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Research Article

Performance Evaluation of Custom A-, D-, and I-Optimal Designs for Non-Standard Second-Order Models

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Abstract

The performances of Custom A-, D-, and I-optimal designs on non-standard second-order models are examined using the alphabetic A-, D-, and G-optimality efficiencies, as well as the Average Variance of Prediction. Designs of varying sizes are constructed with the help of JMP Pro 14 software and are customized for specified non-standard models, optimality criteria, prespecified experimental runs, and a specified range of input variables. The results reveal that Custom-A optimal designs perform generally better in terms of G-efficiency. They show high superiority to A-efficiency as the worst G-efficiency value of the created Custom-A optimal designs exceeds the best A-efficiency value of the designs, and also does well in terms of D-efficiency. Custom-D optimal designs perform generally best in terms of G-efficiency, as the worst G-efficiency value exceeds all A- and D-efficiency values. Custom-I optimal designs perform generally best in terms of G-efficiency as the worst G-efficiency value is better than the best A-efficiency value and performs generally better than the corresponding D-efficiency values. For the Average Variance of Prediction, Custom A- and I-optimal designs perform competitively well, with relatively low Average Variances of Prediction. On the contrary, the Average Variance of Prediction is generally larger for Custom-D optimal designs. Hence when seeking designs that minimize the variance of the predicted response, it suffices to construct Custom A-, D-, or I-optimal designs, with a preference for Custom-D optimal designs.

Keywords

Custom A-, D-, and I-optimal Designs, Non-Standard Second-Order Model, Average Variance of Prediction, D-, G-, A-efficiency

1. Introduction

In most response surface experiments, the full second-order model is assumed to be a true approximation of the underlying mechanism. Montgomery noted that experimenters may have a foreknowledge of the process being studied, which could suggest the need for a non-standard model in Montgomery, D.C. [13]. In like manner, Gaifman, H. [2] observed that one may have doubts about standard models and opt for an alternative model. According to Myers *et al*. [14], non-standard second-order models are reduced models which is a result of the removal of some insignificant terms in the full second-order models. Iwundu, M. P. [7] observed that model fitting may reveal that not all model parameters are significant after data have been collected. Hence, there is a need to remove insignificant parameters thus resulting in a reduced model. Some literature on the Design of Experiments (DOE) sees non-standard models as models that contain different

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types of variables (both categorical and continuous) or models that have underlying forms that may not comply with the usual standard linear models Johnson *et al*. [9].

As far back as the 20th century, Kiefer and Wolfowitz [11], Kiefer and Wolfowitz [12] introduced the use of computers to create optimal designs in most non-standard situations. Hence, with the availability of computers, statistical software, and programming languages, experimenters can go beyond the limitations of classical or standard designs to create optimal designs that align with specific experimental objectives. Warren F. K. [19] supported that when faced with non-standard situations, the computer can be used to generate efficient designs whereby the precision of the parameter estimate is maximized. Furthermore, when a suitable orthogonal design does not exist, computer-generated non-orthogonal designs can be used as a good alternative.

Although some standard designs are robust to model misspecification it is necessary to use a more appropriate design, computer algorithms can be used to generate optimal designs for any specified model but with strict adherence to design optimality criterion depending on the goal of the experiment Montgomery, D.C. [13]. Computer-generated designs (CGDs) have also shown usefulness in mixture experiments, constrained design spaces, and situations where a botched experiment needs to be salvaged Kiefer and Wolfowitz [11].

As its name, computer-generated designs are designs that are generated automatically using a computer algorithm or software programs that are based on predefined statistical principles and do not require manual input from the researcher. The software has built-in mathematical optimization techniques that enable it to generate efficient experimental designs under given design conditions. Closely related to the computer-generated design is custom design which allows experimenters to carefully choose the factors, the levels, and how the treatments should be arranged to solve the research questions effectively. Custom designs are situated in most high-level statistical software such as JMP and Design Expert. They provide a platform for flexibility in the design of experiments. Custom designs involve designing an experiment either manually or with the help of computer programs, based on specific research objectives, constraints, and available resources in a way that allows experimenters to gather relevant data to draw meaningful insights. Rather than force a standard design into the space of the research problem, custom designs can be readily tailored to the problem and resource limitations Johnson *et al*. [9]. Researchers can bring in their knowledge of the process under study and make appropriate adjustments based on practical considerations to effectively address their research questions.

According to Zhou and Xu [22], an essential part of process optimization is the need to obtain an approximation that expresses the relationship between the response variable and the set of factors (independent variables). The second-order model provides a robust approximation and it is widely used for approximating a continuous underlying relationship between the response (y) and a set of experimental factors (k) Walsh *et al*. [18]. For second-order experiments, the assumed model is of the form

$$y = \beta_0 + \sum_{i=1}^{k} \beta_i x_i + \sum_{i=1}^{k} \beta_{ii} {x_{ii}}^2 + \sum_{i<j} \sum \beta_{ij} x_i x_j + \varepsilon \tag{1}$$

where y represents the predicted response, β_0 represents the model intercept, β_i, β_{ii}, β_{ij} are the regression coefficients for the linear, quadratic, and interactive effects of the model respectively.

The error term (ε) is usually assumed to be independently and identically distributed with mean 0 and variance δ^2. The variables X_i and X_j are the factors, and could be k dimensional, where k is the number of factors considered by the experimenter. The model in equation (1.1) is usually known as a p parameter model and an interest could be to obtain the best model parameter estimate containing some desirable statistical properties including unbiasedness of the estimators, minimum variance of the estimators, etc. Interestingly, these properties may be easily obtained if a good design of the experiment is achieved.

Standard models are intended models for a process under study using standard designs. However, there are certain situations when standard designs are unsuitable for expressing the relationship between the dependent variable and the independent variables in these models. Johnson *et al.* [9] observed that when the experimental problem involves unusual resource restrictions, when there is a presence of constraints on the design region, or when the model is non-standard, a standard experimental design becomes unfit to solve such research problem and hence an alternative design is required to explain the response appropriately. Smucker *et al.* [17] stated that the presence of constraints in some experiments may prevent the use of standard designs. Akinlana D. M. [1] described some experimental conditions where standard designs are unsuitable such as, when the model of interest is in a particular order, when a smaller sample size is required, or when there are constraints on the design region. For such situations listed by Akinlana D. M. [1], Johnson *et al.* [9], and Smucker *et al.* [17], it is in doubt how well a standard response surface design is appropriate. Although some standard response surface designs are robust to model misspecification, there is a need for alternative designs that are more economical and efficient. For example, Akinlana D. M. [1] considered the estimation of multiple responses using a computer algorithm based on D-optimality and compared the performance of the design to that of a Unique Factor-Central Composite Design (UF-CCD).

To avoid misapplication of experimental designs when standard designs do not seem appropriate, it is good to opt for custom designs. Researchers can customize their designs in two ways; (i) by manually specifying the factors, levels, and other properties of the design or (ii) by using the custom design platform in some statistical software that involves specifying the factors, levels, and other experimental parameters to create a tailored experimental design. The JMP software includes a platform for custom design to provide users with the flexibility and capability to create experimental designs that are tailored to their specific research objectives and constraints Akinlana D. M [1]. The custom design platform constructs an optimal design to fit the research problem, taking into account one's ability to manipulate factors, constraints on factor settings, information from covariates, and other experimental conditions and resource restrictions. To use the custom design platform in JMP, a first-step requirement is to define the goal of the experiment. Also, the optimality criterion must be specified as it helps to reflect the objective of the experiment.

The purpose of this research is to evaluate the performance of custom A-, D-, and I-optimal designs for non-standard second-order models and this will be achieved by;

i. Creating custom designs of varying sizes for non-standard second-order models based on the A-optimality criterion;
ii. Creating custom designs of varying sizes for non-standard second-order models based on the D-optimality criterion;
iii. Creating custom designs of varying sizes for non-standard second-order models based on the I-optimality criterion; and
iv. Evaluating the quality or performance of the custom designs using design efficiency metrics.

2. Methodology

2.1. The Experimental Models

This research considers three non-standard models in three input variables and one non-standard model in four input variables. The non-standard models considered are;

$$\hat{y}\,(x_1, x_2, x_3) = \hat{\beta}_0 + \hat{\beta}_1 x_1 + \hat{\beta}_2 x_2 + \hat{\beta}_3 x_3 + \hat{\beta}_{11} {x_1}^2 \tag{2}$$

Source: Myers *et al*. [14].

$$\hat{y}\,(x_1, x_2, x_3) = \hat{\beta}_0 + \hat{\beta}_1 x_1 + \hat{\beta}_2 x_2 + \hat{\beta}_3 x_3 + \hat{\beta}_{23} x_2 x_3 + \hat{\beta}_{33} {x_3}^2 \tag{3}$$

Source: Ossia and Big-Alabo [15]

$$\hat{y}\,(x_1, x_2, x_3) = \hat{\beta}_0 + \hat{\beta}_1 x_1 + \hat{\beta}_2 x_2 + \hat{\beta}_3 x_3 + \hat{\beta}_{12} x_1 x_2 + \hat{\beta}_{13} x_1 x_3 + \hat{\beta}_{11} {x_1}^2 \tag{4}$$

Source: Iwundu M. P. [7].

$$\hat{y}\,(x_1, x_2, x_3, x_4) = \hat{\beta}_0 + \hat{\beta}_1 x_1 + \hat{\beta}_2 x_2 + \hat{\beta}_3 x_3 + \hat{\beta}_4 x_4 + \hat{\beta}_{12} x_1 x_2 + \hat{\beta}_{23} x_2 x_3 + \hat{\beta}_{11} {x_1}^2 + \hat{\beta}_{44} {x_4}^2 \tag{5}$$

Source: Iwundu and Otaru [5].

When constructing custom designs using JMP Pro 14 statistical software, some general rules are followed. The rules include stating the model, defining the region of interest, selecting the number of experimental runs, choosing an optimality criterion, and from a set of candidate points, choosing the design points one would like to consider, and which should satisfy the goal of the experimentation.

2.2. Design Optimality and Design Efficiencies

Design optimality are mathematical functions that reflect the objective of the experimental designs and are closely related to Design efficiency, being a function of design optimality. As in the literature of optimal design of experiments, design efficiencies are measures used to assess, evaluate, and compare the qualities of different experimental designs. They offer experimenters insight into the performance of designs such that the most appropriate designs can be selected for a given experimental objective Iwundu and Cosmos [8]. In this study, the A-, D-, G-, design efficiencies, and the Average Variance of Prediction (AVP) are employed to assess the qualities of the custom A-, D-, and I-optimal designs for non-standard second-order models.

2.2.1. A-efficiency

The A-efficiency is related to minimizing the individual variances of the model parameters. It allows comparison of designs across different sample sizes and is given b

$$A - efficiency = \frac{100 * p}{trace\,[N(X'X)^{-1}]} \tag{6}$$

where $(X'X)^{-1}$ is the variance-covariance matrix, N is the sample size, and p denotes the number of parameters in the model.

2.2.2. D-efficiency

The D-efficiency as in Goos and Jones [3] compares the determinant of the information matrix of a design to an "ideal" determinant related to an orthogonal design. The D−efficiency serves as a useful tool for evaluating the quality of the estimated model parameters and it is usually expressed as a percent. The D-efficiency is symbolically written as

$$D-efficiency = 100 * \frac{|X\prime X|^{\frac{1}{p}}}{N} \quad (7)$$

where p denotes the number of parameters in the model, N is the sample size, and $|X'X|$ is the determinant of the information matrix.

2.2.3. G-efficiency

The G-efficiency which is expressed in percentage compares the maximum value of the scaled prediction variance within the design region to its theoretical minimum variance, p Iwundu M. [6]. Myers *et al.* [14] stated that “the G-efficiency emphasizes the use of designs for which the maximum scaled prediction variance, $v(x)$ in the design region is not too large”. That is, it handles worst-case prediction variance. Iwundu M.P. [7] defined the G-efficiency as

$$G-efficiency = 100 \left(\frac{p}{\mathrm{N}* \mathrm{SPV}_{max}}\right) \quad (8)$$

where p denote the parameters in the model, N represent the design size, and SPV_{max} is the maximum scaled prediction variance at any point, $\underline{x}$ in the design region and is given as;

$$\mathrm{SPV} = N\underline{x}'(X'X)^{-1}\underline{x}$$

2.2.4. I-optimal Designs and the Average Variance of Prediction (AVP)

Johnson *et al.* [9] defined the Average Variance of Prediction as “a single measure of prediction performance that is created by the integration of the prediction variance”. The I-optimal designs are designs that minimize the Average Variance of Prediction. Hence, the smaller the value of the AVP, the better the design. According to Goos *et al.* [4], it can be computed as

$$Average\ Variance = \frac{\int_{\chi} f'(x)M^{-1}f(x)dx}{\int_{\chi} dx} = \frac{1}{\int_{\chi} dx} \cdot tr\,[M^{-1}B] \quad (9)$$

over the design region χ.
where $B = \int_{\chi} f(x)f'(x)dx$ is the moment matrix over the design region.

3. Numerical Illustrations

3.1. Custom A Designs and Efficiency Values

Case 1: An Illustration using Equation (2)

Considering the three-variable non-standard second-order model having p = 5 model parameters given in Equation (2), an N-point custom design is obtained from a continuum of points $\tilde{N}$ on the design space, Ω. The design size N satisfies $p \leq N \leq \tilde{N}$. The N points of the custom designs need not be discrete as in the case of standard designs. This allows flexibility in the choice of the points. However, if an experimenter desires to have a discrete point, a mathematical approximation to an integer-valued number is recommended. The construction of custom designs requires specifying the model, the number of factors to be included, the input variable constraints, and the number of center points. The center point is a very important factor as it helps in the estimation of pure error, thereby providing information at a minimum cost and also in detecting model adequacy or inadequacy through a test for lack of fit.

For this illustration, $N = 9, 10, \ldots 15$ well as $N = 27$ design points are considered. The choice of each N is to allow a good understanding of the effect of small-sized designs. In this section, the custom designs are created to satisfy the A-optimality criterion. The custom A-optimal designs for $N = 9, 10, 11, 12, 13, 14, 15, and\ 27$, with $n_c = 1$ are given as;

$$\xi_9 = \begin{pmatrix} 0 & 1 & 1 \\ 1 & -1 & -1 \\ 0 & 1 & -1 \\ 0 & 0 & 0 \\ -1 & -1 & 1 \\ 0 & -1 & 1 \\ -1 & 1 & -1 \\ 0 & -1 & -1 \\ 1 & 1 & 1 \end{pmatrix}$$

$$\xi_{10} = \begin{pmatrix} 1 & -1 & -1 \\ 1 & 1 & 1 \\ -0.08 & -1 & -1 \\ -1 & 1 & 1 \\ 0 & -1 & 1 \\ -1 & 1 & -1 \\ 0 & 1 & 1 \\ 0 & 0 & 0 \\ 0 & 1 & -1 \\ -1 & -1 & 1 \end{pmatrix}$$

$$\xi_{11} = \begin{pmatrix} -1 & -1 & -1 \\ 1 & 1 & 1 \\ 0 & 1 & 1 \\ 0.03 & -1 & 1 \\ 1 & -1 & -1 \\ -0.03 & 1 & -1 \\ -1 & 1 & -1 \\ 0 & -1 & -1 \\ 1 & 1 & -1 \\ 0 & 0 & 0 \\ -1 & -1 & 1 \end{pmatrix}$$

$$\xi_{12} = \begin{pmatrix} 1 & -1 & -1 \\ -1 & -1 & 1 \\ -1 & 1 & -1 \\ 1 & 1 & 1 \\ 0 & -1 & -1 \\ -1 & -1 & 1 \\ 0 & 1 & 1 \\ 1 & -1 & 1 \\ 0 & 1 & -1 \\ 0 & 0 & 0 \\ 0 & -1 & 1 \\ 0 & -1 & 1 \end{pmatrix}$$

$$\xi_{13} = \begin{pmatrix} 0 & 0 & 0 \\ 1 & 1 & 1 \\ -1 & -1 & -1 \\ -1 & 1 & -1 \\ 1 & 1 & -1 \\ 0.03 & -1 & 1 \\ 1 & -1 & -1 \\ -1 & 1 & 1 \\ 0 & -1 & -1 \\ -1 & -1 & 1 \\ 0 & 1 & -1 \\ -0.04 & 1 & -1 \\ 0 & 1 & 1 \end{pmatrix}$$

$$\xi_{14} = \begin{pmatrix} 1 & -1 & 1 \\ 0 & 0 & 0 \\ 1 & -1 & -1 \\ 0.07 & 1 & -1 \\ 1 & 1 & 1 \\ -1 & -1 & 1 \\ 0 & 1 & 1 \\ 1 & 1 & -1 \\ -1 & 1 & -1 \\ 0 & 1 & 1 \\ 0 & -1 & -1 \\ -1 & 1 & -1 \\ 0 & -1 & -1 \\ -0.05 & -1 & 1 \end{pmatrix}$$

$$\xi_{15} = \begin{pmatrix} -1 & -1 & 1 \\ 1 & -1 & 1 \\ 0 & 0 & 0 \\ 0 & 1 & -1 \\ 0 & -1 & 1 \\ -1 & -1 & -1 \\ 1 & 1 & -1 \\ -1 & 1 & 1 \\ 1 & -1 & 1 \\ 0 & 1 & -1 \\ 0 & -1 & 1 \\ -1 & 1 & -1 \\ 0 & -1 & -1 \\ 1 & -1 & -1 \\ 0 & 1 & 1 \end{pmatrix}$$

$$\xi_{27} = \begin{pmatrix} 0 & -1 & -1 \\ 0 & -1 & 1 \\ 0 & 1 & -1 \\ 0 & 1 & 1 \\ 0 & -1 & 1 \\ 0 & -1 & 1 \\ -1 & 1 & -1 \\ 0 & 0 & 0 \\ 0 & 1 & -1 \\ -1 & 1 & 1 \\ 1 & -1 & -1 \\ 1 & -1 & -1 \\ 0 & -1 & -1 \\ 1 & 1 & -1 \\ -1 & 1 & -1 \\ 1 & 1 & 1 \\ 1 & -1 & 1 \\ 1 & 1 & 1 \\ -1 & -1 & 1 \\ 0 & -1 & -1 \\ 1 & -1 & 1 \\ 0 & 1 & 1 \\ 0 & 1 & 1 \\ -1 & -1 & -1 \\ -1 & -1 & -1 \\ 0.03 & 1 & -1 \\ -1 & -1 & 1 \end{pmatrix}$$

Case 2: An Illustration using Equation (3)

The illustration considers a three-variable non-standard model with 6 parameters given in Equation (3). For $N = 9, 10, \ldots 15$ and 27, the custom A-optimal designs for each of the N design points with $n_c = 1$ is given as;

$$\xi_{9} = \begin{pmatrix} 0 & 0 & 0 \\ 1 & 1 & 1 \\ -1 & 1 & 0 \\ 1 & 1 & -1 \\ -1 & -1 & 1 \\ -1 & 1 & 0 \\ -1 & -1 & -1 \\ 1 & -1 & 0 \\ 1 & -1 & 0 \end{pmatrix}$$

$$\xi_{10} = \begin{pmatrix} 1 & 1 & 0 \\ -1 & 1 & 1 \\ -1 & 1 & -1 \\ 0 & 0 & 0 \\ -1 & -1 & -0.05 \\ 1 & -1 & -1 \\ 1 & -1 & 1 \\ -1 & -1 & 0 \\ 1 & 1 & 0 \\ 1 & -1 & -1 \end{pmatrix}$$

$$\xi_{11} = \begin{pmatrix} 1 & 1 & -0.04 \\ 1 & -1 & -1 \\ -1 & 1 & -1 \\ -1 & 1 & 1 \\ 1 & 1 & 0 \\ -1 & -1 & 0 \\ 1 & -1 & 1 \\ -1 & 1 & -1 \\ 0 & 0 & 0 \\ 1 & -1 & -1 \\ -1 & -1 & 0 \end{pmatrix}$$

$$\xi_{12} = \begin{pmatrix} 0 & -1 & 1 \\ 0 & 0 & 0 \\ -1 & -1 & 0 \\ 1 & 1 & 1 \\ -1 & 1 & 0 \\ -1 & 1 & 1 \\ 1 & 1 & 0 \\ 1 & -1 & -1 \\ 1 & 1 & -1 \\ 1 & -1 & 0.01 \\ -1 & 1 & -1 \\ -1 & -1 & -1 \end{pmatrix}$$

$$\xi_{13} = \begin{pmatrix} 1 & 1 & -1 \\ 0 & 0 & 0 \\ -1 & 1 & 0 \\ 1 & -1 & 0 \\ 1 & -1 & 1 \\ 1 & 1 & 0 \\ -1 & 1 & -1 \\ 1 & -1 & -1 \\ -1 & -1 & 0 \\ -1 & -1 & 1 \\ -1 & 1 & 1 \\ 1 & 1 & 1 \\ -1 & -1 & -1 \end{pmatrix}$$

$$\xi_{14} = \begin{pmatrix} -1 & -1 & 0 \\ 1 & 1 & 0 \\ 1 & -1 & -1 \\ 1 & -1 & 0 \\ -1 & -1 & 0 \\ -1 & -1 & -1 \\ 0 & 0 & 0 \\ 1 & -1 & 1 \\ 1 & 1 & 1 \\ -1 & 1 & 0 \\ -1 & 1 & -1 \\ 1 & 1 & -1 \\ -1 & 1 & 1 \\ -1 & -1 & 1 \end{pmatrix}$$

$$\xi_{15} = \begin{pmatrix} 1 & 1 & 1 \\ 1 & 1 & 0 \\ -1 & -1 & 0 \\ 1 & 1 & 0 \\ -1 & 1 & 0 \\ -1 & -1 & -1 \\ 1 & -1 & -1 \\ 0 & 0 & 0 \\ 1 & 1 & -1 \\ 1 & -1 & 1 \\ -1 & -1 & 1 \\ -1 & -1 & 0 \\ -1 & 1 & -1 \\ -1 & 1 & 1 \\ 1 & -1 & 0 \end{pmatrix}$$

$$\xi_{27} = \begin{pmatrix} 1 & 1 & 1 \\ 0 & 0 & 0 \\ -1 & -1 & -1 \\ -1 & -1 & 1 \\ 1 & 1 & 1 \\ 1 & -1 & -1 \\ -1 & 1 & -1 \\ 1 & -1 & 1 \\ 1 & 1 & 0 \\ 1 & 1 & 0 \\ -1 & 1 & 0 \\ 1 & 1 & 0 \\ 1 & 1 & -1 \\ 1 & -1 & 1 \\ -1 & 1 & 0 \\ 1 & -1 & 0 \\ -1 & -1 & -1 \\ -1 & 1 & -1 \\ -1 & -1 & 0 \\ 1 & -1 & 0 \\ -1 & 1 & 1 \\ -1 & -1 & 0 \\ -1 & -1 & 0 \\ 1 & 1 & -1 \\ -1 & 1 & 1 \\ 1 & -1 & -1 \\ -1 & -1 & 1 \end{pmatrix}$$

Case 3: An Illustration using Equation (4)

The illustration considers a three-variable non-standard model with 7 parameters given in Equation (4). For $N = 9, 10, \ldots, 15,$ and 27, the custom A-optimal designs for the N design points with $n_c = 1$ are given as;

$$\xi_9 = \begin{pmatrix} 0 & -1 & 1 \\ -1 & 1 & 0.15 \\ -1 & -1 & -1 \\ 0 & 1 & -1 \\ 0 & 0 & 0 \\ 1 & 1 & 1 \\ -1 & -1 & 1 \\ 1 & -0.35 & -1 \\ 1 & -1 & 1 \end{pmatrix}$$

$$\xi_{10} = \begin{pmatrix} 0 & 0 & 0 \\ 0 & 1 & -1 \\ 0 & -1 & 1 \\ 1 & -1 & -0.37 \\ -1 & 1 & 1 \\ -1 & -1 & -1 \\ 1 & 1 & 1 \\ -1 & -1 & 1 \\ -1 & 1 & -1 \\ 1 & 1 & -1 \end{pmatrix}$$

$$\xi_{11} = \begin{pmatrix} -1 & -1 & 1 \\ 1 & 1 & -1 \\ 0 & 1 & 1 \\ -1 & 1 & -1 \\ 1 & 1 & 1 \\ 0 & -1 & -1 \\ -1 & 1 & 1 \\ 0 & 0 & 0 \\ 1 & -1 & -1 \\ -1 & -1 & -1 \\ 1 & -1 & 1 \end{pmatrix}$$

$$\xi_{12} = \begin{pmatrix} 1 & 1 & -1 \\ 0 & 0 & 0 \\ -1 & -1 & -1 \\ -1 & -1 & 1 \\ -1 & 1 & 1 \\ 1 & -1 & 1 \\ -1 & 1 & -1 \\ 0 & -1 & -0.29 \\ 1 & 1 & 1 \\ 0 & 0 & 1 \\ 0 & 1 & -1 \\ 1 & -1 & -1 \end{pmatrix}$$

$$\xi_{13} = \begin{pmatrix} 1 & -1 & -1 \\ -1 & 1 & -1 \\ 1 & 1 & -1 \\ -1 & 1 & 1 \\ -1 & -1 & -1 \\ 0 & 1 & 1 \\ 0 & 0 & 0 \\ 0 & 1 & -1 \\ 0 & -1 & 1 \\ 1 & 1 & 1 \\ -1 & -1 & 1 \\ 1 & -1 & 1 \\ 0 & -1 & -1 \end{pmatrix}$$

$$\xi_{14} = \begin{pmatrix} 1 & 1 & 1 \\ 0 & -1 & 1 \\ 0 & -1 & -1 \\ 0 & 0 & 0 \\ 0 & 1 & -1 \\ 0 & 1 & 1 \\ 1 & -1 & 1 \\ 1 & 1 & -1 \\ -1 & -1 & 1 \\ -1 & -1 & -1 \\ -1 & 1 & 1 \\ 0 & -1 & -1 \\ 1 & -1 & -1 \\ -1 & 1 & -1 \end{pmatrix}$$

$$\xi_{15} = \begin{pmatrix} 1 & 1 & -1 \\ 1 & -1 & 1 \\ -1 & -1 & -1 \\ 0 & 1 & -1 \\ 1 & -1 & -1 \\ 0 & -1 & -1 \\ -1 & 1 & 1 \\ -1 & 1 & -1 \\ 0 & -1 & 1 \\ 0 & 0 & 0 \\ -1 & -1 & 1 \\ 0 & 1 & 1 \\ 0 & -1 & -1 \\ 1 & 1 & 1 \\ 0 & 1 & 1 \end{pmatrix}$$

$$\xi_{27} = \begin{pmatrix} 1 & 1 & -1 \\ 0 & -1 & -1 \\ 0 & 1 & -1 \\ 0 & -1 & 1 \\ 1 & 1 & 1 \\ 0 & -1 & -1 \\ 1 & -1 & 1 \\ -1 & -1 & 1 \\ 0 & 1 & -1 \\ -1 & -1 & -1 \\ 0 & 1 & 1 \\ -1 & 1 & -1 \\ -1 & -1 & -1 \\ 0 & -1 & 1 \\ 1 & -1 & 1 \\ -1 & 1 & -1 \\ 0 & -1 & -1 \\ -1 & 1 & 1 \\ 0 & 1 & 1 \\ 1 & -1 & -1 \\ 0 & 1 & 1 \\ 0 & 0 & 0 \\ -1 & -1 & 1 \\ 1 & 1 & -1 \\ 1 & -1 & -1 \\ -1 & 1 & 1 \\ 1 & 1 & 1 \end{pmatrix}$$

Case 4: An Illustration using Equation (5)

The illustration considers a four-variable non-standard model with 9 parameters, given in Equation (5).

For $N = 13, 14, \dots, 18$, 21 and 25 the custom A-optimal designs for the N design points with $n_c = 1$ are given as;

$$\xi_{13} = \begin{pmatrix} -1 & -1 & 1 & 1 \\ 0 & 1 & -1 & 0 \\ -1 & 1 & -1 & 0.1 \\ 1 & 1 & 1 & 0 \\ -1 & 1 & 1 & -1 \\ 1 & 1 & -1 & -1 \\ 1 & -1 & 1 & 0 \\ 0 & 1 & 1 & 1 \\ 0 & -1 & 1 & -1 \\ 0 & 0 & 0 & 0 \\ 0 & -1 & -1 & -0.28 \\ 1 & -1 & -1 & 1 \\ -1 & -1 & -1 & 0 \end{pmatrix}$$

$$\xi_{14}=\begin{pmatrix}1&1&1&0\\0&-1&-1&-1\\1&-1&1&0\\-1&1&1&-1\\0&1&1&0\\-1&1&-1&0\\-1&-1&-1&-0.06\\0&1&0&1\\0&-1&1&-1\\1&1&-1&-1\\-1&-1&1&1\\0&0&0&0\\0&1&-1&0\\1&-1&-1&1\end{pmatrix}$$

$$\xi_{15}=\begin{pmatrix}0&-1&1&-1\\0&-1&-1&-1\\1&-1&-1&1\\-1&-1&-1&0\\-1&-1&1&1\\0&1&-1&1\\0&0&0&0\\0&-1&0&0\\1&1&-1&-1\\-1&1&-1&0\\0&1&0&0\\0&1&1&1\\-1&1&1&-1\\1&1&1&0\\1&-1&1&0\end{pmatrix}$$

$$\xi_{16}=\begin{pmatrix}0&-1&-1&0\\-1&-1&1&0\\1&1&1&0\\-1&-1&-1&1\\-1&1&-1&0\\-1&1&1&-1\\1&-1&-1&0\\1&-1&1&1\\0&-1&1&0\\0&1&1&1\\1&1&-1&-1\\0&0&0&0\\0&1&-1&1\\0&1&0&0\\0&-1&1&-1\\0&-1&-1&-1\end{pmatrix}$$

$$\xi_{17}=\begin{pmatrix}-1&1&-1&0\\0&1&-1&-1\\0&-1&1&0\\0&-1&-1&0\\1&-1&-1&1\\0&1&-1&1\\0&0&0&0\\1&1&-1&0\\0&-1&-1&0\\-1&1&1&0\\0&1&1&-1\\0&-1&1&0\\0&1&1&1\\-1&-1&-1&-1\\1&-1&1&-1\\1&1&1&0\\-1&-1&1&1\end{pmatrix}$$

$$\xi_{18}=\begin{pmatrix}-1&-1&-1&-1\\-0.1&1&1&0\\-1&1&-1&0\\-1&1&1&-1\\-1&1&-1&1\\1&-1&1&-1\\0&-1&1&1\\0&-1&-1&0\\1&1&1&1\\0&0&0&0\\0&-1&1&0\\1&1&-1&0\\-1&-1&1&0\\0&1&1&0\\0&-1&-1&1\\1&-1&-1&0\\0&1&-1&-1\\0&1&-1&-1\end{pmatrix}$$

$$\xi_{21}=\begin{pmatrix}0&0&0&0\\-1&-1&-1&0\\0&-1&1&0\\0&1&1&1\\0&1&-1&0\\-1&1&1&-1\\0&1&-1&0\\1&-1&-1&1\\1&1&1&0\\-1&1&1&0\\1&-1&-1&-1\\-1&-1&1&1\\-1&1&-1&1\\0&-1&-1&1\\1&1&1&1\\1&-1&1&0\\1&1&-1&-1\\0&1&1&-1\\0&-1&1&-1\\0&-1&-1&0\\-1&-1&-1&-1\end{pmatrix}$$

$$\xi_{25}=\begin{pmatrix}0&0&0&0\\1&1&-1&-1\\1&-1&-1&1\\0&0&-1&1\\0&-1&1&-1\\0&-1&-1&-1\\1&-1&-1&-1\\1&1&1&1\\0&1&-1&0\\-1&-1&1&1\\0&1&1&0\\0&-1&1&0\\-1&-1&-1&0\\-1&-1&-1&0\\-1&1&1&0\\1&1&-1&0\\-1&-1&1&-1\\0&-1&1&1\\-1&1&-1&1\\-1&1&-1&-1\\0&-1&-1&0\\0&1&-1&0\\1&-1&1&-0.06\\1&-1&1&0\\0&1&1&-1\end{pmatrix}$$

Table 1 below shows the results of the efficiency measures and AVP values of the custom A-optimal designs for non-standard models obtained from John's Macintosh Project (JMP) statistical software. The result shows that the A-optimal design which is a function of the A-optimality criterion had the highest A-efficiency values compared to the custom D- and I-optimal designs. The result also showed that the A-optimal design had high D- and G-efficiency values (above 50%). This means that the A-optimal designs are also D- and G- efficient. Lastly, the result of the AVP showed that the design produced smaller prediction variances compared to the D-optimal design. Hence, they are more appropriate for prediction than the custom D-optimal designs.

Table 1. *Efficiency Measures of A-optimal designs for Non-standard models.*

Number of factors ($\boldsymbol{k}$)	Number of parameters ($\boldsymbol{p}$)	Number of design points (N)	D-efficiency (%)	G-efficiency (%)	A-efficiency (%)	Average Variance of Prediction (AVP)
		9	61.32132	74.07407	48.30918	0.323333
		10	61.77937	71.05871	47.20342	0.298081
		11	62.80609	79.03737	46.8311	0.27298
3	5	12	61.17072	69.28839	47.25415	0.25488
		13	63.43927	92.31354	47.5631	0.231168
		14	63.14763	60.47968	48.04881	0.208608
		15	64.68813	80	48.9083	0.191468
		27	65.15811	83.22195	49.24383	0.105461
		9	58.11824	66.66667	47.61905	0.351111
		10	58.70716	60.00001	46.51177	0.326014
		11	59.90774	58.2449	46.2004	0.300606
3	6	12	61.81098	89.0614	47.27213	0.271109
		13	65.1364	85.2071	49.01293	0.242778
		14	63.71614	82.20551	49.09363	0.22378
		15	62.64027	73.84615	49.5941	0.205357
		27	65.38677	85.82375	49.74763	0.114556
		9	57.44635	57.60852	43.30225	0.432184
		10	61.98699	58.6284	44.39605	0.385574
		11	66.98854	84.84848	46.28099	0.341667
3	7	12	64.36823	81.63543	48.55338	0.29485
		13	64.6098	80.76923	50.48077	0.256667
		14	62.73272	77.35849	50.10183	0.237669
		15	61.21732	74.66667	50.09585	0.219246
		27	64.47407	80.65844	50.9151	0.121501
		13	57.28011	65.42829	42.28961	0.352008
		14	56.75164	80.16152	42.78596	0.323169
4	9	15	56.19102	74.49687	43.4051	0.295676
		16	56.00956	73.65331	43.93409	0.273887
		17	55.95376	70.8992	44.33641	0.25519
		18	56.24087	70.28544	43.77273	0.24469

Number of factors (k)	Number of parameters (p)	Number of design points (N)	D-efficiency (%)	G-efficiency (%)	A-efficiency (%)	Average Variance of Prediction (AVP)
		21	58.53976	72.40759	43.80603	0.208551
		25	57.67718	79.99164	44.21452	0.176553

3.2. Custom D Designs and Efficiency Values

Case 1

Considering the 5-parameter non-standard model in three variables stated in Equation (2). For $N = 9, 10, \ldots 15$ and 27, the custom D-optimal designs for each of the N design points are given as;

$$\xi_9 = \begin{pmatrix} 1 & -1 & 1 \\ -1 & 1 & 1 \\ 0 & 0 & 0 \\ -1 & -1 & -1 \\ 1 & -1 & 1 \\ 1 & 1 & -1 \\ 0 & 1 & 1 \\ 0 & -1 & -1 \\ 1 & 1 & -1 \end{pmatrix}$$

$$\xi_{10} = \begin{pmatrix} 1 & 1 & -1 \\ -1 & 1 & 1 \\ 0 & 0 & 0 \\ -1 & 1 & -1 \\ 1 & -1 & 1 \\ -1 & -1 & -1 \\ 1 & -1 & -1 \\ 0.07 & 1 & -1 \\ 1 & 1 & 1 \\ -0.07 & -1 & 1 \end{pmatrix}$$

$$\xi_{11} = \begin{pmatrix} 1 & 1 & -1 \\ 1 & 1 & 1 \\ -1 & 1 & -1 \\ 0 & 0 & 0 \\ -1 & -1 & 1 \\ 0 & -1 & 1 \\ -1 & -1 & -1 \\ 0 & 1 & -1 \\ 1 & -1 & 1 \\ -1 & 1 & 1 \\ 1 & -1 & -1 \end{pmatrix}$$

$$\xi_{12} = \begin{pmatrix} 1 & -1 & 1 \\ 0 & -1 & -1 \\ 0 & -1 & 1 \\ 1 & 1 & 1 \\ 1 & 1 & -1 \\ -1 & 1 & 1 \\ 1 & -1 & -1 \\ -1 & 1 & -1 \\ -1 & -1 & -1 \\ 0 & 1 & -1 \\ 0 & 0 & 0 \\ -1 & -1 & 1 \end{pmatrix}$$

$$\xi_{13} = \begin{pmatrix} 1 & -1 & -1 \\ 0 & 1 & -1 \\ -1 & 1 & 1 \\ 1 & 1 & -1 \\ 0 & 1 & 1 \\ 1 & -1 & 1 \\ -1 & -1 & -1 \\ 0 & -1 & 1 \\ -1 & -1 & 1 \\ 0 & -1 & -1 \\ -1 & 1 & -1 \\ 1 & 1 & 1 \\ 0 & 0 & 0 \end{pmatrix};$$

$$\xi_{14} = \begin{pmatrix} -1 & -1 & 1 \\ 1 & -1 & 1 \\ -1 & 1 & -1 \\ 0 & 0 & 0 \\ -1 & 1 & 1 \\ 1 & 1 & -1 \\ 0 & 1 & 1 \\ 0 & -1 & -1 \\ 0 & -1 & -1 \\ -1 & -1 & -1 \\ 1 & 1 & -1 \\ -0.05 & 1 & 1 \\ -1 & -1 & -1 \\ 1 & -1 & 1 \end{pmatrix}$$

$$\xi_{15} = \begin{pmatrix} 1 & -1 & 1 \\ -1 & 1 & -1 \\ 0 & 1 & 1 \\ -1 & -1 & 1 \\ 1 & 1 & 1 \\ 1 & -1 & -1 \\ 0 & -1 & -1 \\ 1 & 1 & 1 \\ 0 & 0 & 0 \\ -1 & -1 & -1 \\ -0.04 & -1 & 1 \\ 1 & -1 & -1 \\ -1 & -1 & 1 \\ -1 & 1 & -1 \\ 0.05 & 1 & -1 \end{pmatrix}$$

$$\xi_{27} = \begin{pmatrix} 0 & 1 & 1 \\ -1 & 1 & -1 \\ 1 & 1 & -1 \\ 0 & -1 & -1 \\ 1 & -1 & -1 \\ 0 & -1 & -1 \\ 0 & 0 & 0 \\ 1 & -1 & 1 \\ -1 & 1 & 1 \\ 0 & 1 & 1 \\ -1 & 1 & -1 \\ 0 & -1 & 1 \\ 1 & -1 & 1 \\ -1 & -1 & 1 \\ 1 & 1 & 1 \\ -1 & -1 & 1 \\ 1 & -1 & 1 \\ -0.02 & 1 & 1 \\ -1 & -1 & -1 \\ 0 & -1 & -1 \\ -1 & 1 & -1 \\ 1 & 1 & 1 \\ 1 & 1 & -1 \\ -1 & -1 & 1 \\ -1 & -1 & -1 \\ 1 & -1 & -1 \\ 0 & 1 & -1 \end{pmatrix}$$

Case 2

The illustration considers a three-variable non-standard model with 6 parameters given in Equation (3). For $N = 9, 10, \ldots 15$ and 27, the custom D-optimal designs for each of the N design points with $n_c = 1$ is given as;

$$\xi_9 = \begin{pmatrix} -1 & -1 & 1 \\ -1 & 1 & 1 \\ 1 & -1 & -1 \\ -1 & -1 & -1 \\ 1 & 1 & 1 \\ -1 & 1 & -1 \\ 1 & -1 & 1 \\ 0 & 0 & 0 \\ 1 & 1 & -1 \end{pmatrix}$$

$$\xi_{10} = \begin{pmatrix} -1 & 1 & -1 \\ -1 & 1 & 1 \\ 1 & -1 & 1 \\ -1 & -1 & 1 \\ 1 & -1 & -1 \\ 0 & 0 & 0 \\ -1 & -1 & -1 \\ 1 & 1 & -1 \\ 1 & 1 & 1 \\ 1 & 1 & 0 \end{pmatrix}$$

$$\xi_{11} = \begin{pmatrix} 0 & 0 & 0 \\ -1 & -1 & -1 \\ -1 & 1 & 0 \\ 1 & -1 & -1 \\ -1 & 1 & -1 \\ 1 & -1 & 1 \\ -1 & 1 & 1 \\ 1 & -1 & 0 \\ 1 & 1 & -1 \\ -1 & -1 & 1 \\ 1 & 1 & 1 \end{pmatrix}$$

$$\xi_{12} = \begin{pmatrix} -1 & -1 & 1 \\ -1 & -1 & -1 \\ -1 & 1 & -1 \\ 1 & -1 & 1 \\ 1 & 1 & 1 \\ 1 & 1 & -1 \\ -1 & 1 & 0 \\ 1 & -1 & -1 \\ 1 & 1 & 0 \\ -1 & 1 & 1 \\ 0 & 0 & 0 \\ -1 & -1 & 1 \end{pmatrix}$$

$$\xi_{13} = \begin{pmatrix} -1 & 1 & 0 \\ 1 & -1 & 0 \\ -1 & -1 & 1 \\ -1 & 1 & 1 \\ -1 & -1 & 1 \\ -1 & -1 & -1 \\ -1 & 1 & -1 \\ 0 & 0 & 0 \\ 1 & -1 & -1 \\ 1 & -1 & 1 \\ -1 & -1 & -1 \\ 1 & 1 & 1 \\ 1 & 1 & -1 \end{pmatrix}$$

$$\xi_{14} = \begin{pmatrix} 1 & 1 & -1 \\ -1 & 1 & -1 \\ -1 & -1 & -1 \\ 1 & -1 & 1 \\ -1 & 1 & 1 \\ 1 & -1 & 1 \\ -1 & -1 & 0 \\ -1 & 1 & 1 \\ -1 & -1 & 1 \\ 1 & -1 & -1 \\ 1 & 1 & 0 \\ 1 & -1 & -1 \\ 0 & 0 & 0 \\ 1 & 1 & 1 \end{pmatrix}$$

$$\xi_{15} = \begin{pmatrix} -1 & 1 & -1 \\ -1 & -1 & 0 \\ 0 & 0 & 0 \\ -1 & 1 & -1 \\ 1 & -1 & -1 \\ 1 & -1 & -1 \\ -1 & 1 & 1 \\ 1 & 1 & 0 \\ 1 & -1 & 1 \\ 1 & 1 & -1 \\ -1 & 1 & 1 \\ -1 & -1 & 1 \\ 1 & 1 & 1 \\ 1 & -1 & 1 \\ -1 & -1 & -1 \end{pmatrix}$$

$$\xi_{27} = \begin{pmatrix} 0 & 1 & 1 \\ -1 & 1 & -1 \\ 1 & 1 & -1 \\ 0 & -1 & -1 \\ 1 & -1 & -1 \\ 0 & -1 & -1 \\ 0 & 0 & 0 \\ 1 & -1 & 1 \\ -1 & 1 & 1 \\ 0 & 1 & 1 \\ -1 & 1 & -1 \\ 0 & -1 & 1 \\ 1 & -1 & 1 \\ -1 & -1 & 1 \\ 1 & 1 & 1 \\ -1 & -1 & 1 \\ 1 & -1 & 1 \\ -0.02 & 1 & 1 \\ -1 & -1 & -1 \\ 0 & -1 & -1 \\ -1 & 1 & -1 \\ 1 & 1 & 1 \\ 1 & 1 & -1 \\ -1 & -1 & 1 \\ -1 & -1 & -1 \\ 1 & -1 & -1 \\ 0 & 1 & -1 \end{pmatrix}$$

Case 3

The illustration considers a three-variable non-standard model with 7 parameters given in Equation (4). For $N = 9, 10, \ldots, 15,$ and 27, the custom D-optimal designs for the N design points with $n_c = 1$ are given as;

$$\xi_9 = \begin{pmatrix} -1 & -1 & 1 \\ 1 & 1 & -1 \\ 1 & 1 & 1 \\ 0 & 0 & 0 \\ 1 & -1 & -1 \\ -1 & 1 & 1 \\ -1 & -1 & -1 \\ -1 & 1 & -1 \\ 1 & -1 & 1 \end{pmatrix}$$

$$\xi_{10} = \begin{pmatrix} -1 & 1 & -1 \\ 0 & 0 & 0 \\ -1 & -1 & -1 \\ 1 & 1 & 1 \\ -1 & 1 & 1 \\ 1 & 1 & -1 \\ 1 & -1 & -1 \\ 0 & -1 & 1 \\ -1 & -1 & 1 \\ 1 & -1 & 1 \end{pmatrix}$$

$$\xi_{11} = \begin{pmatrix} -1 & -1 & -1 \\ -1 & 1 & 1 \\ 1 & 1 & -1 \\ 0 & 1 & 1 \\ 1 & 1 & 1 \\ -1 & 1 & -1 \\ 0 & 0 & 0 \\ 1 & -1 & 1 \\ 0 & -1 & -1 \\ -1 & -1 & 1 \\ 1 & -1 & -1 \end{pmatrix}$$

$$\xi_{12} = \begin{pmatrix} -1 & -1 & -1 \\ 1 & 1 & -1 \\ -1 & -1 & 1 \\ 0 & -1 & 1 \\ -1 & 1 & -1 \\ 0 & 1 & -1 \\ -1 & 1 & 1 \\ 1 & -1 & 1 \\ 0 & 0 & 0 \\ 1 & 1 & 1 \\ 1 & -1 & -1 \\ -1 & -1 & -1 \end{pmatrix}$$

$$\xi_{13} = \begin{pmatrix} -1 & -1 & -1 \\ -1 & 1 & 1 \\ 1 & 1 & 1 \\ 0 & 0 & 0 \\ -1 & -1 & -1 \\ 1 & -1 & -1 \\ 0 & 1 & -1 \\ -1 & -1 & 1 \\ 0 & -1 & 1 \\ 1 & 1 & -1 \\ 1 & -1 & 1 \\ -1 & 1 & -1 \\ 1 & -1 & -1 \end{pmatrix}$$

$$\xi_{14} = \begin{pmatrix} 0 & 1 & -1 \\ 1 & -1 & 1 \\ -1 & 1 & 1 \\ 0 & 0 & 0 \\ 1 & -1 & -1 \\ 1 & -1 & -1 \\ -1 & -1 & 1 \\ -1 & -1 & -1 \\ -1 & 1 & -1 \\ -1 & 1 & 1 \\ 1 & 1 & -1 \\ 1 & 1 & 1 \\ -1 & -1 & -1 \\ 0 & -1 & 1 \end{pmatrix}$$

$$\xi_{15} = \begin{pmatrix} 0 & -1 & 1 \\ 0 & 1 & -1 \\ -1 & -1 & -1 \\ 1 & 1 & 1 \\ 1 & -1 & -1 \\ 1 & -1 & -1 \\ -1 & 1 & 1 \\ -1 & -1 & -1 \\ 0 & 0 & 0 \\ -1 & -1 & 1 \\ -1 & 1 & 1 \\ 1 & 1 & -1 \\ 1 & 1 & 1 \\ 1 & -1 & 1 \\ -1 & 1 & -1 \end{pmatrix}$$

$$\xi_{27} = \begin{pmatrix} -1 & -1 & -1 \\ -1 & -1 & 1 \\ -1 & 1 & 1 \\ 1 & -1 & -1 \\ -1 & 1 & -1 \\ -1 & 1 & -1 \\ 0 & -1 & 1 \\ 1 & -1 & 1 \\ 1 & -1 & -1 \\ -1 & -1 & -1 \\ 1 & 1 & -1 \\ 1 & 1 & 1 \\ -1 & 1 & 1 \\ -1 & 1 & 1 \\ 0 & 1 & -1 \\ 0 & 1 & -1 \\ 1 & -1 & 1 \\ 0 & -1 & 1 \\ 1 & -1 & -1 \\ 0 & 0 & 0 \\ -1 & -1 & -1 \\ 1 & 1 & 1 \\ 1 & 1 & 1 \\ 1 & 1 & -1 \\ -1 & -1 & 1 \\ -1 & -1 & 1 \\ 1 & 1 & -1 \end{pmatrix}$$

Case 4

The illustration considers a four-variable non-standard model with 9 parameters given in Equation (5). For $N = 13, 14, \ldots, 18$, 21, and 25 the custom D-optimal designs with $n_c = 1$ are given as;

$$\xi_{13} = \begin{pmatrix} -1 & -1 & 1 & 0 \\ 0 & -1 & -1 & 1 \\ 0 & -1 & 1 & 1 \\ -1 & -1 & -1 & -1 \\ -1 & 1 & -1 & 0 \\ 1 & 1 & 1 & 0 \\ 0 & 0 & 0 & 0 \\ 1 & 1 & -1 & 1 \\ 0 & 1 & -1 & -1 \\ 1 & -1 & 1 & -1 \\ 1 & -1 & -1 & 0 \\ 0 & 1 & 1 & -1 \\ -1 & 1 & 1 & 1 \end{pmatrix}$$

$$\xi_{14} = \begin{pmatrix} -1 & 1 & 1 & 0 \\ 1 & 1 & 1 & -1 \\ -1 & -1 & 1 & 0 \\ 0 & 1 & -1 & 1 \\ -1 & -1 & -1 & 1 \\ 0 & 0 & 0 & 0 \\ 1 & -1 & -1 & -0.04 \\ 0.13 & -1 & 1 & -1 \\ 1 & 1 & -1 & 0 \\ -1 & 1 & -1 & -1 \\ 0 & 1 & 1 & 1 \\ 1 & -1 & 1 & 1 \\ 0 & -1 & -1 & -1 \\ -1 & -1 & 1 & -1 \end{pmatrix}$$

$$\xi_{15} = \begin{pmatrix} 1 & -1 & 1 & -1 \\ -1 & 1 & -1 & 1 \\ 0 & -1 & 1 & 1 \\ 1 & -1 & -1 & 0 \\ 1 & 1 & 1 & -1 \\ -1 & -1 & -1 & 1 \\ -1 & -1 & 1 & 0 \\ 0 & 0 & 0 & 0 \\ 1 & 1 & -1 & 0 \\ 0 & 1 & -1 & -1 \\ 1 & -1 & -1 & 1 \\ 1 & 1 & 1 & 1 \\ -1 & 1 & 1 & 0.08 \\ -1 & -1 & -1 & -1 \\ -1 & 1 & 1 & -1 \end{pmatrix}$$

$$\xi_{16} = \begin{pmatrix} 0 & 1 & -1 & -1 \\ 1 & -1 & 1 & 1 \\ -1 & 1 & 1 & 1 \\ -1 & -1 & -1 & 1 \\ 1 & -1 & 1 & 0 \\ 0 & -1 & 1 & 1 \\ -1 & 1 & 1 & -1 \\ -1 & -1 & 1 & -1 \\ 1 & -1 & -1 & -1 \\ 0 & -1 & -1 & 0 \\ 1 & 1 & 1 & -1 \\ 0 & 0 & 0 & 0 \\ 1 & 1 & 1 & 0.03 \\ -1 & -1 & 1 & -0.08 \\ -1 & 1 & -1 & 0 \\ 1 & 1 & -1 & 1 \end{pmatrix}$$

$$\xi_{17} = \begin{pmatrix} 1 & 1 & -1 & 1 \\ 1 & -1 & -1 & -1 \\ -1 & 1 & -1 & 0 \\ 1 & 1 & 1 & -1 \\ 0 & -1 & -1 & 1 \\ -1 & -1 & -1 & 1 \\ 0 & 1 & 1 & 1 \\ 0 & 1 & -1 & -1 \\ -1 & -1 & -1 & -1 \\ -1 & -1 & 1 & 0 \\ -1 & 1 & 1 & -1 \\ 0 & 0 & 0 & 0 \\ 1 & -1 & 1 & 1 \\ 0 & -1 & 1 & -1 \\ 1 & -1 & -1 & 0 \\ 1 & 1 & 1 & 0 \\ -1 & 1 & 1 & 1 \end{pmatrix}$$

$$\xi_{18} = \begin{pmatrix} -1 & -1 & -1 & 1 \\ 0 & 1 & -1 & 1 \\ -1 & 1 & 1 & 0 \\ -1 & 1 & -1 & 1 \\ -1 & -1 & 1 & -1 \\ 1 & 1 & -1 & -1 \\ 1 & -1 & 1 & 0 \\ -0.11 & 1 & 1 & -1 \\ 1 & 1 & 1 & -1 \\ 1 & 1 & 1 & 1 \\ 1 & -1 & -1 & -1 \\ 1 & -1 & -1 & 1 \\ 0 & -1 & -1 & -1 \\ -1 & -1 & -1 & 0 \\ 0 & 0 & 0 & 0 \\ 1 & 1 & -1 & 0 \\ 0 & -1 & 1 & 1 \\ -1 & 1 & -1 & -1 \end{pmatrix}$$

$$\xi_{21} = \begin{pmatrix} -1 & 1 & -1 & -1 \\ 1 & -1 & 1 & -1 \\ 1 & 1 & -1 & 0 \\ -1 & -1 & -1 & -1 \\ -1 & 1 & 1 & 1 \\ -1 & -1 & 1 & 1 \\ 1 & 1 & 1 & -1 \\ -1 & -1 & 1 & 0 \\ 1 & -1 & 1 & 1 \\ 1 & 1 & 1 & -1 \\ -1 & 1 & -1 & -1 \\ 0 & -1 & -1 & -1 \\ 0 & -1 & 1 & -1 \\ 1 & 1 & -1 & 1 \\ 0 & 1 & 1 & 1 \\ 0 & 1 & -1 & 1 \\ 1 & -1 & -1 & 1 \\ -1 & -1 & -1 & 1 \\ 0 & 0 & 0 & 0 \\ -1 & 1 & 1 & 0 \\ 1 & -1 & -1 & 0 \end{pmatrix}$$

$$\xi_{25} = \begin{pmatrix} 1 & -1 & -1 & 0 \\ 1 & -1 & -1 & 1 \\ 0 & 1 & 1 & 1 \\ 1 & 1 & -1 & 1 \\ 1 & 1 & 1 & -1 \\ 1 & 1 & 1 & 0 \\ -0.06 & -1 & 1 & 0 \\ -1 & -1 & -1 & 0 \\ 1 & -1 & 1 & 0 \\ 0 & 1 & -1 & 1 \\ -1 & -1 & -1 & 1 \\ -1 & 1 & -1 & 0 \\ -1 & 1 & 1 & -1 \\ -1 & 1 & 1 & 1 \\ -1 & -1 & 1 & 1 \\ -1 & -1 & 1 & -1 \\ 1 & -1 & 1 & 1 \\ 1 & -1 & 1 & -1 \\ -1 & 1 & -1 & -1 \\ 1 & 1 & -1 & -1 \\ 0 & -1 & -1 & -1 \\ 0 & -1 & -1 & -1 \\ 1 & 1 & 1 & 0 \\ 0 & 0 & 0 & 0 \\ -1 & 1 & -1 & 0 \end{pmatrix}$$

Results of the efficiency measures and AVP values of custom A-optimal designs for non-standard models are tabulated in Table 2 below. From the result, it is observed that for each of the non-standard models, the custom D-optimal design which is constructed to satisfy the D-optimality criterion produces high (above 50%) D-efficiency values which increase slightly as the design size increases. This indicates that the custom D-optimal designs are D-efficient that is, they produce designs that minimize the variance and covariance of the parameter estimates. In terms of G-efficiency, the result showed that they performed very well with G-efficiency values higher than their related D-efficiency values. But, for the A-efficiencies, the result revealed low efficiency values

($< 50\%$). This means that the D-optimal design does not fare well in terms of A-efficiency. Again, the AVP values of the D-optimal design are high compared to other custom designs. This implies that the D-optimal design is not appropriate for prediction purposes.

***Table 2**. Efficiency Measures of Custom D-optimal designs for Non-standard models.*

Number of factors (k)	Number of parameters (p)	Number of design points (N)	D-efficiency (%)	G-efficiency (%)	A-efficiency (%)	Average Variance of Prediction (AVP)
3	5	9	63.59863	74.07407	43.01075	0.603333
		10	64.0722	82.85965	41.49901	0.336215
		11	64.82191	77.92208	40.40404	0.313889
		12	65.13999	71.9697	43.18182	0.269883
		13	65.88084	92.30769	47.09576	0.22889
		14	65.59811	90.40147	45.50675	0.21977
		15	65.64985	93.83373	44.2516	0.210578
		27	67.00405	97.65296	44.96045	0.115005
3	6	9	62.85394	53.33333	25.39683	0.697222
		10	64.75482	60	34.83871	0.455556
		11	66.07711	87.27273	43.63636	0.327778
		12	65.6757	81.25	41.6	0.315171
		13	65.66822	76.0181	39.96828	0.303042
		14	65.9953	71.42857	38.6681	0.29142
		15	66.61465	80	37.64706	0.280093
		27	67.79991	95.2381	43.31013	0.134206
3	7	9	66.04419	62.22222	28.28283	0.711111
		10	66.74042	70	37.89474	0.469444
		11	66.98854	84.84848	46.28099	0.341667
		12	66.51685	77.77778	44.14414	0.328968
		13	66.51036	85.34107	42.47021	0.41627
		14	66.70295	79.24528	41.07579	0.303968
		15	67.23916	80	40	0.291667
		27	68.71212	86.9281	39.11621	0.167515
4	9	13	59.49831	82.48773	39.16084	0.376323
		14	59.18462	77.6559	38.06724	0.363664
		15	59.39471	67.37465	32.53158	0.408748
		16	59.76306	81.60601	38.02047	0.326061
		17	60.1428	77.51599	36.68532	0.320008
		18	60.21471	75.41108	35.99499	0.311856
		21	61.47599	82.6686	34.77996	0.283406
		25	61.47872	89.83834	37.93374	0.213251

3.3. Custom I Design and Efficiency Values

Case 1

Consider the three-variable non-standard second-order model having p = 5 model parameters given in Equation (2), for $N = 9, 10, \ldots 15$ and 27, the custom I-optimal designs for each of the N design points are given as;

$$\xi_9 = \begin{pmatrix} 0 & 0 & 0 \\ 1 & 1 & -1 \\ -1 & 1 & 1 \\ 0 & 1 & -1 \\ 0 & 1 & 1 \\ 0 & -1 & -1 \\ 1 & -1 & 1 \\ 0 & -1 & 1 \\ -1 & -1 & -1 \end{pmatrix}, \quad \xi_{10} = \begin{pmatrix} 1 & -1 & -1 \\ -1 & 1 & -1 \\ -1 & -1 & 1 \\ -0.08 & -1 & 1 \\ 0 & -1 & -1 \\ 0 & 1 & 1 \\ 1 & 1 & 1 \\ 0.15 & 1 & -1 \\ -1 & 1 & -1 \\ 0 & 0 & 0 \end{pmatrix}$$

$$\xi_{11} = \begin{pmatrix} 0 & 0 & 0 \\ 0 & 1 & -1 \\ 0 & -1 & 1 \\ -1 & -1 & -1 \\ -0.15 & -1 & 1 \\ 1 & -1 & -1 \\ -1 & 1 & 1 \\ 1 & 1 & 1 \\ 0.08 & 1 & -1 \\ 1 & -1 & -1 \\ -1 & 1 & -1 \end{pmatrix}, \quad \xi_{12} = \begin{pmatrix} -1 & 1 & -1 \\ 0 & 1 & 1 \\ 0 & 0 & 0 \\ 1 & -1 & 1 \\ -1 & -1 & -1 \\ 0 & -1 & 1 \\ -1 & -1 & 1 \\ 0 & -1 & -1 \\ -0.18 & 1 & 1 \\ 1 & -1 & -1 \\ 0.26 & 1 & -1 \\ 1 & 1 & 1 \end{pmatrix}$$

$$\xi_{13} = \begin{pmatrix} 0.48 & -1 & -1 \\ 0 & -1 & -1 \\ -0.3 & 1 & 1 \\ 1 & 1 & 1 \\ -1 & 1 & -1 \\ 1 & 1 & -1 \\ -1 & -1 & -1 \\ 0 & 0 & 0 \\ 1 & -1 & 1 \\ 0 & 1 & 1 \\ -1 & -1 & 1 \\ 0 & 1 & -1 \\ 0 & -1 & 1 \end{pmatrix} \quad \xi_{14} = \begin{pmatrix} -1 & 1 & -1 \\ -1 & -1 & 1 \\ 0 & -1 & 1 \\ -1 & -1 & 1 \\ 0.14 & 1 & 1 \\ 0.2 & 1 & 1 \\ 1 & -1 & -1 \\ 1 & 1 & 1 \\ 0 & -1 & -1 \\ -1 & 1 & -1 \\ 0 & -1 & -1 \\ 0 & 0 & 0 \\ 0 & 1 & -1 \\ 1 & -1 & -1 \end{pmatrix}$$

$$\xi_{15} = \begin{pmatrix} 0 & 1 & -1 \\ 0 & 1 & -1 \\ 0 & 0 & 0 \\ 1 & 1 & -1 \\ 0 & -1 & 1 \\ 1 & -1 & 1 \\ 0 & 1 & 1 \\ 1 & -1 & 1 \\ -1 & -1 & -1 \\ 0 & -1 & -1 \\ -1 & -1 & -1 \\ 1 & 1 & -1 \\ 0 & -1 & 1 \\ -1 & 1 & 1 \\ -1 & 1 & 1 \end{pmatrix} \quad \xi_{27} = \begin{pmatrix} 0 & -1 & 1 \\ 1 & -1 & -1 \\ 0 & -1 & -1 \\ 0 & 0 & 0 \\ 1 & -1 & 1 \\ -1 & 1 & 1 \\ 0 & 1 & -1 \\ 0 & 1 & -1 \\ 1 & -1 & -1 \\ 0 & 1 & 1 \\ 0 & -1 & 1 \\ 1 & 1 & 1 \\ 1 & 1 & -1 \\ 0 & -1 & 1 \\ 1 & 1 & -1 \\ 0 & -1 & -1 \\ -1 & -1 & -1 \\ 0 & 1 & -1 \\ 1 & 1 & 1 \\ -1 & -1 & -1 \\ -1 & -1 & -1 \\ -1 & 1 & 1 \\ -1 & -1 & 1 \\ -0.05 & 1 & 1 \\ -1 & 1 & -1 \\ 0 & 1 & -1 \\ 0 & -1 & 1 \end{pmatrix}$$

Case 2

The illustration considers a three-variable non-standard model with 6 parameters given in Equation (3). For $N = 9, 10, \ldots 15$ and 27, the custom I-optimal designs for each of the N design points with $n_c = 1$ is given as;

$$\xi_9 = \begin{pmatrix} 1 & 1 & 0 \\ -1 & 1 & -1 \\ -1 & 1 & 1 \\ -1 & -1 & 0 \\ -1 & -1 & 0 \\ 1 & 1 & 0 \\ 0 & 0 & 0 \\ 1 & -1 & 1 \\ 1 & -1 & -1 \end{pmatrix} \quad \xi_{10} = \begin{pmatrix} -1 & 1 & -1 \\ -1 & 1 & 1 \\ 1 & 1 & 0.19 \\ 1 & 1 & -1 \\ -1 & -1 & -0.01 \\ 1 & 1 & 0 \\ 1 & -1 & -1 \\ 0 & 0 & 0 \\ -1 & -1 & 0 \\ 1 & -1 & 1 \end{pmatrix}$$

$$\xi_{11} = \begin{pmatrix} 0 & 0 & 0 \\ -1 & -1 & 0.26 \\ -1 & 1 & 1 \\ -1 & 1 & -1 \\ 1 & 1 & 1 \\ 1 & 1 & -0.17 \\ -1 & -1 & -1 \\ 1 & -1 & -1 \\ -1 & -1 & 0 \\ 1 & 1 & 0 \\ 1 & -1 & 1 \end{pmatrix} \quad \xi_{12} = \begin{pmatrix} 1 & 1 & 0 \\ 1 & -1 & 1 \\ 1 & 1 & -1 \\ -1 & -1 & 0 \\ 1 & -1 & 0 \\ 0 & 1 & 1 \\ 1 & -1 & -1 \\ -1 & 1 & -1 \\ -1 & 1 & 0.14 \\ 0 & 0 & 0 \\ -1 & -1 & -1 \\ -1 & -1 & 1 \end{pmatrix}$$

$$\xi_{13}=\begin{pmatrix}-1&-1&1\\1&-1&0\\-1&1&1\\-1&1&-1\\1&-1&1\\1&-1&-1\\1&1&-1\\-1&1&0\\1&1&1\\1&1&0\\-1&-1&0\\-1&-1&-1\\0&0&0\end{pmatrix}\ \xi_{14}=\begin{pmatrix}-1&1&1\\-1&1&-1\\1&-1&-1\\-1&-1&1\\0&0&0\\1&1&-1\\-1&-1&0\\1&1&0\\-1&-1&-1\\1&-1&0\\-1&-1&0\\1&-1&1\\-1&1&0\\1&1&1\end{pmatrix}$$

$$\xi_{15}=\begin{pmatrix}-1&-1&1\\1&1&0\\-1&-1&0\\-1&-1&0\\-1&1&-1\\1&1&-1\\-1&1&1\\-1&-1&-1\\1&-1&-1\\1&-1&0\\-1&1&0\\1&1&0\\0&0&0\\1&1&1\\1&-1&1\end{pmatrix}\ \xi_{27}=\begin{pmatrix}1&-1&-1\\-1&1&1\\-1&-1&-1\\-1&-1&0\\-1&-1&1\\-1&-1&0\\-1&1&1\\1&-1&0\\-1&-1&0.12\\1&-1&1\\-1&1&-1\\1&-1&1\\-1&-1&0\\1&1&-1\\1&1&0\\1&1&0\\1&1&0\\0&0&0\\1&-1&-1\\1&-1&0\\-1&-1&-1\\-1&1&0\\-1&1&1\\1&1&0\\-1&1&-1\\-1&1&0\\1&1&1\end{pmatrix}$$

Case 3

Considering the three-variable non-standard model with 7 parameters, given in Equation (4), for $N = 9, 10, \ldots, 15,$ and 27, the custom I-optimal designs for the N design points with $n_c = 1$ are given as;

$$\xi_{9}=\begin{pmatrix}-1&-1&1\\0&-1&-1\\-1&-1&-1\\1&-1&1\\1&0.35&-1\\0&0&0\\1&1&1\\-1&1&-0.37\\0&1&1\end{pmatrix}$$

$$\xi_{10}=\begin{pmatrix}1&-1&1\\-0.82&1&1\\-1&1&-1\\1&0&-1\\0&1&-1\\1&1&1\\0&-1&1\\0&-1&-1\\-1&-1&0\\0&0&0\end{pmatrix}\ \xi_{11}=\begin{pmatrix}-1&-1&-1\\0.34&1&1\\0&-1&-1\\-1&1&-1\\-1&1&1\\-1&-1&1\\1&1&-1\\0.53&-1&-1\\0&1&1\\0&0&0\\1&-1&1\end{pmatrix}$$

$$\xi_{12}=\begin{pmatrix}-1&-1&1\\1&-1&-1\\0&0&0\\0&-1&1\\-1&1&-1\\1&-1&1\\0.18&1&1\\0&-1&-1\\1&1&-0.24\\0&1&-1\\-1&-1&-1\\-1&1&1\end{pmatrix};\ \xi_{13}=\begin{pmatrix}-1&-1&-1\\1&1&-1\\0&-1&-1\\1&-1&-1\\-1&1&-1\\-1&-1&1\\0&1&1\\-1&1&1\\0&1&-1\\0&0&0\\1&1&1\\0&-1&1\\1&-1&1\end{pmatrix},$$

$$\xi_{14}=\begin{pmatrix}-1&1&-1\\-1&1&1\\0&0&0\\1&1&-1\\0&-1&-1\\1&-1&1\\-1&-1&-1\\0&1&-1\\0&1&1\\0&1&1\\1&1&1\\0&-1&1\\1&-1&-1\\-1&-1&1\end{pmatrix}\ \xi_{15}=\begin{pmatrix}0&-1&1\\-1&-1&1\\-1&1&-1\\-1&-1&-1\\0&-1&1\\0&-1&-1\\1&-1&-1\\0&1&-1\\1&1&1\\1&1&-1\\1&-1&1\\0&1&-1\\0&0&0\\-1&1&1\\0&1&1\end{pmatrix},$$

$$\xi_{27}=\begin{pmatrix}-1&-1&1\\-1&1&-1\\0&-1&-1\\1&1&-1\\1&-1&-1\\1&-1&1\\1&1&1\\-1&-1&-1\\-1&-1&-1\\1&1&-1\\0&-1&1\\0&-1&-1\\0&1&-1\\0&0&0\\0&1&1\\0&-1&1\\-1&-1&1\\-1&1&-1\\0&1&-1\\1&-1&1\\0&1&1\\1&-1&-1\\1&1&1\\-1&1&1\\-1&1&1\\0&-1&-1\\0&1&1\end{pmatrix}$$

Case 4

This illustration considers the 9-parameter non-standard model in four variables given in Equation (5). For $N = 13, 14, \ldots, 18$, 21 and 25 the custom I-optimal designs for the N design points with $n_c = 1$ are given as;

$$\xi_{13} = \begin{pmatrix} -1 & 1 & -1 & 0.03 \\ -1 & -1 & 1 & -0.57 \\ 0 & -1 & -1 & -1 \\ 0 & 0 & 0 & 0 \\ 0 & 1 & 1 & 1 \\ 1 & -1 & -1 & 0 \\ 0 & -1 & 1 & 0 \\ 0 & 1 & -1 & 0 \\ -1 & 1 & 1 & -1 \\ -1 & -1 & -1 & 1 \\ 1 & -1 & 1 & 1 \\ 1 & 1 & 1 & 0 \\ 1 & 1 & -1 & -1 \end{pmatrix}$$

$$\xi_{14} = \begin{pmatrix} 0 & 0 & 0 & 0 \\ 1 & -1 & 1 & -1 \\ 0 & 1 & 1 & -1 \\ 1 & 1 & -1 & 1 \\ -1 & -1 & 1 & 0 \\ -1 & 1 & 1 & 1 \\ 0 & 1 & -1 & -1 \\ 1 & -1 & -1 & 0 \\ 0 & -1 & -1 & 0.42 \\ 0 & 1 & 0 & 0 \\ -1 & -1 & -1 & -1 \\ -1 & 1 & -1 & -0.04 \\ 1 & 1 & 1 & 0 \\ 0 & -1 & 1 & 1 \end{pmatrix}$$

$$\xi_{15} = \begin{pmatrix} -1 & -1 & -1 & 1 \\ 1 & -1 & 1 & 1 \\ 0 & 1 & 1 & 1 \\ 0 & -1 & 0 & 0 \\ -1 & 1 & 1 & -1 \\ 0 & 0 & 0 & 0 \\ -1 & 1 & -1 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & -1 & -1 & -1 \\ 1 & -1 & -1 & 0 \\ 1 & 1 & 1 & 0 \\ 0 & -1 & 1 & -1 \\ 1 & 1 & -1 & -1 \\ 0 & 1 & -1 & 1 \\ -1 & -1 & 1 & 0 \end{pmatrix} \quad \xi_{16} = \begin{pmatrix} 0 & 1 & -1 & 0 \\ -1 & 1 & 1 & 1 \\ 0 & -1 & 1 & -1 \\ 0 & 0 & 0 & 0 \\ 0 & 1 & 1 & 0 \\ 0 & -1 & -1 & 1 \\ -1 & -1 & 1 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & -1 & 1 & 1 \\ 1 & -1 & 1 & 0 \\ -1 & 1 & -1 & -1 \\ 1 & 1 & -1 & 1 \\ -1 & -1 & -1 & 0 \\ 1 & 1 & 1 & -1 \\ 0 & -1 & -1 & -1 \\ 1 & -1 & -1 & 0 \end{pmatrix}$$

$$\xi_{17} = \begin{pmatrix} 0 & 1 & -1 & -1 \\ -1 & 1 & 1 & 1 \\ 0 & 0 & 0 & 0 \\ 0 & 1 & -1 & 0 \\ 0 & -1 & -1 & 0 \\ 0 & 1 & 1 & -1 \\ 0 & -1 & -1 & 1 \\ 1 & 1 & -1 & 1 \\ -1 & 1 & -1 & 0 \\ 1 & 1 & 1 & 0 \\ -1 & -1 & -1 & 0 \\ 1 & -1 & -1 & -1 \\ 0 & -1 & 1 & 0 \\ 0 & 1 & 1 & 0 \\ 0 & -1 & 1 & 1 \\ 1 & -1 & 1 & 0 \\ -1 & -1 & 1 & -1 \end{pmatrix},$$

$$\xi_{18} = \begin{pmatrix} 1 & -1 & -1 & -1 \\ 0 & 1 & -1 & 1 \\ 1 & 1 & -1 & -1 \\ -1 & -1 & 1 & 0 \\ 0 & -1 & 1 & -1 \\ -1 & 1 & -1 & 0 \\ 0 & -1 & 1 & 0 \\ -0.25 & -1 & -1 & -1 \\ -1 & -1 & -1 & 1 \\ 0 & -1 & -1 & 0 \\ 0 & 1 & 1 & 1 \\ 0 & 0 & 0 & 0 \\ -1 & 1 & 1 & -1 \\ 1 & 1 & 1 & 0 \\ 1 & -1 & 1 & 1 \\ 1 & -1 & -1 & 0 \\ 0 & 1 & 1 & 0 \\ 0 & 1 & -1 & 0 \end{pmatrix} \quad \xi_{21} = \begin{pmatrix} 1 & 1 & -1 & 0 \\ 0 & -1 & 1 & -1 \\ 1 & 1 & -1 & -1 \\ 0 & 1 & -1 & -1 \\ 1 & -1 & 1 & -1 \\ 0 & 1 & -1 & 1 \\ 1 & -1 & 1 & 1 \\ -1 & -1 & 1 & 1 \\ 0 & -1 & -1 & 1 \\ -1 & 1 & -1 & 0 \\ 0 & 1 & 1 & 0 \\ 1 & 1 & 1 & 1 \\ 0 & -1 & -1 & 0 \\ 0 & 1 & 1 & 0 \\ -1 & 1 & 1 & -1 \\ -1 & -1 & 1 & 0 \\ 0 & 0 & 0 & 0 \\ -1 & -1 & -1 & -1 \\ 1 & -1 & -1 & 0 \\ 0 & -1 & 1 & 0 \\ -1 & 1 & -1 & 1 \end{pmatrix}$$

$$\xi_{25} = \begin{pmatrix} 0 & 0 & 0 & 0 \\ -1 & 1 & -1 & 0 \\ -1 & -1 & -1 & -1 \\ 1 & 1 & 1 & 0 \\ 0 & 1 & -1 & 1 \\ 0 & 1 & -1 & -1 \\ -1 & -1 & 1 & 1 \\ 1 & -1 & 1 & 0 \\ 1 & 1 & -1 & -1 \\ 1 & 1 & -1 & 0 \\ 0 & -1 & -1 & 0 \\ -1 & 1 & -1 & 0 \\ 0 & 1 & 1 & 0 \\ 0 & 1 & 1 & 1 \\ -1 & -1 & 1 & 1 \\ 0 & -1 & 1 & 0 \\ -0.17 & -1 & -1 & 0 \\ 0 & -1 & -1 & 0 \\ 1 & -1 & 1 & -1 \\ -1 & 1 & 1 & -1 \\ 1 & -1 & -1 & 1 \\ 0 & -1 & 1 & -1 \\ 0 & 1 & 1 & 0 \\ 0 & 1 & -1 & 1 \\ 1 & -1 & -1 & 1 \end{pmatrix}$$

Table 3 below shows the result of the efficiency measures and AVP values of custom I-optimal designs for non-standard models. From the result, it is observed that the I-optimal design performed well (above 50%) in terms of D- and G-efficiency. It also performed well in terms of A-efficiency and the values in most cases are similar to that of A-optimal design. Thus, it can be said that the I-optimal designs are D, A, and G efficient. Also, from the result, it was observed that the I-optimal designs had the smallest average variance of prediction compared to other custom designs thus, making it a good choice for prediction.

Table 3. *Efficiency Measures of I-optimal designs for Non-standard models.*

Number of factors (k)	Number of parameters (p)	Number of design points (N)	D-efficiency (%)	G-efficiency (%)	A-efficiency (%)	Average Variance of Prediction (AVP)
3	5	9	61.32132	74.07407	48.30918	0.323333
		10	61.81643	66.77774	46.9793	0.297374
		11	62.87172	66.42324	46.73369	0.272618
		12	61.87742	72.80956	45.73915	0.249532
		13	61.96404	69.21453	46.55971	0.226197
		14	63.18278	85.76883	47.71272	0.208198
		15	64.68813	80	48.9083	0.191468
		27	65.15931	83.36667	49.24094	0.105458
3	6	9	58.11824	66.66667	47.61903	0.351111
		10	58.86504	59.82963	46.20002	0.324658
		11	60.30197	58.83521	45.5094	0.297414
		12	61.88824	89.08194	47.11375	0.270582
		13	65.1364	85.2071	49.01293	0.242778
		14	63.71614	79.12088	49.09363	0.22378
		15	62.64027	73.84615	49.5941	0.205357
		27	62.43969	68.53836	49.21173	0.113965
3	7	9	57.69692	51.59114	43.3002	0.429518
		10	53.80632	53.15039	41.48247	0.378536
		11	58.18175	54.23887	43.80323	0.328886
		12	59.70504	84.75852	46.83452	0.292052
		13	64.6098	80.76923	50.48077	0.256667
		14	62.73272	77.35849	50.10183	0.237669
		15	61.21732	70	50.09585	0.219246
		27	64.47407	77.77778	50.9151	0.121501
4	9	13	57.21456	77.00078	41.93254	0.350826
		14	56.7514	77.71704	42.55255	0.322023
		15	56.19102	74.49687	43.4051	0.295676
		16	56.00956	73.65331	43.93409	0.273887
		17	55.95376	70.8992	44.33641	0.25519
		18	56.33369	68.83533	43.70558	0.244087

Number of factors (k)	Number of parameters (p)	Number of design points (N)	D-efficiency (%)	G-efficiency (%)	A-efficiency (%)	Average Variance of Prediction (AVP)
		21	58.53976	72.40759	43.80603	0.208551
		25	57.08659	66.10358	43.44466	0.175454

4. Discussion of Findings

Based on the computation of the efficiency properties of the custom D-, A-, and I-optimal design for the non-standard models, it is seen that the D, G, and A-efficiency values of the custom designs are less than 100%. This is in line with Kiefer and Wolfowitz [11] who proposed that the optimality criteria consider experimental design as an N-point design. Therefore, optimal designs will generally be less than 1.0 (or 100%).

Again, from the results, it is observed that without much loss in efficiency, small-size designs are as efficient as large-size designs. For example, the custom A 13-point design for the 5-parameter non-standard model has the highest G-efficiency of 92.31354%, D-efficiency of 63.43927%, A-efficiency of 47.5631%, and AVP of 0.231168. In comparison, the custom A 27-point design has a G-efficiency of 65.15811%, D-efficiency of 83.22195%, A-efficiency of 49.24383%, and AVP of 0.105461. Hence, small-size economical designs can be selected to meet specific research objectives.

For custom A-optimal designs, the result in Table 1 showed that the custom A-optimal designs had the highest A-efficiency value compared to other custom designs. This owes to the fact that the design is created based on the A-optimality criterion thus, they are A-efficient. In terms of D-efficiency, it was observed that the values were moderately high but less than those of a D-optimal design. This implies that custom A-optimal designs are also D-efficient. Hence, they can be used to identify both the main factors and interactions in second-order experiments. Again, custom A-optimal design is efficient in terms of G-efficiency. This is in contrast with Wong W.K. [20]. This implies that custom A-optimal designs minimize the worst-case prediction variance. Lastly, the result of the Average Variance of Prediction (AVP) showed a smaller variance compared to that of the D-optimal design for each of the design points. Hence, the custom A-optimal design is more suitable for prediction than the custom D-optimal design. Therefore, for the non-standard models, we can say that the custom A-optimal design is D-efficient, G-efficient, and A-efficient, and is more suitable for prediction than the custom D-optimal design.

The result in Table 2 showed that the custom D-optimal design which was created based on the D-optimality criterion had the highest D-efficiency values compared to other custom designs. This implies that custom D-optimal designs are good at estimating all the parameters of interest in the model. Also, it was observed that the custom D-optimal design produced the best G-efficiency (60% and above) compared to other custom designs. This means that the custom D-optimal designs are G-optimal hence, minimize the worst-case prediction variance. This corresponds with the work of Kiefer and Wolfowitz [11] who proposed that a D-optimal design is also G-optimal.

In terms of A-efficiency and Average Variance of Prediction (AVP), the result revealed that the D-optimal design does not fare well. This is contrary to the work of Wong W. K. [20] that D-optimal designs are A-efficient. The A-efficiency values were generally less than 50% this implies that the D-optimal design is not an appropriate design for identifying only the significant factors in a model. Also, the AVP values were high compared to other custom designs. Indicating high prediction variance thereby, making the D-optimal design unsuitable for prediction purposes.

Table 3 shows the efficiency and AVP values of the I-optimal design. From the result, it is observed that custom I-optimal design performed moderately well (above 50%) in terms of D- and G-efficiency. In terms of A-efficiency, they performed as well as the A-optimal design. This corresponds with the work of Jones and Goos [10], and Rady *et al*. [16]. For the AVP values, it is observed that the custom I-optimal design had the lowest values compared to custom D- and A-optimal designs. This corresponds with the works of Johnson *et al*. [9], Jones and Goos [10], and Yeh *et al*. [21], that the I-optimal design has a lower average prediction variance than the D-optimal design. This justifies the fact that the I-optimality criterion seeks designs that minimize the Average Variance of Prediction. Generally, for non-standard models, the I-optimal designs performed well in terms of D-efficiency, G-efficiency, and A-efficiency and have the smallest Average Variance of Prediction.

From the results of the analysis, it is appropriate to describe custom designs as efficient designs for fitting second-order non-standard models. As earlier mentioned, custom designs are suitable in situations that involve non-standard models, fewer experimental runs, and irregularly shaped design regions where standard designs are not suitable to use or not economical to utilize. The efficiency value is a function of the optimality criterion. The custom D-optimal design performed best in terms of D- and G-efficiency. Custom A-optimal design had the best

A-efficiency value. The custom I-optimal design had the smallest average variance of prediction.

5. Conclusion

The efficiency of custom D-, A-, and I-optimal designs have been thoroughly examined and demonstrated in this research work in second-order non-standard models under varying design points. This study is applied mostly in situations where the experimenter knows the model. Also, in situations where some constraints (such as time, materials, and resources) may limit the use of commonly known classical designs. Thus, custom designs can be used in non-standard models to effectively construct designs that align with the goal of the experiment and available resources.

Design efficiency metrics such as D-, G-, A-efficiency, and AVP are functions of design optimality criterion and they help experimenters evaluate the quality of designs based on the specific goal and objectives of the experiment even before the experiment is conducted.

Abbreviations

AVP	Average Variance of Prediction
DOE	Design of Experiment
CGD	Computer-generated Designs
JMP	John's Macintosh Project
SPV	Scaled Prediction Variance

Author Contributions

Iwundu Mary Paschal: Datacuration, Formal Analysis
Israel Chinomso Fortune: Methodology, Resources

Conflicts of Interest

The authors declare no conflicts of interest.

References

[1] Akinlana, D. M. (2022). New Developments in Statistical Optimal Designs for Physical and Computer Experiments. University of South Florida.

[2] Gaifman, H. (2004). Non-standard models in a broader perspective. In Nonstandard Models of Arithmetic and Set Theory (pp. 1–22). American Mathematical Society. https://doi.org/10.1090/conm/361/06585

[3] Goos, P., & Jones, B. (2011). Optimal Designs of Experiments: A Case Study Approach, 1st Edition, Wiley, New York. ISBN: 978-0-470-74461-1

[4] Goos, P., Jones, B., & Syafitri, U. (2016). I-optimal design of mixture experiments. Journal of the American Statistical Association, 111(514), 899–911. https://doi.org/10.1080/01621459.2015.1136632

[5] Iwundu M. P. & Otaru O. A. P. (2019). Construction of Hat-Matrix Composite Designs for Second-Order Models. American Journal of Computational and Applied Mathematics. https://doi.org/10.5923/j.ajcam.20190903.03

[6] Iwundu, M. (2017). Missing observations: The loss in relative A-, D- and G-efficiency. International Journal of Advanced Mathematical Sciences, 5(2), 43. https://doi.org/10.14419/ijams.v5i2.7786

[7] Iwundu, M. P. (2018). Construction of Modified Central Composite Designs for Non-standard Models. Canadian Center of Science and Education. https://doi.org/10.5539/ijsp.v7n5p95

[8] Iwundu, Mary Paschal, & Cosmos, J. (2022). The efficiency of seven-variable box-Behnken experimental design with varying center runs on full and reduced model types. Journal of Mathematics and Statistics, 18(1), 196–207. https://doi.org/10.3844/jmssp.2022.196.207

[9] Johnson, R. T., Montgomery, D. C., & Jones, B. A. (2011). An expository paper on optimal design. Quality Engineering, 23(3), 287–301. https://doi.org/10.1080/08982112.2011.576203

[10] Jones, B., & Goos, P. (2012). I-optimal versus D-optimal split-plot response surface designs. Journal of Quality Technology, 44(2), 85–101. https://doi.org/10.1080/00224065.2012.11917886

[11] Kiefer, J., & Wolfowitz, J. (1959). Optimum Designs in Regression Problems. The Annals of Mathematical Statistics, 30(2), 271–294. https://doi.org/10.1214/aoms/1177706252

[12] Kiefer, J., & Wolfowitz, J. (1960). The equivalence of two extremum problems. Canadian Journal of Mathematics. Journal Canadien de Mathematiques, 12(0), 363–366. https://doi.org/10.4153/cjm-1960-030-4

[13] Montgomery, D. C. (2001). Design and Analysis of Experiment 5th ed. John Wiley & Sons Inc.

[14] Myers R. H, M. D. C. &. A.-C. C. M. (2009). Response surface methodology: Process and product using designed experiments (3rd ed.). Wiley-Blackwell.

[15] Ossia C. V. and Big-Alabo, A. (2022). Performance Evaluation of Apricot Kernel Oil-Based Cutting-Fluid Using L27 Orthogonal Arrays Design. Journal of the Egyptian Society of Tribology. https://doi.org/10.21608/jest.2022.216109

[16] Rady E. A., M. M. E. Abd El-Monsef, and M. M. Seyam. (2009). Relationships among Several Optimality Criteria. Cairo University.

[17] Smucker, B., Krzywinski, M., & Altman, N. (2018). Optimal experimental design. Nature Methods, 15(8), 559–560. https://doi.org/10.1038/s41592-018-0083-2

[18] Walsh, S. J., Lu, L., & Anderson-Cook, C. M. (2024). I -optimal or G -optimal: Do we have to choose? Quality Engineering, 36(2), 227–248. https://doi.org/10.1080/08982112.2023.2194963

[19] Warren F. Kuhfeld, SAS Institute, Inc. (1997). Efficient Experimental Designs Using Computerized Searches. Sawtooth Software, Inc.

[20] Wong, W. K. (1994). Comparing robust properties of A, D, E, and G-optimal designs. Computational Statistics & Data Analysis, 18(4), 441–448. https://doi.org/10.1016/0167-9473(94)90161-9

[21] Yeh Mei-Fen, Anthony Cece, Mark Presser. (2010). Custom Designs Using JMP® Design of Experiments and SAS® PROC OPTEX. Unilever, Trumbull, CT.

[22] Zhou, Y. D., & Xu, H. (2017). Composite designs based on orthogonal arrays and definitive screening designs. Journal of the American Statistical Association, 112(520), 1675–1683. https://doi.org/10.1080/01621459.2016.1228535

Research Field

Iwundu Mary Paschal: Modelling and Response Surface optimization, Sequential design of experiments, Missing observations and loss functions, Optimal design and efficiency, Exploration of nonstandard model, Development of search algorithms for global optimization.

Israel Chinomso Fortune: Optimal experimental design, Exploration of Non-standard Models, Design Optimality and efficiency, Response Surface Methodology, Design of Experiments, Statistics.