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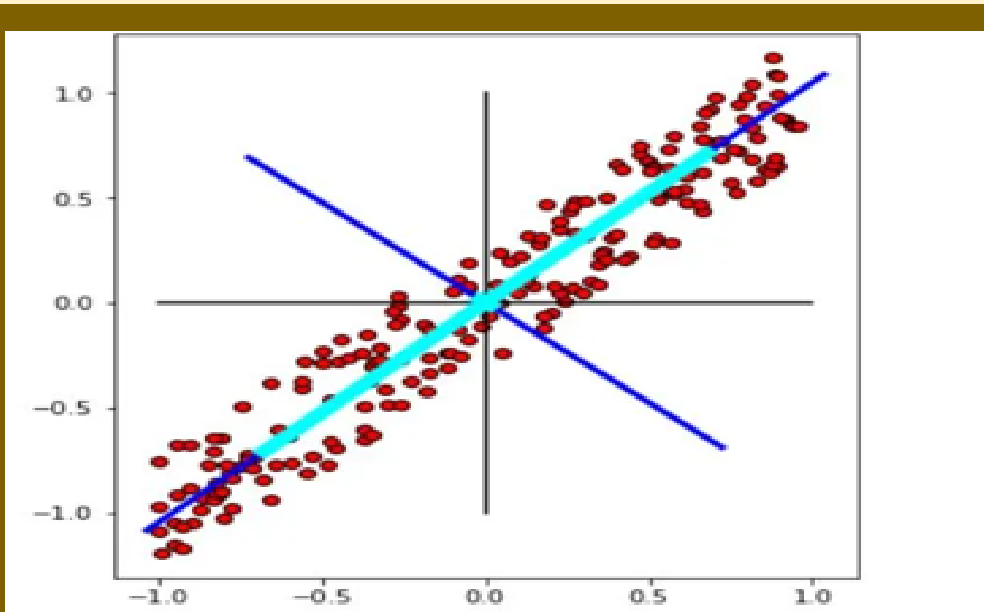

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ABSTRACT

The optimization of parameters to achieve desired performance outcomes presents significant challenges due to high dimensionality, collinearity among variables, and data noise. Traditional optimization methods, such as Response Surface Methodology (RSM), often face limitations when tackling these complexities. Additionally, the lack of efficient techniques for identifying and prioritizing influential parameters further exacerbates the difficulties in the optimization process. To address these intertwined issues, we propose an enhanced optimization methodology that integrates Principal Component Analysis (PCA) with Multi- Response Surface Methodology (MRSM). This integration aims to reduce dimensionality and highlight the most significant parameters, facilitating a more effective optimization process. We evaluated the effectiveness of the PCA-MRSM approach using a simulated dataset. Our findings indicate that the PCA-MRSM technique significantly outperforms traditional MRSM, leading to improved optimization outcomes and reduced variability. The analysis of response surface plots reveals a curved relationship between the principal components and the response variable, suggesting intricate interactions among the components. The results highlight the potential of the PCA-MRSM approach for optimizing complex systems characterized by multiple responses and correlated input variables. By effectively addressing the challenges of high dimensionality and collinearity, this methodology paves the way for more robust and insightful optimization techniques in intricate contexts.

Keywords: – MRSM, PCA, DOE, Complex system, Optimization, Parameter Design

1. INTRODUCTION:

Background to the study

Multi objective optimization helps to achieve simultaneous improvement of more than one output characteristic in machining processes where complex interaction between the input parameter exists. In today's evolving human society, economy, and culture, the industry plays a crucial role in shaping future lifestyle, cultural trends, energy consumption patterns, and environmental dynamics. Notably, conceptual design emerges as a pivotal stage in product development that reflects human ingenuity and determines the quality of the final concept.

As core product technologies approach maturity, the visual aesthetic of the product becomes increasingly vital for gaining competitiveness and swiftly capturing market share. Over time, significant research efforts have focused on developing methods for automated and intelligent product modeling design processes [1]. Users and designers have a shared objective of achieving optimal product functionality, which entails employing various technical methods to create products that efficiently meet user needs. Calibrating component parameters is vital for ensuring the quality of assembled products, as any deviations from target values can lead to a decline in quality. Furthermore, tighter tolerances in part design increase costs and the likelihood of losses. Therefore, identifying the optimal parameters for components is crucial for maintaining product quality and reducing overall expenses. Throughout the design process, it is essential to consider how controllable factors influence product quality while also striving to make the product resilient to variations from external influences.

Response surface methodology (RSM)

Response surface methodology (RSM) is a well known up to date approach for constructing approximation models based on either physical experiments, computer experiments (simulation) and it was invented by Box and Wilson, is a collection of mathematical and statistical techniques for empirical model building. By careful design of experiments, the objective is to optimize a response (output variable) which is influenced by several independent variables (input variables). An experiment is a series of tests, called runs, in which changes are prepared in the input variables in order to recognize the reasons for changes in the output response [2]. RSM involves two basic concepts:

(1)The choice of the approximate model, and

(2)The plan of experiments where the response has to be evaluated.

The performance of a manufactured product often characterize by a group of responses. These responses in general are correlated and measured via a different measurement scale. Consequently, a decision-maker must resolve the parameter selection problem to optimize each response. This problem is regarded as a multi-response optimization problem, subject to different response requirements. Most of the common methods are incomplete in such a way that a response variable is selected as the primary one and is optimized by adhering to the other constraints set by the criteria. Many heuristic methodologies have been developed to resolve the multi-response problem.

[3] A regression technique was used; however, this method increases the complexity of the computational process and may not account for possible correlations among the responses. Additionally, a factor that proves significant in a single-response scenario may not hold the same significance in a multi-response context. Therefore, a more effective approach is needed to address this complex issue. Response Surface Methodology (RSM) is primarily applied in situations where multiple input variables potentially impact a performance measure or quality characteristic of a process, referred to as the response. The input variables, often termed independent variables, are controlled by the scientist or engineer. The goal is to model and analyze scenarios in which the response of interest is influenced by several variables, with the aim of optimizing that response.

For two independent variables, the first order model is given as

$$n = \beta_o + \beta_1 x_1 + \beta_2 x_2 \qquad (1)$$

This is called a main effect model, because it represents the main effect of two variables X_1 and X_2

If there is an interaction, we have

$$n = \beta_o + \beta_1 x_1 + \beta_2 x_2 + \beta_{12} x_1 x_2 \qquad (2)$$

A second-order mode will likely be required in this situation for the case of two variables as

$$n = \beta_o + \beta_1 x_1 + \beta_2 x_2 + \beta_{11} x_1^2 + \beta_{22} x_2^2 + \beta_{12} x_1 x_2 \qquad (3)$$

The general first - order model

$$n = \beta_o + \beta_1 x_1 + \beta_2 x_2 + \dots\dots + \beta_k x_k \qquad (4)$$

The general quadratic response surface methodology (RSM) model

The model encompasses linear, quadratic and interaction term for a system with k factors.

$$Y = \beta_o + \sum_{i=1}^{k} \beta_i x_i + \sum_{i=1}^{k} \beta_{ii} x^2{}_i \sum_{i<j} \sum \beta_{ij} x_i x_j + \varepsilon \qquad (5)$$

Where

Y is the response variable

β_o Is the intercept

β_i Represent the linear coefficient for factor

β_{ii} Represent the quadratic coefficient for factor x_i

β_{ij} Represent the interaction coefficient between factors x_i and x_j

Principal component Analysis (PCA).

Principal component analysis (PCA) is a very flexible tool and allows analysis of datasets that may contain, for example multicollinearity, missing values, categorical data, and imprecise measurements. The goal is to extract the important information from the data and to express this information as a set of summary indices called principal components. Statistically, PCA finds lines, plane and hyper- planes in the k-dimensional space that approximate the data as well as possible in the least squares sense, A line or plane that is the least squares approximation of a set of data points make the variance of the coordinates on the line or plane as large as possible.

PCA is a multivariate statistical technique capable of shrinking the dimensions of a data set consisting of innumerate correlated variables while ensuring most variations in the data set are captured [4]. Dimension reduction is achieved by converting the correlated variables from the original data sets into linearly uncorrelated variables, called principal components (PC). Traditionally, PCs' are determined by solving the inverse eigenvector of the covariance matrix. [5] It has been noted that traditional covariance-based PCA does not effectively represent data when dealing with variable combinations that have different units of measurement. To address this, a correlation method that involves normalizing the original data sets is employed. PCA serves as the foundation for multivariate data analysis utilizing projection methods. Its primary purpose is to condense a multivariate data table into a smaller set of variables

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(summary indices), enabling the identification of trends, significant changes, and outlier clusters. This approach can reveal relationships among observations and between variables. PCA was initially introduced in statistics by Pearson in 1901, who described it as the process of finding "lines and planes of closest fit to systems of points in space" (Jackson, 1991).

Optimizing a multi-response manufacturing process is a complex challenge. Many researchers have sought to address the specific difficulties in this field by leveraging various techniques, including design of experiments, response surface methodology (RSM), principal component analysis (PCA), and mathematical programming. The Taguchi method, developed in the 196s, has been widely adopted across industries to improve product quality. This method assesses product quality through the signal-to-noise (SN) ratio, allowing for the identification of the optimal combination of factors and levels to minimize quality variation and align the mean with the target value. However, despite its extensive use in industry, the Taguchi method is limited to single-response optimization. As product designs become more complex, the need to optimize multiple responses simultaneously is increasingly critical, especially in high-tech sectors, given that these responses are often moderately or highly correlated.

[6] The new implementation of PCA has been formalized. PCA, or Principal Component Analysis, is a widely recognized multivariate analytical technique used to identify the principal components among interrelated variables, simplifying complex data sets into lower-dimensional forms.

[7] A hybrid approach combining the Taguchi, Grey Relational Analysis (GRA), and Principal Component Analysis (PCA) methods was employed to evaluate and optimize multiple responses—specifically wears rate, frictional force, and specific wear rate—related to the wear behavior of matrix composites. The influence of three process variables (optimal normal load, sliding distance, and weight percentage of SiC) on response characteristics was analyzed to determine the best levels of these parameters. Grey Relational Analysis (GRA), which quantifies the dynamic evolution of complex systems, has proven to be an effective technique for uncovering the relationships between influential factors and multiple responses.

[8] The process parameters were optimized through the Taguchi method of experimental design, leading to reduced tool wear. Numerous researchers from various scientific fields, including mechanical manufacturing and different machining processes, utilize Principal Component Analysis (PCA). In recent years, PCA has become a widely adopted analytical tool for process optimization involving multiple performance characteristics.

[9] Explore current optimization techniques designed to identify optimal outcomes in complex systems. After recognizing suitable methods, researchers conduct experiments and analyses to determine which technique produces the best response. Optimization is recognized as a crucial process for selecting the most favorable option from various alternatives. However, many existing optimization methods fail to account for the correlations between multiple responses, which can lead to less than ideal outcomes. Moreover, the often complex mathematical nature of these techniques can make them challenging for engineers to apply in practice. The interdependencies among responses add further difficulty to the simultaneous optimization of multiple objectives, which can hinder the success of traditional optimization approaches. To improve their practical usability, it is vital to develop optimization techniques that consider response correlations while also reducing mathematical complexity, making them more accessible for engineers in real-world scenarios.

In recent years, response surface methodology (RSM) has brought many attentions of many quality engineers in different industries. Most of the published literature on robust design methodology is basically concerned with optimization of a single response or quality characteristic which is often most critical to consumers. For most products, however, quality is multidimensional, so it is common to observe multiple responses in an experimental situation. It is believed that the procedure can resolve a complex parameter design problem with more than two responses using readymade standard statistical packages (Raissi,and Fasrsani 2009).

In complex engineering manufacturing, and scientific systems, the optimization of parameters to achieve desired performance outcomes is often challenge due to the high dimensionality of input variables, collinearity among parameters, and noise in the data. Traditional optimization techniques, such as Response Surface Methodology (RSM), may struggle to effectively handle these complexities. Furthermore, the lack of efficient methods to identify and prioritize the most influential parameters hinders the optimization process. Hence, there is a need to enhance optimization methodologies by integrating advanced techniques like Principal Component Analysis (PCA) with RSM. The primary objective of this research is to develop a comprehensive framework that leverages PCA to reduce

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dimensionality, identify key parameters, and improve the accuracy and efficiency of RSM based optimization for complex parameter designs.

2. MATERIALS AND METHODS

The research methodology need to resolve complex parameter design problem by integrating principal component Analysis (PCA) for multi response surface methodology (MRS) which generally fallows a structured approach simulations.

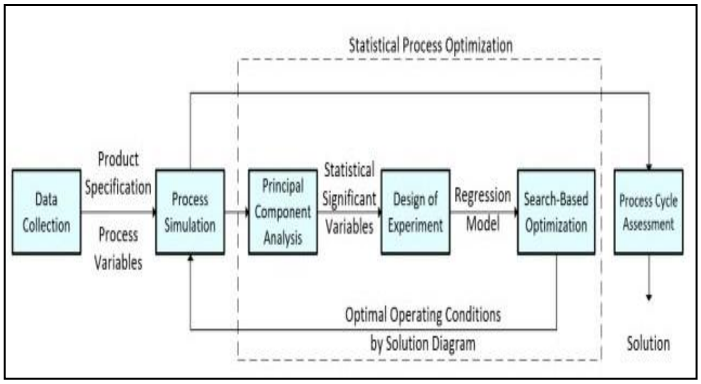

Fig. 1 (source**:** Sin Yong Teng, PASPO 2019**)**

Data Collection: gather data on multiple parameters and response from experiments.

PCA Application: apply PCA to the collected dataset to reduce the dimensionality while retaining as much variance as possible. This involves computing eigenvectors and eigenvalues of the covariance matrix and selecting principal components

Model Fitting: develop the response surface model using the reduced set of principal components instead of original parameters.

$$Y = \beta_o + \sum_{i=1}^{k} \beta_i x_i + \sum_{i=1}^{k} \beta_{ii} x^2{}_i \sum_{i<j} \sum \beta_{ij} x_i x_j + \varepsilon$$

(6)

The goal is to optimize the response variable Y. ε is a random error. The β coefficients, which should be determined in the second-order model, are obtained by the least square method.

It is assumed that the independent variables are continuous and controllable by experiments with negligible errors. It is required to find a suitable approximation for the true functional relationship between independent variables and the response surface.

Montgomery also considers unlikely that a specific polynomial model approximates a real model for the whole experimental space covered for the independent variables. For a specific region, the approximation usually is efficient. The OLS method is used to estimate the parameters (β) that in matrix form could be written as:

$$\hat{\boldsymbol{\beta}} = (\mathbf{X'X})^{-1}\mathbf{X'y}$$

(7)

Where X is the matrix of factor levels and y is the response. The evaluation of the presence of curvature in the model is based on the analysis of center points for the factors levels.

Pearson and Hotelling (1933) Principal component analysis (PCA) was first introduced by Pearson and then developed by Hotelling. PCA is a multivariate technique for forming new uncorrelated variables through a linear composite of the original variables.

Assume there are p original variables $x_1, x_2, \ldots, x_p$; PCA generates p uncorrelated linear combinations as follows:

$$\begin{aligned} Y_1 &= a_{11}x_1 + a_{12}x_2 + \ldots\ldots\ldots + a_{1p}x_p \\ Y_2 &= a_{21}x_1 + a_{22}x_2 + \ldots\ldots\ldots + a_{2p}x_p \\ &\vdots \qquad\qquad\qquad \vdots \\ Y_k &= a_{k1}x_1 + a_{k2}x_2 + \ldots\ldots\ldots + a_{kp}x_p \end{aligned}$$

(8)

Further, $Y_1$is called the first principal component; Y_2 is called the second principal component and so on. The coefficients of the k^{th} component are the elements of the eigenvector corresponding to the k^{th} largest eigenvalues.

1. The principal components are created in order of the decreasing variances. Therefore, the first principal component accounts for the most variance in the data, the second principal component accounts for the maximum of the variances that is not accounted for by the first variable and so on.

$a^2{}_{k1} + a^2{}_{k2} + \ldots\ldots\ldots + a^2{}_{kp} = \quad 1$ where $k = 1; 2; \ldots ; p$

Since we assume that there are p responses. The proposes procedure is described in the following.

Step 1: Compute the quality loss for each response. Let L_{ij} be the quality loss for i^{th} response at j^{th} trial. L_{ij}can be computed on the basis of Taguchi's loss function.

Step 2: Normalize L_{ij} . To reduce the variability, the scale of the quality loss for each response is normalized. L_{ij} is transformed into Y_{ij} ($0<Y_{ij}< 1$) by using the following formula:

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$$Y_{ij} = \frac{L^{+}_{i} - L_{ij}}{L^{+}_{i} - L^{-}_{i}} \qquad (9)$$

where Y_{ij} is the normalized quality loss for i^{th} response at j^{th} trial; L^{+}_{i} is max{L_{i1} , L_{i2}, . . . , L_{ij}}; L^{-}_{i} is min{L_{i1} , L_{i2} , . . . , L_{ij}}.

Step 3: Perform the PCA on the basis of the computed data, Y_{ij}.

Step 4: Determine the number of principal components k, and compute

$$Y_{kj} = \sum_{i=1}^{p} a_{k1} x_{ij} \qquad (10)$$

Where $a_{k1}, a_{k2}, \ldots\ldots\ldots, a_{kp}$ are the elements of the eigenvector corresponding to the k^{th} largest eigenvalue. Y can be considered as a multi-response performance index, which can be used to determine the optimal conditions.

This new equation is modeled through OLS algorithm. To force the solution to fall inside the experimental region, a constrained nonlinear programming problem written in terms of principal components could be expressed as shown in the following equation:

Minimize PC_1 =

$$\beta_o + \sum_{i=1}^{k} \beta_i x_i + \sum_{i=1}^{k} \beta_{ii} x^2{}_i \sum_{i<j} \sum \beta_{ij} X_i X_j \qquad (11)$$

Subject to: $x^T x \leq \rho^2$ (12)

Treating the principal components rather than the original response variables has several advantages. If the first principal component represents a high proportion of the total variance in the data, it provides a univariate summary of the multivariate responses. Inspection of the loadings (eigenvectors) will reveal the kind of relationship among the i^{th} principal component score equation and the original

3 RESULTS AND DISCUSSION

The section illustrated the flexibility of enhancing multi- response surface methodology through integrating principal component analysis (PCA) for complex parameter design optimization; **python** software was employed to analyze the fallowing results.

Dep. Variable:	y1	R-squared:	0.962
Model:	OLS	Adj. R-squared:	0.961
Method:	Least Squares	F-statistic:	618.7
Date:	Fri,05Jul 2024	Prob(Fstatistic):	5.98e-63
Time:	15:30:12	Log-Likelihood:	-59.774
No. Observations	100	AIC:	127.5
Df Residuals	96	BIC:	137.9
Df Model:	3		
Covariance Type:	nonrobust		

Table 3.1 Present Model summary Response for y1 of OLS Regression Results.

Table 3.2 Represent Model summary Response of

	coef	std err	t	P>|t|	[0.025	0.975]
Const	10.0408	0.046	216.396	0.000	9.950	10.131
PC1	0.3870	0.027	14.242	0.000	0.334	0.440
PC2	0.8012	0.021	38.285	0.000	0.759	0.844

OLS Regression and PCA.

Table 3.3 Represent Model summary of OLS and

Omnibus:	0.451	Durbin-Watson:	2.185
Prob(Omnibus):	0.798	Jarque-Bera (JB):	0.613
Skew:	0.020	Prob(JB):	0.736
Kurtosis:	2.626	Cond. No.	3.19e+16

Durbin waston for Autocorrelation det.

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Since the DW statistic is very close to 2, it suggests that there: **No significant autocorrelation** in the residuals, meaning that the residuals appear to be randomly distributed with no evidence of autocorrelation.

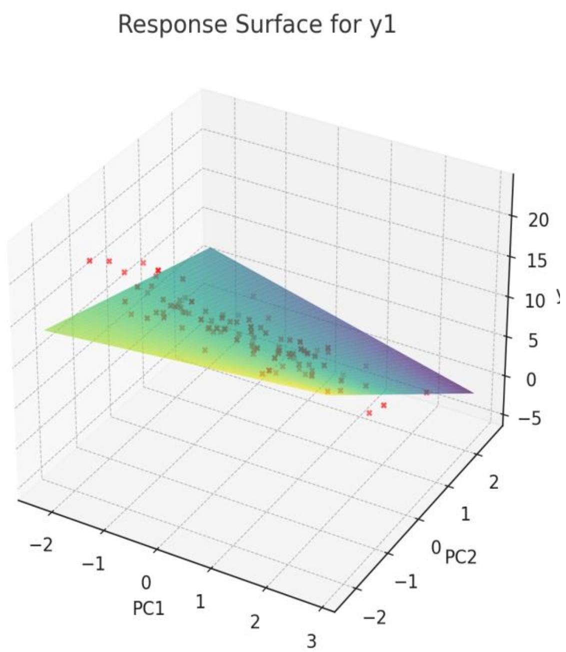

Fig 3.1

Shows visualizations of the predicted values of y2 based on the principal components PC1 and PC2. The red dots represent the actual data points in the transformed space.

- The response surface plot shows a negative (+ve) relationship between PC_1 and y_1, meaning that as PC_1 increases, y_1 tends to inecrease.
- The plot also shows a positive (+ve) relationship between PC_2 and y_1, meaning that as PC_1 increases, y_2 also tends to increase.

Table 3.4 Represent Model summary Response for y2 of OLS Regression Results.

Dep. Variable:	y_2	R-squared:	0.966
Model:	OLS	Adj. R-squared:	0.964
Method:	Least Squares	F-statistic:	674.7
Date:	Fri, 05 Jul 2024	Prob(F-statistic):	1.56e-64
Time:	15:30:12	Log-Likelihood:	-60.511
No. Observations:	100	AIC:	129.0
Df Residuals:	96	BIC:	139.4
Df Model:	3		
Covariance Type:	nonrobust		

Table 3.5 Represent Model summary of OLS Regression and PCA

Table 3.6 Represent Model summary of OLS and Durbin waston for Autocorrelation det.

	coef	std err	t	P>|t|	[0.025	0.975]
Const	15.0516	0.050	299.007	0.000	14.951	15.152
PC1	0.3860	0.029	-13.489	0.000	-0.444	-0.328
PC2	0.7421	0.023	32.383	0.000	0.697	0.787

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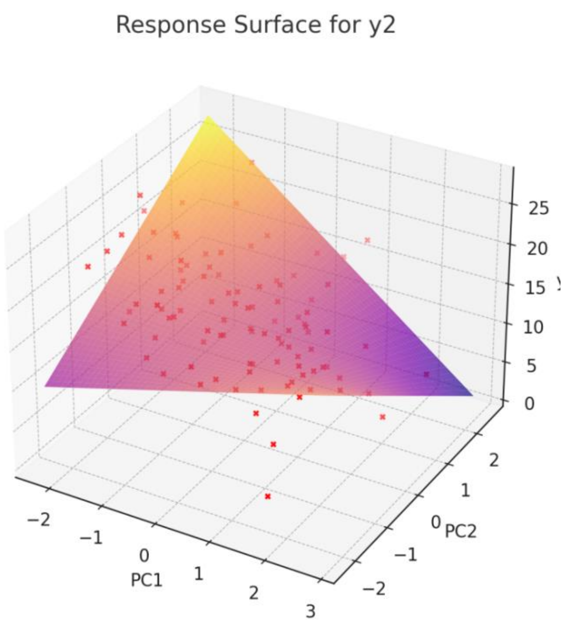

Fig. 3.2

Shows visualizations of the predicted values of y2 based on the principal components PC1 and PC2. The red dots represent the actual data points in the transformed space.

- The response surface plot shows a negative (-ve) relationship between PC_1 and y_2, meaning that as PC_1 increases, y_2 tends to decrease.
- The plot also shows a positive (+ve) relationship between PC_2 and y_2, meaning that as PC_2 increases, y_2 also tends to increase.

Omnibus:	1.168	Durbin-Watson:	2.109
Prob (Omnibus)	0.558	Jarque Bera (JB):	1.263
Skew:	-0.134	Prob(JB):	0.532
Kurtosis:	2.610	Cond. No.	3.19e+16

Residuals Plot for y1 and y2 (Histogram & QQ Plot)

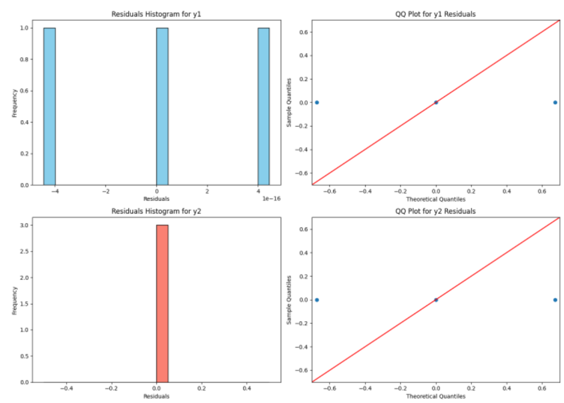

Fig. 3.3

A residuals plot will help assess how well the models fit by showing the distribution of the errors.

- ➢ It uses to assess the goodness of fit of the regression model.
- ➢ Residuals are symmetric around zero: meaning that the distribution it fallows normal

SUMMARY, CONCLUSION AND RECOMMENDATIONS

- ➢ The multiresponse surface methodology (MRSM) model successively fits the data, capturing the relationships between the principal components (PCs) and both response variables (y1 and y2), the model includes significant terms for the PCs and their interaction, indicating that the PCs have a significant impact on both responses.
- ➢ The coefficients of the model represent the estimated effects of the PCs and responses, allowing for the optimization of the input variables (x_1, x_2,x_3) to achieve desired responses.

- While R-squared values indicate the proportion of variance in the responses explained by the PCs, suggesting a strong relationship between the inputs and outputs, enabling the identification of optimal input settings to achieve desired response values.
- The PCA Analysis successfully reduced the dimensionality of the input data (x_1, x_2, x_3) to two principal component (PCs), PCs captured a significant amount of the variability in the original data, with PC1 explaining a larger proportion of the variance.

By incorporating PCA, which reduces the dimensionality of data while preserving variance, one can simplify the analysis of multiple responses, this integration helps in identifying the most significant factors affecting the responses and can streamline the optimization process. It allows for a more efficient exploration of the design space, leading to better decision making and improved performance in complex system. In summary, the combination of MRSM and PCA provides a robust framework for tackling complex parameter design optimization, enabling practitioners to achieve more effective and efficient results.

RECOMMENDATIONS:

Recommendations bases on simulation can made through the following:

1. When dealing with multiple inputs, use PCA to reduce the dimensionality and identify the most important features
2. When optimizing multiple responses, use multi response surface methodology MRSM to model the relationships between the inputs and responses.
3. Validate the MRSM model through statistical metrics and visualization to ensure its accuracy and reliability, and also use model to identify optimal inputs settings that achieve desired response values.
4. Consider including interaction terms and non linear effects in the MRSM model to capture complex relationships between the inputs and responses, so also by using other techniques such as machine learning algorithms, to complement or alternative to MRSM.
5. Monitor the process and update the model as needed to ensure its continued accuracy and relevance.
6. Be cautious of over fitting the model, especially when using high degree polynomials or complex models, by following these recommendations, you can effectively optimizing complex parameter designs with multiple responses using PCA and MRSM.

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