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Comparisons of Bayes factors for 2^4 full, fractional, and reduced factorial designs

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ABSTRACT

The effect of factors in full and fractional factorial designs is being studied ubiquitously in all fields of science and engineering. At times, researchers would want to gather additional information than the fractional factorial design provided, there is no restriction to conducting more experimental runs. In this study, we propose a reduced fractional factorial design consisting of all significant factors. This paper illustrates the effectiveness of factors through real data application and simulation by comparing the full factorial, reduced factorial, and fractional factorial designs. The actual weightage of the main/interaction effects in these three designs was found by identifying and quantifying the Bayes factors through the simulation datasets. It is observed that the reduced factorial design produces better results when there are no constraints to select or add factors to the model.

1. Introduction

Factorial designs are being widely used in experiments involving several factors and where it is necessary to study the impact of the factors or combination of factors on a process. The commonly used method in scientific experiments is a special case of general factorial designs and they form the basis for other designs of considerable practical value. The most important among these special cases is the factorial design with p factors, each having two levels and it may be quantitative or qualitative with levels corresponding to the "high" and "low" levels of a factor. The recent developments in the non-regular fractional factorial designs such as generalized minimum aberration criteria, optimality results, and analysis strategies were explained by Xu et al. (2009). A full replicate of such a design is called a 2^p full factorial design and requires 2^p observations. Wang and Ma (2013) discussed how to identify the effects that are to be included in the model by applying the Bayesian approach. The construction of hierarchical ANOVA models was discussed and the different comparison strategies to the models were based on the Bayes factors (Rouder et al., 2017). In the hierarchical Bayesian ANOVA with a simulation dataset (Dong and Wedel, 2017), the Bayesian approach is applied to the multi-way ANOVA models and compared to their hierarchical ANOVA model (Rouder et al., 2017). The framework of hypothesis-based Bayesian decision theory with robust loss function and step-by-step guidelines was given to apply the Bayes factor to get optimal decisions was presented (Schwaferts and Augustin, 2021) and the best extraction condition of factors was identified from the application of six-factors fractional factorial design (Khaw et al., 2019). Lakens et al. (2020) have provided comprehensive explanations of the calculation and interpretation of Bayes factors for several tests. In educational research, the Bayesian analysis for treatment and control groups was discussed through factorial designs (Kassler et al., 2020). The limitations of optimization and mathematical model for improving composting processes are addressed (Sokac et al., 2022). Outlined a thorough knowledge of Bayesian variable selection, Bayesian evaluation of cognitive models (Heck et al., 2022), and opportunities for Bayes factor applications. Gardini et al. (2021) gave an idea on the log-transformation of a response variable by applying the Bayesian analysis of variance mixed models to examples and simulation datasets. Egburonu and Abidoye (2021) discussed a balanced two-way analysis of variance of three cases such as the factors are fixed, random, and mixed by applying the Bayesian techniques. Grömping (2021)

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developed an algorithm for a two-level regular fractional factorial design with two-factor interactions. Chang (2022) used the Bayesian approach for the minimum aberration criteria for many applications.

2. Factorial design for four factors with two levels

In this paper, we have taken up 2^4 factorial examples to identify the vital and significant factors in the full factorial reduced factorial and fractional factorial designs. In general, we propose to study fractional factorial design when the experimental run is huge, integrating all significant factors in the design. Xu et al. (2009) discussed recent developments in non-regular fractional factorial designs, particularly optimality criteria, projection properties, resolutions, and aberration criteria. Baba et al. (2013) proposed the usefulness of the empirical Bayesian approach to the saturated factorial designs and observed predictions and inferences for the parameters. Espinosa et al. (2016) proposed a new approach to screen for active factorial effects from replicated factorial design using the potential outcomes framework and based on sequential posterior predictive model checks. Rouder et al. (2017) presented the Bayes factor approach to multi-way ANOVA with hierarchical models for fixed, random effects, with-subjects, between-subjects, and mixed designs. The models which we have employed for this study are explained in the following session.

2.1. 2^4 Full factorial design

The factorial design of 2^4 was employed to give a 16-step experimental run with the four factors each at low and high levels. We considered four factors A, B, C, and D each at two levels. The standard order of treatment combinations is (1), A, B, AB, C, AC, BC, ABC, D, AD, BD, ABD, CD, ACD, BCD, and ABCD, i.e., four main effects, six first-order interactions, four second-order interactions, and one third-order interaction. These fifteen effects are mutually orthogonal contrasts of the treatment means. The experimental matrix for the 2^4 factorial design is given in Table 1.

2.2. 2^{4-1} Fractional factorial design

In a 2^p factorial design, as the number of factors increases then the number of trials required for a full replicate of the design rapidly increases in the experiments. In such cases, we cannot perform a full replicate of the design and a fractional factorial design has to be run. Assume that certain interactions involving a large number of factors are negligible, the information on the lower order effects can be obtained by running a suitable fraction of the 2^p full factorial design. Two-level fractional factorial designs are broadly divided into regular and non-regular fractional factorial designs discussed by Deng and Tang (1999). Statisticians have designated fractional factorial experiments to reduce the number of runs or trials, only selected treatment combinations are tried instead of all combinations. A fractional factorial design employs a systematic approach to reduce the number of experimental conditions to allow meaningful study. To run-size the economy and be cost-effective, we used fractional factorial designs, which are widely applied in various fields such as engineering, industrial and scientific research.

The higher-order interactions are confounded, or aliased, with lower-order effects such that they are negligible in size in the fractional factorial designs. The experimenters have found that higher-order interactions of three or more factors tend to be small and can be ignored. Furthermore, for the objective of improving the process with 8 runs, we constructed 2^{4-1}fractional factorials by selecting ABCD as the generator. Also, this choice of generator will result in a design of the highest possible resolution IV. To construct the design, we used the defining relation, each main effect is aliased with a three-factor interaction, A=BCD, B=ACD, C=ABD, and D=ABC. Moreover, every two-factor interaction is aliased with other two-factor interactions, the alias relationships AB=CD, AC=BD, BC=AD. Therefore, the four main effects plus the three two-factor interaction alias pairs account for the seven degrees of freedom for the design. The experimental matrix for the 2^{4-1} fractional factorial design is shown in Table 2.

2.3. 2^4 Reduced factorial design

If the number of significant factors in the full factorial design is more than the factors in the half-fraction factorial design, our choice may be a reduced factorial design. The idea is to construct a reduced factorial design with significant factors alone. One cannot predetermine this before doing the full factorial design. Suppose, the experimenter decides never to lose any kind of reduced factorial design that will be useful and more informative. This screening design is preferable if there is no constraint or deliberately wanted by the experimenter, for adding all the main and interaction factors except the non-significant factors. Once the significant factors from the full factorial design are identified, this reduced factorial design is demonstrated in the full and fractional factorial designs. This experiment is used to compare the efficacy of reduced and fractional factorial designs.

3. Priors and Bayes factors

In this study, we used five different priors to find the Bayes factors for full, reduced, and fractional factorial designs. The estimating Bayes factor for repeated-measures analysis of variance design 1 was addressed by Faulkenberry (2020). These priors are considered in the comparison of hierarchical two-way ANOVA models 10 by Vijayaragunathan and Srinivasan (2020). Bayes factors were conceptually extensively discussed by Maruyama (2009), Wetzels et al. (2012), and Wang and Sun (2014).

Table 1: Experimental matrix for the 2^4 factorial design

Runs		1	2	3	4	5	6	7	8	9	10	11	12	13	14	15	16
Factors	A	-1	1	-1	1	-1	1	-1	1	-1	1	-1	1	-1	1	-1	1
	B	-1	-1	1	1	-1	-1	1	1	-1	-1	1	1	-1	-1	1	1
	C	-1	-1	-1	-1	1	1	1	1	-1	-1	-1	-1	1	1	1	1
	D	-1	-1	-1	-1	-1	-1	-1	-1	1	1	1	1	1	1	1	1

Table 2: Experimental matrix for the 2^{4-1} fractional factorial design with the defining relation I=ABCD

Runs		1	2	3	4	5	6	7	8
Factors	A	-1	1	-1	1	-1	1	-1	1
	B	-1	-1	1	1	-1	-1	1	1
	C	-1	-1	-1	-1	1	1	1	1
	D=ABC	-1	1	1	-1	1	-1	-1	1

3.1. Zellner's g prior

Zellner's priors were most commonly used prior to Bayesian hypothesis testing Many authors such as George and Foster (2000), Kass and Wasserman (1995), and others have discussed extensively on this prior. We consider two priors by setting the value of$g$, (i) Unit Information Prior (UIP) if $g = n$ and (ii) Risk Inflation Criterion (RIC) if $g = k^2$, where n=number of observations and k= the number of predictors in the regression model. The Bayes Factor for the full model to the null model is

$$BF = (1+g)^{(n-k-1)/2}[1+g(1-R^2)]^{-(n-1)/2} \tag{1}$$

3.2. Jeffreys-Zellner-Siow prior

Jeffreys-Zellner-Siow (JZS) prior is a mixture of priors we estimate g from the data, (Liang et al., 2008). The Bayes Factor for the full model to the null model is in Eq. 2.

3.3. Hyper-g prior

Hyper-g prior is a family of prior distributions on g and this hyper-g approach. The term a varies from 2 to 4, it produces different behavior of hyper-g prior, for our convenience, we take only two values such as $a = 3$ and $= 4$. The Bayes Factor for the full model to the null model is in Eq. 3.

Algorithm for comparison of Bayes Factor for full, reduced, and fractional factorial designs.

The following steps were made for comparing and identifying the effect of factors in the full, fractional and reduced factorial designs:

Step 1: Apply full factorial design for the suitable data and identify the significant and non-significant main and interaction effects.
Step 2: Generate a reduced factorial design according to the significant factors from the full factorial design
Step 3: Construct a fractional factorial design with minimum aberration then check its significance in the model.
Step 4: Compute the Bayes factor values for these designs to compare the strength and weaknesses of factors while incorporating them into these designs.
Step 5: To generalize the results we used different simulation datasets to find a substantial number of Bayes factors to conclude the ample and instructive conclusions.

$$BF = \frac{(n/2)^{1/2}}{\Gamma(\frac{1}{2})}\int_0^\infty (1+g)^{(n-k-1)/2}\,[1+g\,(1-R^2)]^{-(n-1)/2}\,g^{-3/2}\,e^{-n/2g}\,dg \tag{2}$$

$$BF = \frac{a-2}{2}\int_0^\infty (1+g)^{\frac{n-k-1-a}{2}}\,[1+g(1-R^2)]^{-\frac{n-1}{2}}\,dg \tag{3}$$

4. Application of 2^4 factorial design

An example of 2^4 factorial design, a team of engineers at a semiconductor manufacturer run in a vertical oxidation furnace (Montgomery, 2019). Four wafers are "stacked" in the furnace, and the response variable of interest is the oxide thickness on the wafers. The four design factors are temperature (A), time (B), pressure (C), and gas flow (D). The experiment is conducted by loading four wafers into the furnace, setting the process variables to the test conditions required by the experimental design, processing the wafers, and then measuring the oxide thickness on all four wafers. The full factorial design was formed by the factors A to D. The effects of these four factors on the oxidation furnace were accessed using the experimental matrix of 2^4 full factorial experiments with four replications.

4.1. Frequentist approach to the 2^4 full, fractional, and reduced factorial designs

The ANOVA for 2^4 full factorial designs was carried out using the R program and presented in Table 3, all the main effects (A, B, C, and D) and the interaction effects (AB, AC, BC, BD, and ABD) are significant, other interaction effects are not significant. Now, we decided to devise a new factorial design consisting of the significant effects alone or we may say a reduced factorial design. To identify the effect of non-significant effects by comparing the full and reduced factorial designs. Furthermore, in 2^4 full factorial designs, the main factors A, B, and C are highly significant but the factor D is not as significant as compared with other main effects and the three or more higher-order interaction effects are not significant except the interaction ABD. In the fractional factorial design, all the effects are highly significant. Particularly, the main effect D is observed to be less significant in the full and fractional factorial design as compared to the reduced factorial design (Tables 3-5). In the 2^4 reduced factorial designs, all the main and interaction effects are significant which is shown in Table 5. Thus, the main effect D is highly significant in the reduced factorial design than the full factorial design.

Table 3: ANOVA output for 2^4 full factorial design

Source of Variations	Sum of Squares	d.f	Mean Sum of Square	F Value	Pr(>F)	
Blocks	22	3	7	1.243	0.3053	
A	29756	1	29756	4931.975	2e-16	***
B	5256	1	5256	871.202	2e-16	***
C	1722	1	1722	285.456	2e-16	***
D	42	1	42	7.003	0.0112	*
AB	4556	1	4556	755.180	2e-16	***
AC	1806	1	1806	299.378	2e-16	***
AD	20	1	20	3.356	0.0736	.
BC	240	1	240	39.820	1.08e-07	***
BD	240	1	20	39.820	1.08e-07	***
CD	20	1	20	3.356	0.0736	.
ABC	2	1	2	0.373	0.5445	
ABD	132	1	132	21.920	2.63e-05	***
ACD	0	1	0	0.041	0.8396	
BCD	6	1	6	1.036	0.3142	
ABCD	0	1	0	0.041	0.8396	
Residuals	272	45	6			

Significant codes 0.001 '***' 0.01 '**' 0.05 '*' 0.1 '.' 1 ' '

Table 4: ANOVA output for 2^{4-1}fractional factorial design

Source of Variations	Sum of Squares	d.f	Mean Sum of Square	F Value	Pr(>F)	
Blocks	3	3	1	0.304	0.82192	
A	14450	1	14450	4059.532	<2e-16	***
B	2592	1	2592	728.187	<2e-16	***
C	450	1	450	126.421	2.40e-10	***
D	32	1	32	8.990	0.00685	**
AB	2592	1	2592	728.187	<2e-16	***
AC	1682	1	1682	472.535	7.04e-16	***
BD	200	1	200	56.187	2.30e-07	***
Residuals	4	21	4			

Significant codes 0.001 '***' 0.01 '**' 0.05 '*' 0.1 '.' 1 ' '

Table 5: ANOVA output for 2^4 reduced factorial design

Source of Variations	Sum of Squares	d.f	Mean Sum of Square	F Value	Pr(>F)	
Blocks	7	3	2	0.59	0.628	
A	932	1	932	22.19	8.88e-14	***
B	1198	1	1198	294.62	5.57e-15	***
C	345	1	345	84.80	2.40e-09	***
D	6933	1	6933	1705.73	<2e-16	***
AB	3691	1	3691	907.92	<2e-16	***
AC	4760	1	4760	1171.05	<2e-16	***
BD	243	1	243	59.78	5.74e-08	***
ABD	11449	1	11449	2816.61	2e-16	***
Residuals	98	24	4			

Significant codes 0.001 '***' 0.01 '**' 0.05 '*' 0.1 '.' 1 ' '

4.2. Bayesian approach to the 2^4 full, fractional, and reduced factorial designs

All five priors of the Bayes factor decisively support the full, fractional, and reduced factorial designs are shown in Table 6. Nevertheless, both the Zellner's g priors support the full factorial design around 35 times. It is also observed that the other priors support the full factorial design around 45 times. The fractional factorial design provides half of the full factorial design results, which may be due to the loss of half of the effects from the original problem. In comparison to the fractional factorial design, our proposed reduced factorial model, which only considers significant effects, gives a better alternative. The reduced factorial design result may provide different results for our example due to inconsistency in the data. The simulated data set will resolve this issue.

5. Simulation of 2^4 full, fractional, and reduced factorial designs

This section also simulated 10,000 data with the error variance is 1 to compute 10,000 Bayes factor values for each of the five prior and also computed Bayes factors for various datasets with the error variances of 5, 25, and 50, respectively. The five prior's Bayes factors for these simulated data to both full and half-fraction factorial designs were shown in Figs. 1-4. The mean and standard deviation of Bayes factor values for 2^4 full and fractional factorial designs were presented in Table 7. All the five priors produce more or less similar results in a full factorial design and the same as in fractional factorial design too. All the Bayes factor values in the full model are almost two times as compared with the fractional factorial model. Thus, we lose half of the information in a fractional factorial design. In the simulation dataset with less error variance, the data support full and fractional design, but if the error variance is high the simulation data support the null model. This trend may cause less variability in the original data.

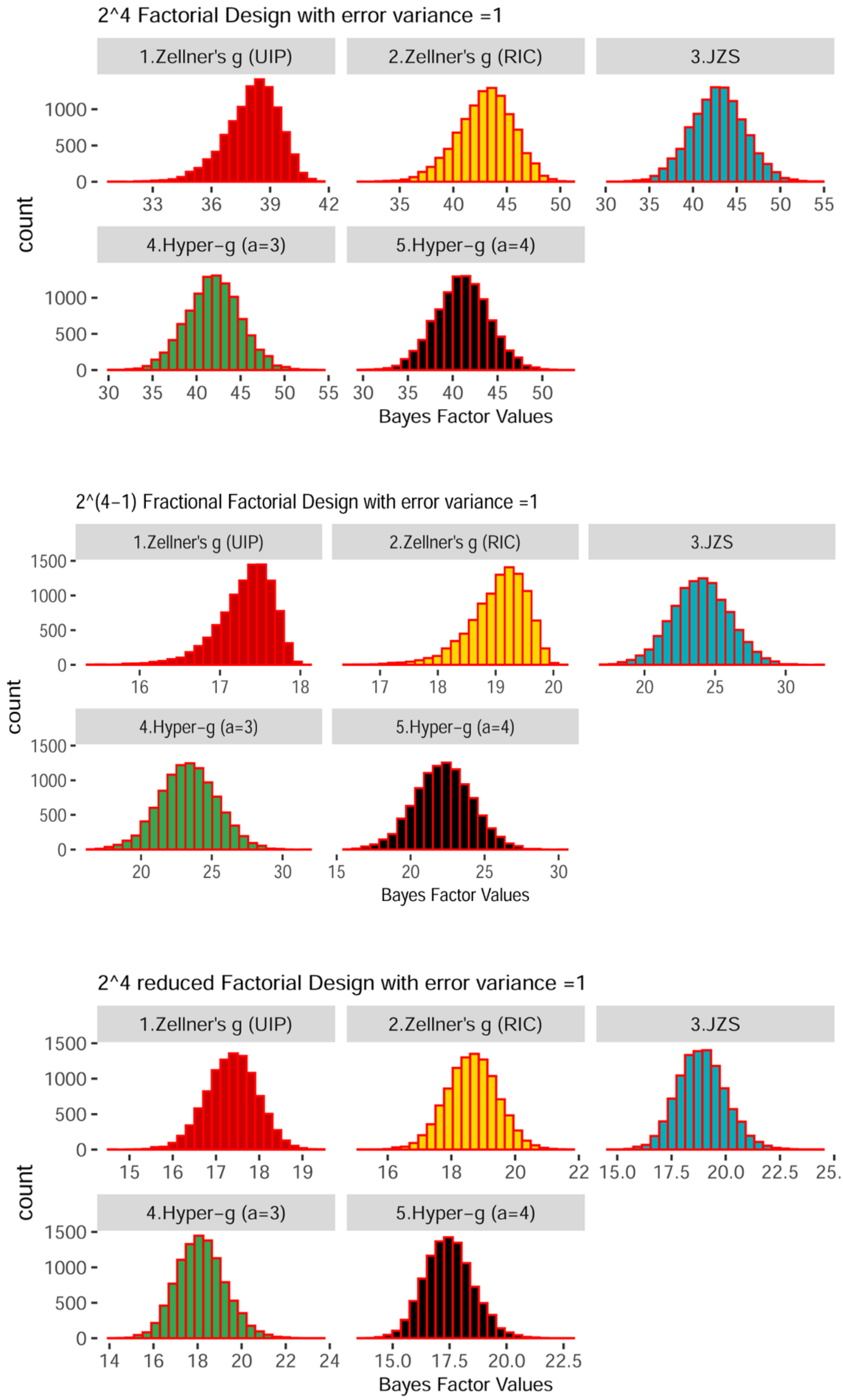

Fig. 1: Bayes factors for 2^4 full, fractional, and reduced factorial designs to the simulation datasets (σ_e^2=1)

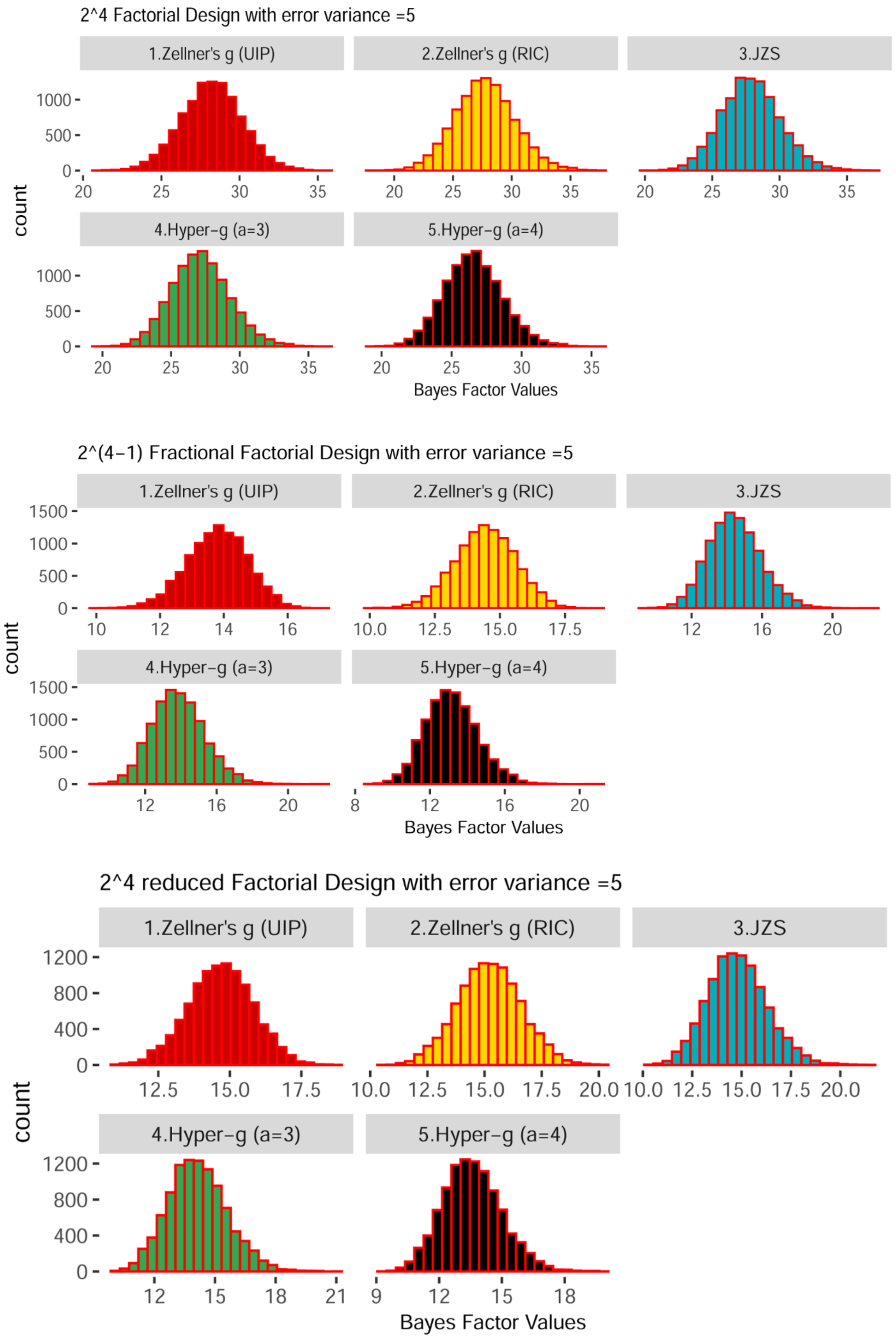

Fig. 2: Bayes factors for 2^4 full, fractional, and reduced factorial designs to the simulation datasets (σ_e^2=5)

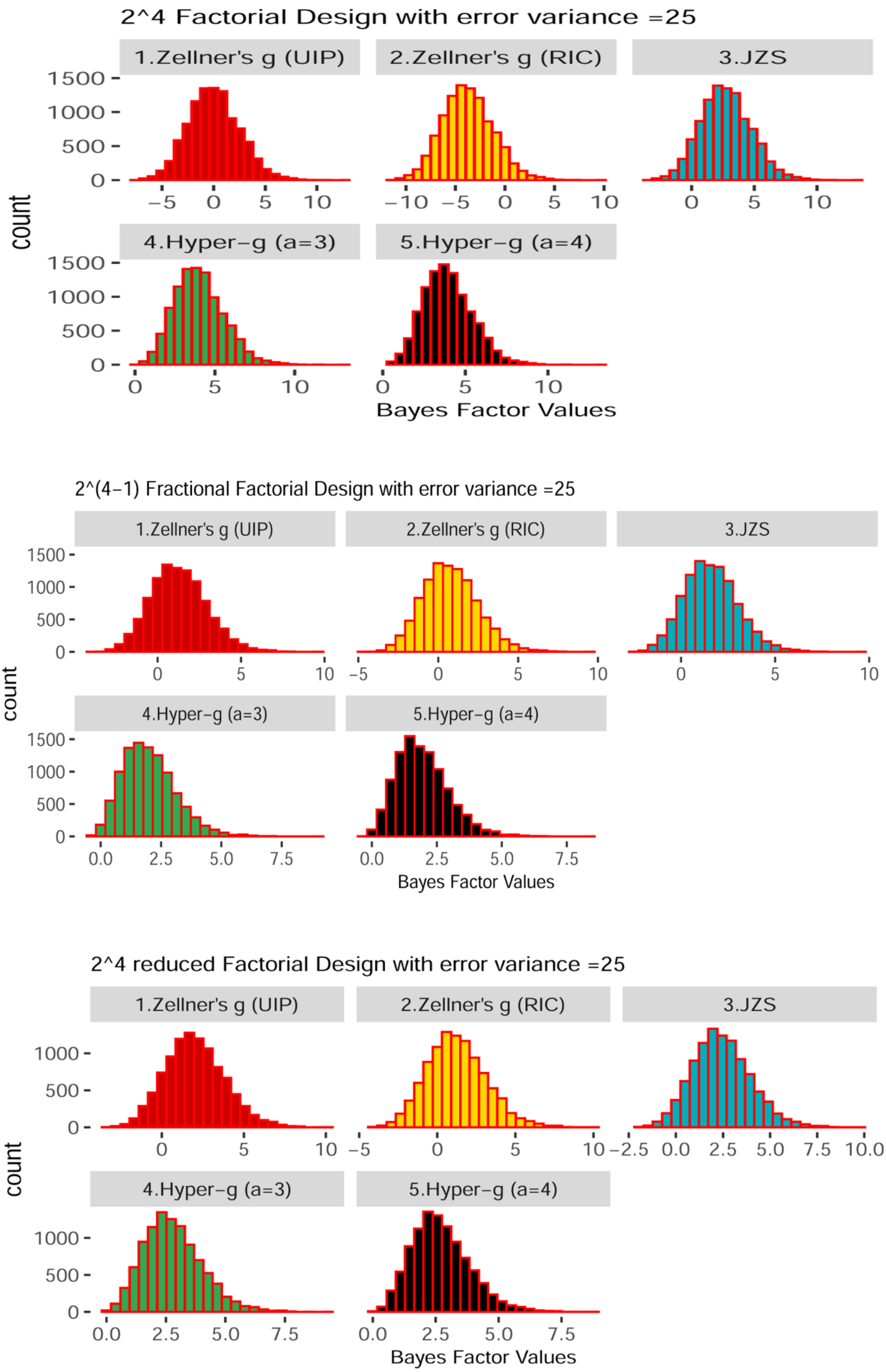

Fig. 3: Bayes factors for 2^4 full, fractional, and reduced factorial designs to the simulation datasets (σ_e^2=25)

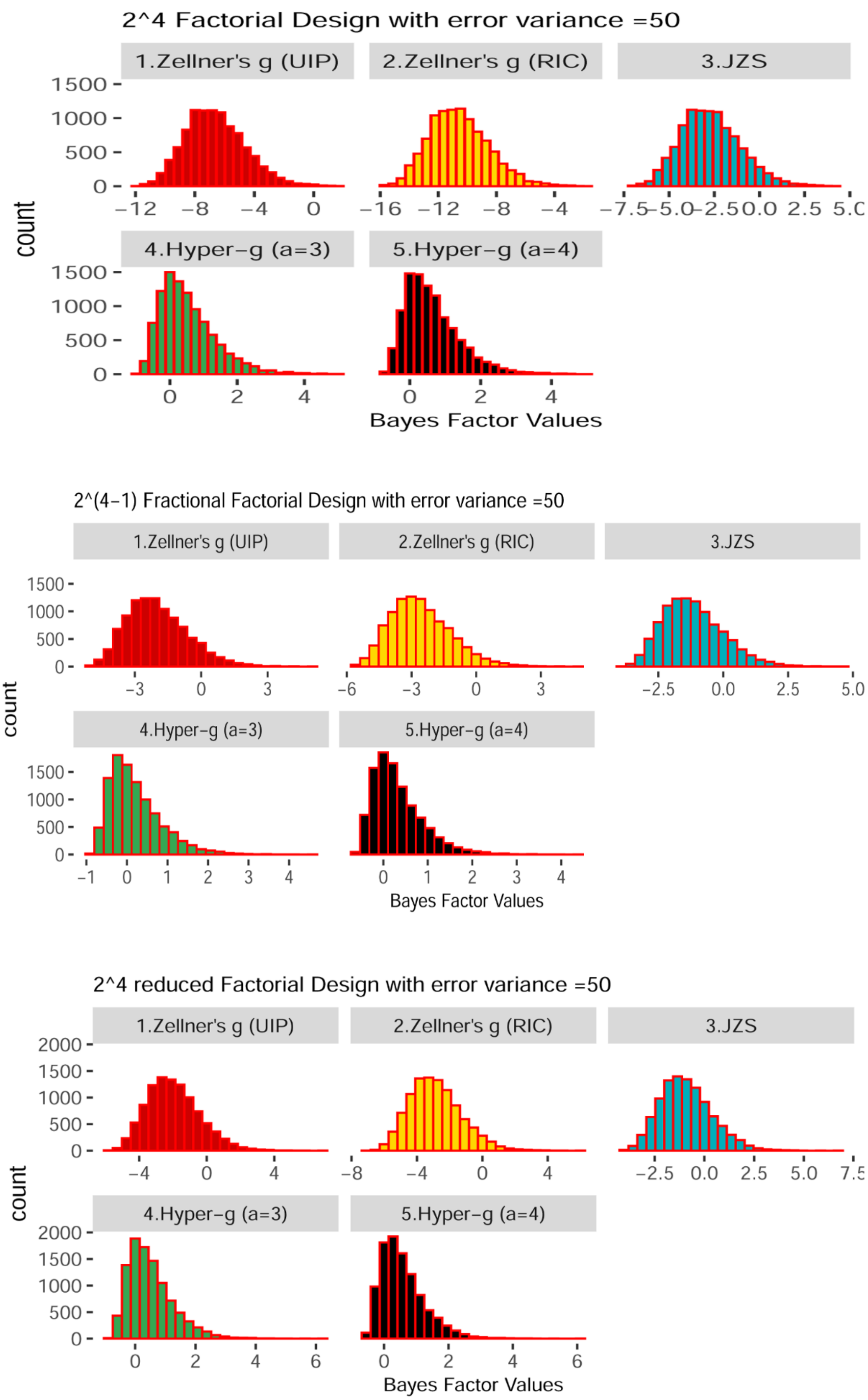

Fig. 4: Bayes factors for 2^4 full, fractional, and reduced factorial designs to the simulation datasets (σ_e^2=50)

Table 6: Bayes factor for 2^4 full, reduced, and fractional factorial designs

Prior	2^4 Full Factorial Design	2^{4-1}Fractional Factorial Design	2^4 reduced Factorial Design
Zellner's g prior (UIP)	34.5580	17.5011	20.2610
Zellner's g prior (RIC)	35.4780	19.3128	22.9253
Jeffreys-Zellner-Siow	45.2391	24.8760	28.0650
Hyper –g prior (a=3)	44.4630	24.2300	27.3944
Hyper –g prior (a=4)	43.4245	23.0776	26.2407

Table 7: Average (SD) of 10000 Bayes factor values to the simulation of (a) 2^4 full factorial, (b) 2^{4-1} fractional factorial and (c) 2^4 reduced factorial designs for five priors when the error variances are 1, 5, 25 and 50

Error Variance (σ_e^2)	Zellner's g-prior (UIP)	Zellner's g-prior (RIC)	Jeffreys-Zellner-Siow	Hyper-g prior (a=3)	Hyper-g prior (a=4)
a). 2^4 full factorial design					
1	38.9888 (1.3818)	43.8288 (2.4902)	44.1892 (3.2031)	43.4177 (3.1927)	42.4013 (3.1255)
5	29.0771 (1.9418)	29.0037 (2.4981)	28.8342 (2.2235)	28.1732 (2.1930)	27.4817 (2.1452)
25	0.9358 (2.4664)	-2.1816 (2.5408)	3.2750 (2.0428)	4.3887 (1.6163)	4.3145 (1.5525)
50	-5.6703 (2.0146)	-8.9420 (2.0518)	-2.2033 (1.6764)	0.6918 (0.9151)	0.8150 (0.8512)
b). 2^{4-1} fractional factorial design					
1	17.3011 (0.3518)	19.0300 (0.4993)	23.9242 (2.0058)	23.2808 (2.0013)	22.1700 (1.9138)
5	13.8103 (0.9421)	14.4622 (1.1496)	14.4712 (1.5001)	13.8886 (1.4792)	13.1936 (1.4123)
25	1.2146 (1.6433)	0.7073 (1.6939)	1.5412 (1.4016)	1.9730 (1.0750)	1.9233 (0.9885)
50	-1.9786 (1.3742)	-2.5615 (1.4007)	-1.1624 (1.1610)	0.2092 (0.6508)	0.3321 (0.5793)
c). 2^4 reduced factorial design					
1	20.0467 (0.3462)	22.5857 (0.5519)	27.0577 (1.8971)	26.3896 (1.8932)	25.2748 (1.8199)
5	16.2577 (0.9866)	17.1918 (1.2810)	17.0600 (1.5810)	16.4499 (1.5619)	15.7237 (1.4998)
25	1.8366 (1.7811)	1.0411 (1.8488)	2.2762 (1.5094)	2.6725 (1.2004)	2.5894 (1.1193)
50	-2.1745 (1.5071)	-3.0848 (1.5409)	-1.0972 (1.2651)	0.3798 (0.7234)	0.4920 (0.6508)

6. Discussion and conclusion

In the study, we explored how to use Bayes factors to determine the intensity of factors in the factorial designs. The Bayesian framework has been widely applied to factorial designs, but we will use it to determine the intensity of the component in the model. We illustrate the full, fractional factorial designs by in the Bayesian principle, furthermore, we construct the reduced factorial design consisting of only significant factors. Through Bayes factors, we can see how much the reduced factorial design will yield the best result if it has fewer factors than full and/or fractional factorial designs.

In general, when a factorial design is planned, it is normal to start with a full factorial design. However, if the number of factors is too large then the size of the design shall be enormous. Therefore, we may use an alternative to the full factorial design i.e., a fractional factorial design that can help to reduce the number of runs for screening designs. In a fractional factorial design, we may lose some significant factors. We propose a reduced factorial design that includes all the significant factors as an alternative to the fractional factorial design. We have considered an example 2^4 of factorial designs and applied the frequentist and Bayesian concepts to find the effects of the factors in the full, fractional and reduced factorial designs.

In the classical approach, we find the significance of factors from the ANOVA output, and based on the results and aliased factors we form a fractional factorial design. The Bayes Factor for five priors, such as Zellner's g (UIP), Zellner's g (RIC), Jeffreys-Zellner-Siow, Hyper-g (a=3), and Hyper-g (a=4) priors, are computed for 2^4 full, fractional, and reduced factorial designs. It provided different results within the respective models. To generalize the Bayesian approach, we generated a large set of data by simulation with different error variances and it gives a wide range of ideas to compare the full, fractional, and reduced factorial design with the existence of the factors. All the Bayes factor values in the full model are almost two times as compared to the fractional factorial model. Nevertheless, in a reduced factorial design, Bayes factor values are better than the fractional factorial designs, since we lose half of the information in a fractional factorial design. In the simulation dataset with less error variance, the data support full, fractional, and reduced design, but if the error variance is high, the simulation data support the null model in these three models. This tendency may be due to the less variability in the original data and more precisely mean squared error is minimum in all three models. If researchers consider including all essential factors in the model, they might prefer a reduced factorial model, since it produces much better results when there are no constraints as to selecting or adding factors to the model.

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Compliance with ethical standards

Conflict of interest

The author(s) declared no potential conflicts of interest with respect to the research, authorship, and/or publication of this article.

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