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Dimensionality Reduction Techniques In Response Surface Designs

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ABSTRACT: *Dimensionality reduction has enormous applications in various fields in industries. It can be applied in an optimal way with respect to time and cost related to the agricultural sciences, mechanical engineering, chemical technology, pharmaceutical sciences, clinical trials, biological studies, image processing, pattern recognitions etc. Several researchers made attempts on the reduction of the size of the model for different specific problems using some mathematical and statistical techniques identifying and eliminating some insignificant variables.This paper presents a review of the available literature on dimensionality reduction.*
Keywords: *Principle component analysis, Factor analysis, Cluster analysis*

I. INTRODUCTION

The study of functional relationship between the response and the factor combinations is said to be response surface study. The response variable is a measured quantity whose value is assumed to be affected with change in the levels of the factors. Mathematically, the response function is denoted as $\mathbf{y} = f(x_1, x_2, \ldots x_k) + \varepsilon$, where $f(x_1, x_2, \ldots x_k)$ is a polynomial function of degree d with k factors. The purpose of response surface is to determine and quantify the relationship between the values of one or more measurable response variable(s) and settings of a group of experimental factors presumed to affect the response(s) and also to find the settings of the experimental factors that produce the best value or best set of values of the response(s).

Let there be v factors X_i (i =1,2…v) each at s levels for experimentation and let D denote the design matrix of the combination of the factor levels, given by

$$D = ((x_{u1}, x_{u2}, \ldots, x_{uv})) \qquad (2.1)$$

Where x_{ui} be the level of the i^{th} factor in the u^{th} treatment combination (i=1,2, ..., v; u = 1, 2, …, N). Let Y_u denote the response at the u^{th} combination. The factor-response relationship given by

$$E(Y_u) = f(x_{u1}, x_{u2}, \ldots, x_{uv}) \qquad (2.2)$$

is called the response surface. Designs used for fitting the response surface models are termed as ‘Response Surface Designs’.

The functional form of the response surface model in ‘v’ factors, can be expressed in the form of a linear model as

$$\underline{\mathbf{Y}} = X\underline{\boldsymbol{\beta}} + \underline{\boldsymbol{\varepsilon}} \qquad (2.3)$$

Where $\underline{\mathbf{Y}} = (Y_1, Y_2, \ldots, Y_N)'$ is the vector of observations,

$\underline{\boldsymbol{\varepsilon}} = (\varepsilon_1, \varepsilon_2, \ldots \varepsilon_N)'$ is the vector of random errors and assume that $\underline{\boldsymbol{\varepsilon}} \sim N(0, \sigma^2 I)$.

If the model is of first order, then

$X_u = (1, x_{u1}, x_{u2}, \ldots x_{uv})$is the u^{th}row of X,

$\underline{\boldsymbol{\beta}} = (\beta_0, \beta_1, \beta_2, \ldots \beta_v)$is the vector of parameters

If the model is of second order, then

$X_u = (1, x_{u1}, x_{u2}, \ldots x_{uv}, x^2_{u1}, x^2_{u2}, \ldots x^2_{uv}, x_{ul}x_{u2}, \ldots x_{uv-1}x_{uv})$is the u^{th}row of X,

$\underline{\boldsymbol{\beta}} = (\beta_0, \beta_1, \beta_2, \ldots \beta_v, \beta_{11}, \beta_{22}, \ldots \beta_{vv}, \beta_{l2}, \ldots \beta_{v-1v})'$ is the vector of parameters

The least square estimate of the parameters $\hat{\beta}$ of the model is given by

$$\hat{\beta} = (X'X)^{-1}X'Y \qquad (2.4)$$

with variance–covariance matrix as

$$D(\hat{\beta})=(X'X)^{-1}\sigma^2 \quad (2.5)$$

The estimated value of the response is

$$\hat{Y} = \mathbf{X}\hat{\beta} \quad (2.6)$$

withvariance function of $\hat{Y}_u$ at the u^{th} design point given as

$$V(\hat{Y}_u)=X_u(X'X)^{-1}X'_u\sigma^2 \quad (2.7)$$

Generally, $V(\hat{Y}_u)$ is a function of the distance(ρ) of the design point from the origin and also a function of variances and covariance's of the estimates of the parameters. In particular, Box and Hunter (1957) noted that "Reasons are advanced for preferring designs having a spherical or nearly spherical variance function. Such designs ensure that the estimated response has a constant variance at all points which have the same distance from the center of the design and designs having this property are called “Rotatable Designs”. The variance of the estimated response at any design point is a function of its distance from the design center (origin).

Several researchers worked on different concepts in response surfaces of different orders such as finding the stationary point of the system, optimization of the function, construction of response surface designs, Orthogonal Designs, Central Composite Designs, Rotatable designs, Group Divisible Designs, Blocking of response surface designs etc.

As the number of factors increases (k>10), the number of relationships between the combinations of factors and response increases. As a result, the difficulty level of the analysis of the model increases and will be relatively inaccurate in higher dimensions. With increase of the number of factors, the size of the data set increases and the difficulty level of the model also increases which leads to the problem of dimensionality. The size of the data or model cannot be reduced directly because it affects the model and analysis of the data sets.

When the number of factors (dimension) is more and only a few factors (or its combinations) are important it is assumed that it is possible to eliminate the insignificant factors or its combinations, which are not affecting much the response. Thus, the loss of information must be as minimum as possible. As a result, the time, cost, effort and data complexity can be minimized.

Dimensionality reduction has enormous applications in various fields in industries. It can be applied in an optimal way with respect to time and cost related to the agricultural sciences, mechanical engineering, chemical technology, pharmaceutical sciences, clinical trials, biological studies, image processing, pattern recognitions etc. For instance, in the structural mechanics of systems with spatially random properties the functional mapping from a high-dimensional work space to a low-dimensional feature space. Defining the raw parameters of a problem here, features are knowledge-laden coordinates that are defined with the help of a domain expert. It is noted that the expert need not know which region of feature space may contain designs of systems with desirable behavior. The expert needs only features that may be relevant to system performance.

II. LITERATURE REVIEW ON THE MODEL REDUCTION

Several researchers made attempts on the reduction of the size of the model for different specific problems using some mathematical and statistical techniques identifying and eliminating some insignificant variables. Most of the literature available on the reduction of the dimensionality is related to the reduction of the size of the multiple regression models. A detailed up to date review on the related work has been presented.

Different authors who made attempts in this direction are: Friedman and Tukey (1974), Breiman, Friedman, Olshen and Stone (1984), Diaconis and Freedman (1984), Breiman and Friedman (1985), Stone (1985, 1986), Engle, Granger, Rice and Weiss (1986), Chipman, Hamada and Wu (1997), Chen (1988), Loh and Vanichsetakul (1988), Haste and Stuetzle (1989), Kramer (1991), Lin (1991), George and Meculloch (1993); Tibshirani (1996), Jin and Shaoping (2000), George and Foster (2000), Fan and Li (2001); Lu and Wu (2004), Efron, John stone, Hastie and Tibshirani (2004), Yuan and Lin (2004), Janathi, Idrissi, Sbihi and Touahni (2004) ...

There are some multivariate techniques that are used for the reduction of dimensionality. Some of them are Principal Component Analysis, Factor Analysis and Multi Dimensional Scaling etc.

Principal Component Analysis is a popular multivariate dimensionality reduction technique by itself. It expresses data as a linear combination of all the available explanatory variables in the data set. This method is suitable for finding the ranking of the parameters given the fact that the parameters contributing most to the first few principal components should explain maximum variance of the data. Also, since the principal components are orthogonal to each other there is no possibility of any interaction affect.

Factor analysis is another multivariate technique proposed by Thurston (1934) for reducing the size of the model. It expresses the information contained in a number of original variables into a new set of factors fewer in number than the original variables so that these factors are common among the original variables. The factors can be identified based on the interrelationships among the variables from the covariance structure. These are underlying but observable random quantities. It is motivated by the variables can be grouped based on their correlations i.e. all variables within a particular group are highly correlated among themselves but relatively small correlations exists among variables from different groups.

Friedman and Tukey (1974) proposed a projection pursuit method for the reduction of dimensionality. This method searches for linear projection onto the lower dimensional space that robustly reveals structures (i.e. their distribution is "interesting"). Interesting is defined as being "far from the normal distribution", (i.e. the normal distribution is assumed to be most uninteresting) in the data. The degree of "far from the normal distribution" is defined as being a projection index.

Hastie and Tibshirani (1984) proposed a flexible method to identify and characterize the effect of potential prognostic factors on an outcome variable in clinical trials. These methods are called generalized additive models. In Logistic regression models, the effects of prognostic factors x_j are expressed in terms of a linear predictor of the form $\Sigma\beta_j x_j$. The additive model replaces $\Sigma\beta_j x_j$ with $\Sigma f_j(x_j)$ where f_j is an unspecified (non-parametric) function. This function is estimated in a flexible manner using a scatter plot smoother. The estimated function $\hat{f}_j(x_j)$ can reveal possible nonlinearities in the effect of the x_j.

Breiman, Friedman, Olshen and Stone (1984) proposed a tree-structured approach in which a regression model can be reduced by constructing tree by splitting the data with respect to the characterization at each step, with a partition of the entire data into several homogenous groups. Since one can split the data in many possible ways, this leaves a great deal of flexibility in constructing the tree.

Diaconis and Friedman (1984) proposed a method of distribution of Projections. The data is set by projections and categorized into Gaussian (or nearly Gaussian) and non Gaussian projections. Many data sets show nearly Gaussian projections. On the other hand, the class of data sets where most projections are close to non-Gaussian, a different criterion seems to project which are close to Gaussian.

Breiman and Friedman (1985) proposed the Alternating Conditional Expectation algorithm for estimating the transformations of a response and a set of predictor variables in multiple regression which produce the maximum linear effect between the transformed independent variables and the transformed response variable. These transformations can give the data analyst insight into the relationships between the variables, so that, relationship between them can be best described and non-linear relationships can be uncovered. The algorithm is used in the context of the ever-growing collection of modern tools for regression wherein robust procedures and diagnostic techniques are used for identifying important factors.

Stone (1985, 1986), developed the additive regression model for easier interpretation of the contribution of each explanatory variable.

In the study of the effect of 'weather' on 'electricity demand' and its analysis, Engle, Granger, Rice and Weiss (1986) proposed a class of partial spline curve models for smoothing data with reduced dimensions.

Chen (1988), Loh and Vanichsetakul (1988), constructed trees based on the information provided from the learning sample of objects with known class for each of the components of classifier construction. Hastie and Stutzle (1989) developed a concrete algorithm to find the principal curve which is represented by a parametric curve. The principal curves of a given distribution are not always unique. Kramer (1991) proposed a non linear principal component analysis approach for training the feed forward network to obtain an identity mapping using sequential networks in cascade. Each network has single bottleneck layer and the output of one is fed into the second and the whole network is trained.

Saund (1991) used a three layer neural network with a single hidden layer which he called a "connectionist network". While training the network, he noticed that in order to obtain a good dimensionality reduction, we need to identify the most effective number of units in the middle bottleneck layer but, he does not provide us with a way of directly identifying it.

Jin and Shaoping (2000) used neural network approach for reduction of dimensionality for Chinese character recognition. Li and Chen (2000) proposed iterative Tree-Structured regression for finding a direction, along which the regression surface bends. The direction is used for splitting the data into two regions, within each region another direction is found and the partition is done in the same manner. The process continues recursively until the entire regressor domain is decomposed into regions, where, the surface no longer bends significantly and linear regression fit becomes appropriate. For implementing the direction search, the Principal Hessian directions are used. Fan and Li (2001) proposed a non-concave penalized likelihood approach for selecting significant variables. Unlike, stepwise variable selection and subset regression, their approaches delete insignificant variables by estimating their coefficients to be Zero. Thus, their approaches estimate the regression coefficients and select significant variables simultaneously.

Very few authors made attempts on the reduction of dimensionality of the response surface design model. Some of them are: Cukier, Fortuin, Shuler (1973), Kaufman, Balabano, Grossman, Manson, Watson and Haftaka (1996), Homma and Saltelli (1996), Venter, Haftaka and Stammer (1998), Vignaux and Scott (1999), Lacey and Steele (2006) etc. Even though, some researchers made attempts on the reduction of the number of factors or factor combinations related to the fitted response surface model, no theoretical work is found in the literature. The methods used by the researchers are related to different aspects used in mathematics and statistics; that are extended to the response surface study. As a result, response surface methodology suffers from lack of procedures for model reduction.

Fourier Amplitude Sensitivity Test proposed by Cukier, Fortuin and Shuler (1978) provides a way to estimate the expected value and variance of the output variable and the contribution of individual factors for this variance. This method is based on Fourier transformation of uncertain model parameters into a frequency domain. i.e. Transform the multi-dimensional data X to single dimensional data by using the transformation function $G_w(s) = (1/\pi)$ arccos (Cos $(2\pi ws)$), by choosing different values for 'w' for different input factors to obtain the outputs.For the above input and output values, compute the model $y = f(x_1, x_2, \ldots, x_k)$. Compute the Sobol indices for the parameters of the model and arrange them in increasing order and ignore the variables corresponding to the parameters whose indices are small.

Venter, Haftaka and Stammer (1998) considered the data on the modeling of a plate with an abrupt change in thickness for a mechanical problem and fitted the data for first order response surface model and tried to reduce the number of variables from nine to seven using finite elements analysis approach by solving the equations obtained through the boundary conditions.

McKay (1999) reduced the fitted model to some specific experimental data using correlation ratios. Lacey and Steele (2006) studied the finite element method for several engineering case studies experimental data based on the Response surface Designs and reduced variables.

Reviews on different global sensitivity analysis methods can be found in the literature. The total variance of the response variable is decomposed into different parts contributed by various sources of input variations. Then sensitivity indices are derived as the ratio of partial variance contributed by an effect of interest over the total variance of the response.

A review of global sensitivity analysis methods including the montecarlo based, sobol, regression, correlation measures, and various forms of differential analysis can also be found in Helton (1993). These authors used fractional factorial design which appears to be capable of identifying a few active factors in systems with thousands of variable parameters. Another approach to sensitivity analysis not included in Helton (1993), is the recent work of Critchfield and Willard (1986), where, global sensitivity analysis is performed with the frame of first order reliability analysis. A comparison of different sensitivity analysis methods can be found in Iman and Helton (1988), Saltelli and Homma and Saltelli et al(1996).

A general approximation to the robust parameter design problem based on response surface methods was first proposed by Box and Jones (1990) and later elaborated by Myers (1992). The noise factors are not controllable in general, and they follow certain distribution. Expectation models can be obtained from the fitted response to provide dual responses which can be optimized to solve Taguchi's robust parameter design problem

Wu, Boos and Stefanski (2007) developed a general simulation based method for estimating the tuning parameter of variable selection techniques to control the false selection rate of variables.

III. CONCLUDING REMARKS

High-dimensional data sets or models make challenges as well as some opportunities bound to give rise to new theoretical developments. This can be studied in two aspects:

(i) Minimizing the number of factors or factor combinations in the model with minimum loss of information in the data and

(ii) Constructing the designs with minimum number of design points keeping in view the factors that are more active.

Though, several methods on the reduction of dimensionality of the regression model are available in the literature, it appears that no significant work has been done to give a proper criterion for the selection of variables in the regression model. No specific exclusive method is used for model reduction. The statistical techniques used for model reduction by the researchers are Principal Component Analysis, Factor Analysis, Multidimensional Scaling, Stepwise regression, Correlation approach, Regression approach, Sobol sensitivity approach, Fourier amplitude and Projection pursuit, Finite element methods etc. All these techniques are well known statistical / mathematical methods used to fit experimental data model and reduce the model by eliminating insignificant variables based on the parameter in the response surface model.

The feasibility of the Principal Component Analysis, Factor Analysis, Multidimensional Scaling, Stepwise regression, Correlation approach, Regression approach are studied for the response surface design models and observed that these methods have given fruitful results. Principal Component Analysis searches lower dimensional space that computes majority of the variation within the data and discovers linear structure in the data. However, this is ineffective in analyzing nonlinear structures, i.e. curves, surfaces or clusters. Hence it is not applicable for response surface model of second and higher orders. Factor Analysis is not applicable for response surface models due to the study of the interaction effects in the model and estimation of main effects of individual factors. Correlation approach, Regression approach, Sobol sensitivity approach, Fourier amplitude test and Projection pursuit can be used for response surface model reduction but Fourier amplitude test and Projection pursuit methods are very time consuming and their time complexity is more.

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