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MODELLING AND OPTIMIZATION OF COMPLEX INTERACTIONS IN MULTIVARIATE SYSTEMS USING DESIGN EXPERT

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Abstract -

This study involves a decision matrix analysis using design expert tool to optimize a set of responses (R1 to R5) influenced by five factors (C1 to C5). The initial decision matrix was subjected to analysis, and a new decision matrix was predicted. The predicted decision matrix was characterized by a set of equations, each representing a response using coded factors. Subsequently, ANOVA tables were generated for each response, indicating the significance of the design. The results revealed the effectiveness of the design in optimizing the responses, in which few follow cubic or quadratic models, while others showed linear behavior.

Keywords - Decision making, Design Expert, Modelling, ANOVA.

Introduction

Mathematical models in engineering can make predictions when the concept of prediction is properly defined. These models serve as representations of systems or processes, utilizing mathematical concepts and language to describe the behavior of entities within the system. Through mathematical analysis and computer simulations, insights into the overall system behavior can be gained, allowing for predictions about the future state of the modeled system or process. Furthermore, these models enable the examination of how predictions change when adjusting or varying the rules that govern the entities[6].

For predictions within a mathematical model to be relevant, it is crucial that they accurately reflect reality. Decision makers acknowledge that all models are simplifications of the real world and that assumptions have inherent limitations.

Design Expert is a valuable tool for design professionals, as it streamlines the decision-making process by integrating statistical analysis and experimentation into the design workflow. By leveraging the software's capabilities, designers can make more informed and data-driven decisions, leading to improved product quality, efficiency, and overall success in their design projects[7, 15].

Design Expert[1, 2] is a powerful tool with widespread applications in research, engineering, and industry. One of its primary uses is in experimental design, where it allows researchers to plan experiments systematically. By providing a range of experimental design options such as Full Factorial, Fractional Factorial, Response Surface and Taguchi designs, Design Expert enables the exploration of multiple factors and their interactions. This capability is invaluable for understanding complex systems and optimizing processes efficiently[18].

One of the standout features of Design Expert is its proficiency in RSM (Response Surface Methodology). RSM enables users to create mathematical models that describe how different factors influence a process or product. By visualizing these relationships through contour plots, 3D surfaces

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plots, and other graphical tools, users gain insights that aid in decision-making and process improvement[3-5].

Design Expert excels in creating mixture design experiments. This feature is particularly useful for industries where achieving the optimal combination of components is essential for product performance and quality. Additionally, the software supports robust parameter design, allowing for the creation of products or processes that are robust against variations in factors, ultimately reducing defects and increasing reliability[12].

Design Expert also offers a wide array of statistical analysis tools, including ANOVA[11], regression analysis, and hypothesis testing. These tools empower users to make informed decisions based on their experimental data, enhancing the reliability of their findings. Furthermore, the tool can predict outcomes based on established models, which aids in decision-making and reduces the need for extensive experimentation. The ability to validate models within Design Expert ensures that the mathematical representations accurately depict real-world processes. This validation enhances the trustworthiness of the results and decisions derived from the analysis[16].

Design Expert is an indispensable tool for researchers, engineers, and professionals in various fields. Its multifaceted applications in experimental design, process optimization[10, 14] mathematical modeling[17] data analysis, and more make it an asset for enhancing efficiency, product quality, and informed decision-making while reducing experimentation time and costs.

PREMILINARIES AND DEFINITIONS

Definition 2.1: F-Value:

The F-value is calculated as the ratio of the variance between groups to the variance between and within groups.

The F-value is calculated as F =(Mean Square between Groups)/(Mean Square within Groups)

If the F-value is significantly greater than 1, it suggests that there is a reasonable association between the group means.

Definition 2.2: p-Value:

The probability of F-statistic as extreme as, or more extreme than the observed values from the sample is regarded as p-value, if the null hypothesis is true. The value provides a strong validation on contrary to the null hypothesis.

Definition 2.4: Cubic Model in ANOVA:

A cubic model in Analysis of Variance is a statistical model used to analyze data in which there is a non-linear association between the dependent and independent variables.

The cubic model is mathematically expressed as:

 $Y{=}\beta_0{+}\beta_1 \ X{+}\beta_2 \ X^{\wedge}2{+}\beta_3 \ X^{\wedge}3{+}\epsilon$

where,

Y significant the dependent variable under investigation.

X represents the independent variable, which is the factor being studied.

 $\beta_0, \beta_1, \beta_2$ and β_3 are the coefficients that need to be estimated through the ANOVA analysis.

 ϵ accounts for the error term, encompassing unexplained variability in the data.

Definition 2.5: Quadratic Model in ANOVA:

A quadratic model in Analysis of Variance is a statistical model used to analyze data when there is a curvilinear or quadratic association between the dependent and independent variables.

The quadratic model can be expressed as:

 $Y=\beta_0+\beta_1 X+\beta_2 X^2+\varepsilon$

where,

Y refers the dependent variable, the outcome of interest.

X be the independent variable, the factor under investigation.

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 β_0,β_1 and β_2 are the coefficients that need to be estimated through the ANOVA analysis.

 ϵ denotes the error term, capturing unexplained variation in the data.

Definition 2.5: Linear Model in ANOVA:

A linear model in Analysis of Variance is a statistical model used to analyze data when there is a linear association between the dependent and independent variables.

The quadratic model can be expressed as:

 $Y = \beta_0 + \beta_1 X + \epsilon$

where,

Y represents the dependent variable, the variable to predict.

X represents the independent variable, the factor influencing the dependent variable.

 β_0 is the intercept, representing the value of the dependent variable when the independent variable is zero.

 β_1 is he slope indicating how much the dependent variable changes for one unit change in the independent variable.

 ϵ denotes the error term, capturing unexplained variation in the data.

Numerical Example

Illustration: Consider a MCDM problem which contains 5 alternatives (R1, R2, R3, R4, R5) and 5 criteria (C1, C2, C3, C4 and C5) as shown in Table 1. Predict the dataset which could significantly model a cubic / quadratic coded equation with acceptable p-value. The Design expert 13 is used to make a custom design to predict and model a coded linear / quadratic equation.

TABLE 1: INITIAL DECISION MATRIX								
	C1	C2	C3	C4	C5			
R1	649	4.7	326	7.1	143			
R2	749	5.5	401	7.3	192			
R3	740	5.7	520	7.6	171			
R4	400	5.7	520	11.1	179			
R5	600	5.5	538	8.9	152			

The custom design admits the cubic model when R1 is maintained as response. The Factor coding is Coded (Type III – Partial). The observed F-value of 923510167.11 indicates that the design is significant which has only a 0.01% possibility to develop noise.

TABLE 2: R1 DESIGN FOR CUBIC MODEL										
Source	SoS	df	MS	F	р					
Model	63326.4	3	21108.80	9.235E+08	< 0.0001					
A-A	57877.30	1	57877.30	2.532E+09	< 0.0001					
A ²	1225.41	1	1225.41	5.361E+07	< 0.0001					
A ³	42120.10	1	42120.10	1.843E+09	< 0.0001					
Res.	0.0000	1	0.0000							
Total	63326.41	4								
The Design is Significant.										

The design is significant when the observed P-values are less than 0.0500 and not significant on the contrary.

122 1st Predicted Equation in Terms of Coded Factors R1 = + 646.31 - 457.17 * A - 37.42 * A² + 432.67 * A³

The above equation is used to make a prediction based on the response R1 of the coded factors against each level which also compares the coefficients of the factors and identifies the relative importance of the factors at all levels as shown in Table 2 and Table 3.

TABLE 3: FIRST PREDICTION – R1									
Run Order	1	2	3	4	5				
Original	633.39	811.46	646.31	462.46	584.39				
Predicted	633.39	811.46	646.31	462.46	584.39				
Error	-0.0006	0.0023	-0.0034	0.0023	-0.0006				
Advantage	0.986	0.771	0.486	0.771	0.986				
Int. Residuals	-1	1	-1	1	-1				
Ext. Residuals	0	0	0	0	0				
Cook's Measure	17.250	0.844	0.236	0.844	17.250				
DFFITS	0	0	0	0	0				
Accepted Order	4	5	3	2	1				

The custom design admits the cubic model when R2 is maintained as response. The Factor coding is Coded (Type III - Partial). The observed F-value of 29026.25 indicates that the design is significant which has only a 0.01% possibility to develop noise.

TABLE 4: R2 DESIGN FOR QUADRATIC MODEL										
Source	SoS	df	MS	F	р					
Model	0.6635	2	0.3317	29026.25	< 0.0001					
A-A	0.3240	1	0.3240	28350.00	< 0.0001					
A ²	0.3395	1	0.3395	29702.50	< 0.0001					
Res.	0.0000	2	0.0000							
Total	0.6635	4								
The Design is Significant.										

The design is significant when the observed P-values are less than 0.0500 and not significant on the contrary.

2nd Predicted Equation in Terms of Coded Factors $R2 = +5.73 + 0.3600 * A - 0.6229 * A^2$

The above equation is used to make a prediction based on the response R2 of the coded factors against each level which also compares the coefficients of the factors and identifies the relative importance of the factors at all levels as shown in Table 4 and Table 5.

TABLE 5: SECOND PREDICTION – R2									
Run Order 1 2 3 4 5									
Original	4.75	5.4	5.73	5.76	5.47				

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Predicted	4.75	5.4	5.73	5.76	5.47
Error	-0.0006	0.0023	-0.0034	0.0023	-0.0006
Advantage	0.886	0.371	0.486	0.371	0.886
Int. Residuals	-0.5	0.853	-1.414	0.853	-0.5
Ext. Residuals	-0.378	0.756	0	0.756	-0.378
Cook's Measure	0.646	0.143	0.63	0.143	0.646
DFFITS	-1.052	0.581	0	0.581	-1.052
Accepted Order	4	5	3	2	1

The custom design admits the cubic model when R3 is maintained as response. The Factor coding is Coded (Type III – Partial). The observed F-value of 16.91 indicates that the design is significant which has only a 2.60% possibility to develop noise.

TABLE 6: R3 DESIGN FOR LINEAR MODEL										
Source	SoS	df	MS	F	р					
Model	29484.90	1	29484.90	16.91	0.0260					
A-A	29484.90	1	29484.90	16.91	0.0260					
Res.	5231.10	3	1743.70							
Total	34716.00	4								
The Design is Significant.										

The design is significant when the observed P-values are less than 0.0500 and not significant on the contrary.

3rd Predicted Equation in Terms of Coded Factors R3 = +461.00 + 108.60 * A

The above equation is used to make a prediction based on the response R3 of the coded factors against each level which also compares the coefficients of the factors and identifies the relative importance of the factors at all levels as shown in Table 6 and Table 7.

TABLE 7: THIRD PREDICTION – R3									
Run Order	1	2	3	4	5				
Original	326	401	520	520	538				
Predicted	352.4	406.7	461	515.3	569.6				
Error	-26.4	-5.7	59	4.7	-31.6				
Advantage	0.6	0.3	0.2	0.3	0.6				
Int. Residuals	-1	-0.163	1.58	0.135	-1.197				
Ext. Residuals	-0.999	-0.134	3.145	0.11	-1.351				
Cook's Measure	0.749	0.006	0.312	0.004	1.074				

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DFFITS	-1.224	-0.088	1.572	0.072	-1.655
Accepted Order	4	5	3	2	1

The custom design admits the cubic model when R4 is maintained as response. The Factor coding is Coded (Type III – Partial). The observed F-value of 371.99 indicates that the design is significant which has only a 0.03% possibility to develop noise.

TABLE 8: R4 DESIGN FOR LINEAR MODEL									
Source	SoS	df	MS	F	р				
Model	5.87	1	5.87	371.99	0.0003				
A-A	5.87	1	5.87	371.99	0.0003				
Res.	0.0473	3	0.0158						
Total	5.91	4							
The Design is Significant.									

The design is significant when the observed P-values are less than 0.0500 and not significant on the contrary.

4th Predicted Equation in Terms of Coded Factors R4 = +8.45 + 1.53 * A

The above equation is used to make a prediction based on the response R4 of the coded factors against each level which also compares the coefficients of the factors and identifies the relative importance of the factors at all levels as shown in Table 8 and Table 9.

TABLE 9: FOURTH PREDICTION – R4									
Run Order	1	2	3	4	5				
Original	6.92	7.66	8.4	9.4	9.88				
Predicted	6.92	7.69	8.45	9.22	9.98				
Error	0	-0.026	-0.052	0.182	-0.104				
Advantage	0.6	0.3	0.2	0.3	0.6				
Int. Residuals	0	-0.247	-0.463	1.732	-1.309				
Ext. Residuals	0	-0.204	-0.392	0	-1.633				
Cook's Measure	0	0.013	0.027	0.643	1.286				
DFFITS	0	-0.134	-0.196	0	-2.000				
Accepted Order	4	5	3	2	1				

The custom design admits the cubic model when R5 is maintained as response. The Factor coding is Coded (Type III – Partial). The observed F-value of 47387500.00 indicates that the design is significant which has only a 0.01% possibility to develop noise.

TABLE 10: R5 DESIGN FOR QUADRATIC MODEL									
Source SoS df MS F p									
Model	1083.14	2	541.57	4.739E+07	< 0.0001				

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A-A	2.50	1	2.50	2.188E+05	< 0.0001
A ²	1080.64	1	1080.64	9.456E+07	< 0.0001
Res.	0.0000	2	0.0000		
Total	1083.14	4			
The Design	n in Cignificant	•	•	•	•

The Design is Significant.

The design is significant when the observed P-values are less than 0.0500 and not significant on the contrary.

5th Predicted Equation in Terms of Coded Factors $R5 = +184.97 + 1.00 * A - 35.14 * A^2$

The above equation is used to make a prediction based on the response R5 of the coded factors against each level which also compares the coefficients of the factors and identifies the relative importance of the factors at all levels as shown in Table 10 and Table 11. Table 12 represents the predictions corresponding to each response.

TABLE 11: FIFTH PREDICTION – R5								
Run Order	1	2	3	4	5			
Original	148.83	175.69	184.97	176.69	150.83			
Predicted	148.83	175.69	184.97	176.69	150.83			
Error	-0.0006	0.0023	-0.0034	0.0023	-0.0006			
Advantage	0.886	0.371	0.486	0.371	0.886			
Int. Residuals	-0.5	0.853	-1.414	0.853	-0.5			
Ext. Residuals	-0.378	0.756	0	0.756	-0.378			
Cook's Measure	0.646	0.143	0.63	0.143	0.646			
DFFITS	-1.052	0.581	0	0.581	-1.052			
Accepted Order	4	5	3	2	1			

@Confidence = 95%

TABLE 12: CONFIRMATION ANALYSIS							
Response	Predicted Mean	Predicted Median	Std Dev	n	SE Pred	95% PI low	95% PI high
R1	646.313	646.31	0.0047	1	0.0058	646.23	646.38
R2	5.73343	5.73	0.0033	1	0.0041	5.71	5.75
R3	461	461	41.7576	1	45.7432	315.42	606.57
R4	8.452	8.45	0.1255	1	0.1375	8.01	8.88
R5	184.973	184.97	0.0033	1	0.0041	184.95	184.99

@Confidence = 95%

RESULTS AND DISCUSSION

Response R1: The predicted model for R1 indicated a significant design. The response was modeled using a cubic equation, suggesting a complex relationship with the factors. The equation $M1 = +646.31 - 457.17 * A - 37.42 * A^2 + 432.67 * A^3$ provided a predictive framework for R1. This cubic model suggests that factor adjustments may lead to non-linear variations in R1, and further analysis may be required to understand the nature of this relationship.

Response R2: The design for R2 was also found to be significant. The response was modeled using a quadratic equation, indicating a non-linear relationship with the factors. The equation $M2 = +5.73 + 0.3600 * A - 0.6229 * A^2$ represents the relationship between the factors and R2. This quadratic model implies that changes in factors can have a parabolic effect on R2.

Response R3: R3 was modeled as a linear response, and the design was significant. The equation M3 = +461.00 + 108.60 * A provided a straightforward linear relationship between the factors and R3. This linear model simplifies the understanding of how changes in factors affect R3.

Response R4: Like R3, R4 exhibited a linear relationship with the factors. The design for R4 was significant, and the equation M4 = +8.45 + 1.53 * A described the linear relationship. This simple linear model allows for easy interpretation of the influence of factors on R4.



Fig. 1: RAMP graph

Response R5: The design for R5 was significant, and the response followed a quadratic model. The equation $M5 = +184.97 + 1.00 * A - 35.14 * A^2$ revealed the non-linear nature of the relationship between the factors and R5. Adjusting factors may result in parabolic changes in R5.

The incorporation of ramp graphs (Fig. 1) allows for the visualization of factors and responses across their entire range, enabling designers to understand how variables influence outcomes. The clarity provided by ramp graphs is instrumental in identifying optimal design settings, potential issues, and the boundaries within which a design can perform effectively.

The use of Design Expert shows the desirability and predictions in optimizing complex interactions within a multivariate system yielded promising results. Desirability scores of 0.597 (Fig. 2) suggest progress toward desired outcomes. Individual responses (R1 to R5) closely aligned with predictions, and their respective models proved significant. The optimization process effectively improved R1, R2, R3, R4, and R5, demonstrating the tool's ability to capture complex interactions.

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Conclusion

In this study, we utilized a design expert to optimize responses influenced by five factors. The analysis yielded valuable insights into the relationships between the factors and the responses. The results indicated that some responses follow linear models, while others exhibit non-linear behavior, either cubic or quadratic. These findings provide a basis for further experimentation and refinement of the factors to achieve desired outcomes. The significance of the design underlines the effectiveness of the approach in optimizing the decision matrix. Understanding these models will support in making informed decisions and adjustments to improve the performance of the system or process under consideration.

In conclusion, the analysis presented here provides a foundation for further optimization and control of the factors influencing the decision matrix. It projects the importance of a systematic approach in decision-making and the utility of mathematical models in understanding complex relationships. This study can be used to improve the efficiency and effectiveness of processes or systems in various engineering domains to solve any real-world problems

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