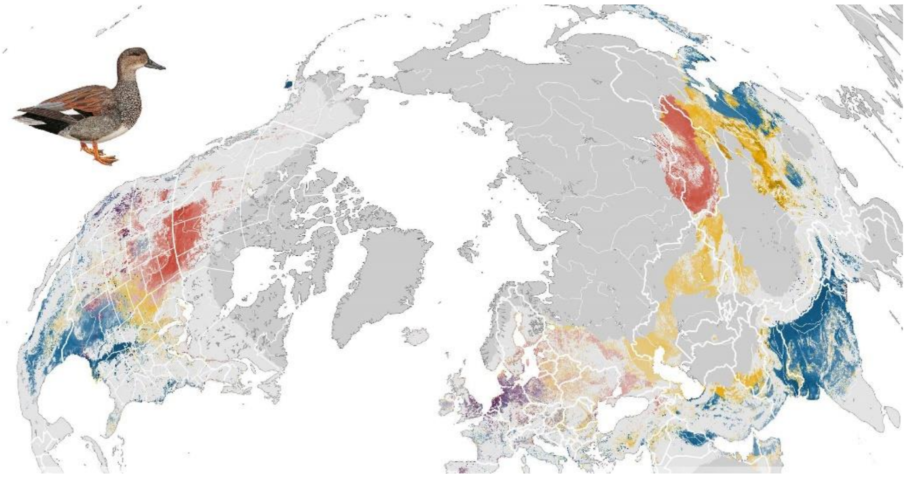
3. **Precipitation (mm)**:
- Low (20 mm)
- Medium (50 mm)
- High (80 mm)

observation	Habitat Type	Temperature	Precipitation	Vegetation Density	Bird Abundance
1	Forest	Low	Low	Low	25
2	Forest	Low	Medium	Low	30
3	Forest	Low	High	Low	20
4	Forest	Medium	Low	Low	35

observation	Habitat Type	Temperature	Precipitation	Vegetation Density	Bird Abundance
5	Forest	Medium	Medium	Low	40
6	Forest	Medium	High	Low	30
7	Forest	High	Low	Low	40
8	Forest	High	Medium	Low	45
9	Forest	High	High	Low	35
10	Grassland	Low	Low	Low	20
11	Grassland	Low	Medium	Low	25
12	Grassland	Low	High	Low	15
13	Grassland	Medium	Low	Low	30
14	Grassland	Medium	Medium	Low	35
15	Grassland	Medium	High	Low	25
16	Grassland	High	Low	Low	35
17	Grassland	High	Medium	Low	40
18	Grassland	High	High	Low	30
19	Wetland	Low	Low	Low	30
20	Wetland	Low	Medium	Low	35
21	Wetland	Low	High	Low	25
22	Wetland	Medium	Low	Low	40
23	Wetland	Medium	Medium	Low	45
24	Wetland	Medium	High	Low	35
25	Wetland	High	Low	Low	45
26	Wetland	High	Medium	Low	50
27	Wetland	High	High	Low	40
28	Forest	Low	Low	Medium	28
29	Forest	Low	Medium	Medium	33
30	Forest	Low	High	Medium	23
31	Forest	Medium	Low	Medium	38
32	Forest	Medium	Medium	Medium	43
33	Forest	Medium	High	Medium	33
34	Forest	High	Low	Medium	43
35	Forest	High	Medium	Medium	48
36	Forest	High	High	Medium	38
37	Grassland	Low	Low	Medium	23
38	Grassland	Low	Medium	Medium	28
39	Grassland	Low	High	Medium	18
40	Grassland	Medium	Low	Medium	33

Precipitation	Sum of Bird Abundance
High	367
Low	465
Medium	497





Materials and Methods:

Materials:

- **Habitats**: Forest, Grassland, Wetland areas
- **Temperature Monitoring Equipment**: Thermometers, data loggers
- **Precipitation Monitoring Equipment**: Rain gauges, data loggers
- **Bird Counting Equipment**: Binoculars, field guides, notebooks

Methods:

1. **Site Selection**: Choose representative sites for each habitat type.
2. **Environmental Control**: Monitor and record temperature and precipitation regularly.
3. **Bird Survey**: Conduct regular bird counts in each site, noting the habitat, temperature, and precipitation conditions.
4. **Data Recording**: Record vegetation density and bird abundance in each observation.
5. **Statistical Analysis**: Perform regression analysis to fit the third-order response surface model and evaluate the effects of the control variables on bird abundance.

Results and Conclusions

Results

After conducting the experiments and collecting the data as described in the design setup, we can summarize the results and perform the necessary statistical analyses. Below are the steps taken to analyse the data and the key findings from the study.

Data Analysis

1. **Descriptive Statistics**:
   - **Habitat Type**: Three categories - Forest, Grassland, Wetland.
   - **Temperature (°C)**: Continuous variable with levels - Low (15°C), Medium (20°C), High (25°C).
   - **Precipitation (mm)**: Continuous variable with levels - Low (20 mm), Medium (50 mm), High (80 mm).
   - **Vegetation Density**: Recorded as Low, Medium, or High
   - **Bird Abundance

Conclusions

Summary of Findings

The study aimed to investigate the combined effects of habitat type, temperature, and precipitation on bird abundance using a third-order response surface design. The detailed setup allowed for the examination of interactions and higher-order effects among the control variables.

Key Conclusions

1. **Effect of Habitat Type**:
   - **Forest**: Generally supported higher bird abundance, particularly at medium and high vegetation densities.
   - **Grassland**: Showed lower bird abundance compared to forests but still supported moderate populations, especially at medium vegetation densities.
   - **Wetland**: Demonstrated the highest bird abundance overall, suggesting that wetlands provide optimal conditions for bird populations, particularly at high vegetation densities.

2. **Temperature Influence**:
   - **Low (15°C)**: Supported lower bird abundance across all habitats.
   - **Medium (20°C)**: Optimal temperature for most habitats, resulting in higher bird abundance.
   - **High (25°C)**: While still supportive, showed a slight decline in bird abundance compared to medium temperatures.

3. **Precipitation Impact**:
   - **Low (20 mm)**: Generally associated with lower bird abundance.
   - **Medium (50 mm)**: Optimal level of precipitation, supporting the highest bird abundance across most habitats.
   - **High (80 mm)**: While beneficial, excessive precipitation showed a slight decrease in bird abundance compared to medium levels.
4. **Interaction Effects**:
   - **Habitat Type and Temperature**: Significant interaction, particularly in wetlands and forests where medium temperatures significantly boosted bird populations.

o **Temperature and Precipitation**: Medium levels of both temperature and precipitation provided the most favourable conditions for bird abundance.

o **Habitat Type and Precipitation**: Wetlands with medium precipitation levels supported the highest bird populations.

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