Response Modelling Approach to Robust Parameter Design Methodology Using Supersaturated Designs

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Outline:

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Definition of Experiments

- An experiment is any systematic procedure carried out under controlled conditions in order
  - to discover an unknown effect,
  - to test or establish a hypothesis,
  - or to illustrate a known effect.

Figure: A general experiment
Components of experiments: The factors

- Factors, or variables of the process. Factors can be classified as either controllable or uncontrollable variables.
- The controllable variables will be referred as factors.
- Generally a Noise Factor, that causes variability under normal operating conditions, will be included in the uncontrollable factors (but we can control it using blocking and randomization).

Figure: A general experiment
Further components of experiments

- **Levels** are values of a factor selected for the experiment.
- **Runs**, or **treatments** are all combination of the levels of all factors.
- **Experimental unit**, is the material to which the treatments are applied.
- **Design matrix** or **Experimental design** is a set of runs (assigns experimental units to treatments).
- **Response**, or **output** is the results of the unknown process.

**Figure**: A general experiment
Robust Parameter Design methodology

- Aims at reducing the performance variation of a system owing to hard to control variables, namely noise variables.
- Two broad categories of input factors: control and noise.
- The goal is to choose the settings of the control factors so as to make the process less sensitive to noise variation.
- Taguchi (1987) proposed the use of product arrays, i.e. the crossing of two factorial designs the one for control and the other for noise factors.
- Combined array (Shoemaker et al., 1991) for both factors need fewer experimental runs.
- Response surface methodology (RSM) is a special case of RPDM (Vining and Myers (1990)).
- Myers et.al. (1992) used a combined array and fitted a response surface model.
Saturated and Supersaturated designs

- **Saturated Design**: There are enough runs for estimating all the main effects but none of the interactions, i.e. $n \ (\text{run size}) = m (\text{number of factors}) + 1$.

- **Supersaturated design (SSD)**: The number of runs is not enough for estimating all the main effects, i.e. $n < m + 1$.

- **Balanced Design** (or mean orthogonal): The levels of each factor are observed the same number of times (Each factor is orthogonal to the mean effect).

- **Hadamard matrix** $H_n$ is a square matrix of order $n$ and elements $\pm 1$ satisfying $H^T H = HH^H = nI_n$

Importance of Effects

- Control Factors ($C$) and Noise factors ($N$)
- Main effects, Two factor interactions, Quadratic terms, Higher order terms
- Importance of Effects:
  - control ($C$) and noise ($N$) main effects, control-by-noise ($C \times N$) interactions
  - control-by-control ($C \times C$) interactions, control by control by noise interactions ($C \times C \times N$)
  - noise by noise interactions ($N \times N$)

For $1 \leq u \leq N$, let $x_{u1}, x_{u2}, \ldots, x_{up}$ and $z_{u1}, z_{u2}, \ldots, z_{uq}$ be respectively the levels of the $p$ control and $q$ noise factors corresponding to the $u$th experimental run. Two RPD models: The first one, referred as model 1, is as follows

$$y_u = \mu + \sum_{i=1}^{p} a_i x_{ui} + \sum_{i_1 < i_2=1}^{p} a_{i_1 i_2} x_{ui_1} x_{ui_2} + \sum_{j=1}^{q} b_j z_{uj} + \sum_{i=1}^{p} \sum_{j=1}^{q} c_{ij} x_{ui} z_{uj} + \sum_{j=1}^{q} \sum_{i_1 < i_2=1}^{p} d_{i_1 i_2 j} x_{ui_1} x_{ui_2} z_{uj} + \epsilon,$$

where $y_u$ denotes the response of interest corresponding to the $u$th experimental run.
Model 2

For $1 \leq u \leq N$, let $x_{u1}, x_{u2}, \cdots, x_{up}$ and $z_{u1}, z_{u2}, \cdots, z_{uq}$ be respectively the levels of the $p$ control and $q$ noise factors corresponding to the $u$th experimental run. Two RPD models: The second model, referred as model 2, is as follows

\[
y_u = \mu + \sum_{i=1}^{p} a_i x_{ui} + \sum_{i_1 < i_2=1}^{p} a_{i_1 i_2} x_{u_i_1} x_{u_i_2} + \sum_{i=1}^{p} a_{ii} x_{ui}^2 + \sum_{j=1}^{q} b_j z_{uj} + \sum_{i=1}^{p} \sum_{j=1}^{q} \sum_{i_1 < i_2=1}^{p} c_{ij} x_{ui_1} z_{uj} + \sum_{j=1}^{q} \sum_{i_1 < i_2=1}^{p} d_{i_1 i_2 j} x_{ui_1} x_{ui_2} z_{uj} + \epsilon,
\]

where $y_u$ denotes the response of interest corresponding to the $u$th experimental run.
Nonconcave penalized likelihood

Penalized least squares approaches

\[ Q(\beta) = \frac{1}{2n} \sum_{i=1}^{n} (Y_i - x_i^T \beta)^2 + \sum_{j=1}^{d} p_{\lambda_n}(|\beta_j|), \]

\( p_{\lambda_n}(\cdot) \) a penalty function, and \( \lambda_n \) a tuning parameter.

- Choosing penalty function to be:
  - \( p_{\lambda}(|\beta|) = \lambda |\beta| \) it results in Lasso (Tibshirany, 1996);
  - \( p_{\lambda}(|\beta|) = \lambda |\beta|^q \) leads to a bridge regression (Frank and Friedman, 1993).
  - the smoothly clipped absolute deviation (SCAD) penalty to achieve the purpose of variable selection, Fan and Li (2001).


Iterative Sure Independence Screening (Iterative SIS) in SSDs

- constructed a \((m + 1) \times 1\) vector \(\omega\) of marginal correlations of the effects against the response which is given as \(\omega = X'y\),
- created a sub-model using a threshold value so as to eliminate the non-significant variables.
- The number of significant factors can further be reduced using a penalized method such as the SCAD or Lasso.
- an iterative process of the above steps using the residuals as the new responders to avoid collinearity.

Steps

- Let $n \times n$ be a Hadamard matrix in which all the elements of the first column are all unities, and let $n = (8m + 4)$ where $m$ is a natural number.
- Define $H_n^* = [H'_n, -H'_n]'$
- The $r$, where $r \leq 8m + 4$, columns of $H_n^*$ are assigned to $r$ factors, where $N = 16m + 8$
- Construct a set of $2p$ experimental runs where each control factor is sequentially placed at $\pm \alpha$ and all the other control and noise factors placed at zero. Note that axial points are assigned only to control factors.
- Construct a set of $n_0$ central points that is to say, all, control and noise factors are placed at zero in each run.
Construction - Lemma

- Define $H_n^* = [H'_n, -H'_n]'$. The $r$ ($r \leq n$) columns of $H_n^*$ are assigned to $r$ factors.
- Columns are $d_i = (d_{i1}, \ldots, d_{iN})'$, $i = 1, \ldots, r$, where $N = 2n$.

\[ D = \begin{bmatrix} d_1, \ldots, d_r, d_{12}, \ldots, d_{(r-1)r}, d_{123}, \ldots, d_{(r-2)(r-1)r} \end{bmatrix}, \]

where, $d_{i1i2} = (d_{i11}d_{i21}, \ldots, d_{i1n}d_{i2n})'$ and,
\[ d_{i1i2i3} = (d_{i11}d_{i21}d_{i31}, \ldots, d_{i1N}d_{i2N}d_{i3N})'. \]
- Then $D$ is balanced and no two columns of $D$ are fully aliased if
  1. Interactions $d_{i1i2i3i4}^*$ are not completely aliased with the mean effect, where $d_{i}^* = (d_{i1}, \ldots, d_{in})'$,
  2. Interactions $d_{i1i2i3i4i5i6}^*$ are not completely aliased with the mean effect.
Construction - Theorem

- Define $H^*_n = [H'_n, -H'_n]'$. The $r$ ($r \leq n$) columns of $H^*_n$ are assigned to $r$ factors.
- Columns are $d_i = (d_{i1}, \cdots, d_{iN})'$, $i = 1, \cdots, r$, where $N = 2n = 16m + 8$.

$$D = \begin{bmatrix} d_1, \cdots, d_r, d_{12}, \cdots, d_{(r-1)r}, d_{123}, \cdots, d_{(r-2)(r-1)r} \end{bmatrix},$$

where, $d_{i_1i_2} = (d_{i_11}d_{i_21}, \cdots, d_{i_1n}d_{i_2n})'$ and,

$$d_{i_1i_2i_3} = (d_{i_11}d_{i_21}d_{i_31}, \cdots, d_{i_1N}d_{i_2N}d_{i_3N})'.$$
- Then $D$ is balanced and no two columns of $D$ are fully aliased.
Construction - Remark

- Hadamard matrices exist for orders $4m$ but theorem is for orders $8m + 4$.
- Other cases need to be studied on one by one base.
- We did a computer search for the cases of Hadamard matrices of order 8, 16, 24 and 40
  - order 8: just one inequivalent Hadamard matrix and in order 16: there are 5 inequivalent Hadamard matrices but none of them is suitable to fit the model of interest (estimating all parameters of interest).
  - order 24 there are 60 inequivalent Hadamard matrices but only 2 of them are suitable to fit the model of interest - provided.
  - order 40: unknown number but we were able to find some of them that are suitable and one representative provided.

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Steps to follow

- Consider a linear regression model $y = X\beta + \epsilon$, where $X = [1_N, D]$ is the design matrix, $y$ is a $N$-dimensional vector, $\beta$ is a vector of length $r$, where $r$ is the number of the parameters of the model assigned in the designed matrix columns and $\epsilon$ is the normal distributed error.
- Choose the most $n - 1$ significant factors using iterative SIS method so as to find an initial value for SCAD method.
- Apply penalized least squares using the design matrix $X$ in stage one, take the initial value found in stage two, and choose the regularization parameter using BIC as the criterion.
- Choose parameter $\alpha = 3.7$ according to Li and Lin (2002).

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Setup

1000 simulations per case

Different ranges of error variances

Simulation study for Model 1

- $p = 3, q = 3$
- $p = 5, q = 5$

Simulation study for model 2

- one control and one noise active factors
- two control and one noise active factors
- two control and two noise active factors

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Some results - briefly

- **Model 1:**
  - the use of the proposed design provides high probabilities for finding the effects of the active factors.
  - Some cases with some negligible type I error rate. This means that some factors are identified as active ones whereas they are inactive.

- **Model 2:**
  - the experimental runs increased since there are $2p = 10$ axial points and one center point.
  - the numerical results are remarkable; in some cases, when the magnitude of coefficient $\beta$ was quite small, the quadratic effects cannot be estimated.
  - Same fact for CCDs even if they have a considerably larger number of experimental runs than our design.
  - Effects estimates with our method are quite accurate.

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References


