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RESPONSE SURFACE METHODOLOGY FOR FUNCTIONAL DATA WITH APPLICATION TO NUCLEAR SAFETY

ANGELINA ROCHE

ABSTRACT. The paper proposes an adaptation of Response Surface Methodology (RSM) when the covariate is a functional data (one or more functions for instance). The key of the method is to combine dimension reduction techniques with usual Design of Experiments. We prove that the good properties of multivariate designs (rotatability, alphabetic optimality,...) are also verified by the functional designs. The good behavior of the method is illustrated on numerical experiments and applied to nuclear safety.

Keywords: Functional data analysis. Response surface methodology. Design of experiments.

AMS Subject Classification 2010: 62K20, 62K15.

1. INTRODUCTION

Response Surface Methodology (RSM) was introduced by Box and Wilson (1951) with the goal of identifying optimal conditions for experiments in chemistry. The target was to minimize the cost of experimentation or maximize the purity of the product obtained by finding the right combination of factors (temperature, pressure, proportion of reactants, ...). Then, its purpose is to find the values of explanatory variables $(x_1, \dots, x_d) \in \mathbb{R}^d$ for which the response variable is optimal $Y \in \mathbb{R}$. This method has been and is still widely used in the industry.

Suppose we want to find the values of $(x_1, \dots, x_d)' \in \mathcal{R}$ – where \mathcal{R} is a given region of \mathbb{R}^d – minimizing an unknown (maybe random) function $m : \mathcal{R} \rightarrow \mathbb{R}$. We assume here that, for all $(x_1, \dots, x_d)' \in \mathcal{R}$ we can observe $y = m(x_1, \dots, x_d)$.

The principle of the method is to find the optimal experimental conditions by performing a limited number of experiments. The function m is approximated using experimentation and modeling. Usually the first step consists in fitting a first-order linear model to the data

$$(1) \quad y = \beta_0 + \sum_{j=1}^d \beta_j x_j + \varepsilon,$$

while $\varepsilon \sim \mathcal{N}(0, \sigma^2)$ is an error term. Second-order models

$$(2) \quad y = \beta_0 + \sum_{j=1}^d \beta_j x_j + \sum_{j=1}^d \beta_{jj} x_j^2 + \sum_{1 \leq j < k \leq d} \beta_{j,l} x_j x_l + \varepsilon$$

are also often considered to take into account surface curvatures. More complex models such as generalized linear models (see Khuri, 2001, and references therein) or nonparametric models (Facer and Müller, 2003) have been considered.

The parameters of the chosen model are often least-squares estimates calculated from observations $\{(y_i, \mathbf{x}_i), i = 1, \dots, n\}$ where, for all $i = 1, \dots, n$, $y_i = m(\mathbf{x}_i)$ and the *design* points $\{\mathbf{x}_i \in \mathcal{R}, i = 1, \dots, n\}$ are chosen by the user.

This question of the choice of an appropriate design is still an open problem, the idea is that the model must be fitted as best as it is possible, realizing a small number of experiments. We refer to Georgiou et al. (2014) and references therein for the recent advances on the subject. We focus here on the designs classically used for RSM but the method we propose can be applied to all multivariate designs.

Let us describe the 2^d *factorial design* which is the simplest. It is a *first-order design* in the sense that it is frequently used to fit a first-order linear model. For each explanatory variable x_1, \dots, x_d , we choose two levels (coded by +1 and -1) and we take all the 2^d combinations of these two levels. If d is large, it may be impossible to achieve the 2^d factorial experiments. The *fractional factorial design* keeps only a certain proportion (e.g. a half, a quarter, ...) of points of a 2^d factorial design. Typically, when a fraction $1/(2^p)$ is kept from the original 2^d design, this design is called 2^{d-p} factorial design. The points removed are carefully chosen, we refer e.g. to Gunst and Mason (2009) for more details.

Traditional second-order designs are factorial designs, central composite designs and Box-Behnken designs.

- 3^d or 3^{d-p} factorial designs are similar to 2^d and 2^{d-p} factorial designs but with three levels (+1, -1 and 0).
- *Central Composite Designs (CCD)* are obtained by adding to the two-level factorial design (fractional or not) two points on each axis of the control variables on both sides of the origin and at distance $\alpha > 0$ from the origin.
- *Box-Behnken Designs (BBD)* are widely used in the industry. It is a well-chosen subset of the 3^d factorial design. For $d \geq 4$, we refer to Myers et al. (2009, 7.4.7).

For all these designs, some or all points may be replicated, this may allow the design to verify some additional properties and perform lack-of-fit tests (Brook and Arnold, 1985, pp. 48-49).

The aim is to choose the design so that the coefficients of the model $\beta_0, \beta_1, \dots, \beta_d$ (plus β_{jk} , $j, k = 1, \dots, d$ for the second-order model (2)) are estimated as effectively as possible. There are different ways of conceiving the properties a design should satisfy and therefore there are different criteria used in the literature. We focus on the most classical ones: orthogonality, rotatability and alphabetic optimality.

The models (1) and (2) and even highest-order polynomial model can be rewritten in a matrix form

$$\mathbf{y} = \mathbf{X}\boldsymbol{\beta} + \boldsymbol{\varepsilon},$$

where $\mathbf{y} = (y_1, \dots, y_n)^t$, $\boldsymbol{\varepsilon} = (\varepsilon_1, \dots, \varepsilon_n)^t$.

For instance, for the first-order model (1),

$$\mathbf{X} = \begin{pmatrix} 1 & x_{1,1} & \dots & x_{1,d} \\ 1 & x_{2,1} & & x_{2,d} \\ \vdots & \vdots & \ddots & \vdots \\ 1 & x_{n,1} & \dots & x_{n,d} \end{pmatrix} \text{ and } \boldsymbol{\beta} = \begin{pmatrix} \beta_0 \\ \beta_1 \\ \vdots \\ \beta_d \end{pmatrix}$$

with $(x_{1,i}, \dots, x_{d,i})$ the coordinates of \mathbf{x}_i . The least-squares estimator of $\boldsymbol{\beta}$ is equal to

$$\hat{\boldsymbol{\beta}} := (\mathbf{X}^t \mathbf{X})^{-1} \mathbf{X}^t \mathbf{Y}$$

and is a random vector of mean $\mathbb{E}[\widehat{\boldsymbol{\beta}}] = \boldsymbol{\beta}$ and variance-covariance matrix given by

$$\text{Var}(\widehat{\boldsymbol{\beta}}) = \mathbb{E}\left[(\widehat{\boldsymbol{\beta}} - \boldsymbol{\beta})(\widehat{\boldsymbol{\beta}} - \boldsymbol{\beta})^t\right] = \sigma^2 (\mathbf{X}^t \mathbf{X})^{-1}.$$

Hence, the matrix $\mathbf{X}^t \mathbf{X}$ appears both in the definition of $\widehat{\boldsymbol{\beta}}$ and in the expression on its variance. The quality of the estimation of $\boldsymbol{\beta}$ then essentially rests on the properties of $\mathbf{X}^t \mathbf{X}$.

An important property is the *orthogonality*. An orthogonal design is a design for which the matrix $\mathbf{X}^t \mathbf{X}$ is diagonal. This implies that the vector $\widehat{\boldsymbol{\beta}}$ is also a Gaussian random vector with independent components and makes it easier to test the significance of the components of $\boldsymbol{\beta}$ in the model. 2^d factorial designs are orthogonal first-order designs. However, fractional designs have to be constructed carefully in order to keep the orthogonality property, for instance $\{(1, 1), (1, -1)\}$ is a 2^{2-1} design but is not orthogonal. Orthogonality for second-order designs is even harder to verify, we refer to Box and Hunter (1957) for general criteria applied to factorial and fractional factorial designs. Central Composite Designs are orthogonal if

$$\alpha = \sqrt{\frac{\sqrt{F(F + 2d + n_0)} - F}{2}},$$

where F is the number of points of the initial factorial design (see Myers et al. 2009).

A design is said to be *rotatable* if $\text{Var}(\widehat{y}(\mathbf{x}))$ depends only on the distance between \mathbf{x} and the origin. The rotatability is a desirable feature since it implies that the prediction variance is unchanged under any rotation of the coordinate axes. We refer to Box and Hunter (1957) for conditions of rotatability. All first-order orthogonal designs are also rotatable. This is not the case for second-order designs, for instance a CCD design is rotatable if $\alpha = F^{1/4}$ which means that a CCD design can be rotatable and orthogonal only for some specific values of n_0 and F . Box-Behnken designs are rotatable for $d = 4$ and $d = 7$. Some measures of rotatability have been introduced (Khuri, 1988; Draper and Guttman, 1988; Draper and Pukelsheim, 1990; Park et al., 1993) in order to measure how close a design is to the rotatability property.

Another important notion is the *D-optimality criterion* which maximizes the determinant of the matrix $\mathbf{X}^t \mathbf{X}$. A justification of such a criterion is to minimize the volume of the confidence region for $\boldsymbol{\beta}$. Another classical criterion is the *G-optimality criterion* which minimizes the maximal value of $\text{Var}(\widehat{y}(\mathbf{x}))$ over $\mathbf{x} \in \mathcal{R}$. *D-optimal* and *G-optimal* designs may be generated by computers and are used as alternatives to classical designs when they are not available (this is the case for instance when the region \mathcal{R} is constrained). Other criteria are *A-optimality* minimizing the average variance of the estimated coefficients or *E-optimality* maximizing the minimal eigenvalue of the matrix $\mathbf{X}^t \mathbf{X}$. We refer to Pázman (1986) for more details.

2. DESIGN OF EXPERIMENTS FOR FUNCTIONAL DATA

2.1. Generation of a functional design of experiment (DoE). Suppose that the response y depends on a variable x in an infinite or high-dimensional space \mathbb{H} . We propose a method of generation of a Design of Experiments for RSM in this context.

General principle. The method is based on dimension reduction coupled with classical multivariate designs. The main idea is the following: suppose that we want to generate a design around $x_0 \in \mathbb{H}$, we choose an orthonormal basis $(\varphi_j)_{j \geq 1}$ of \mathbb{H} , a dimension d and

a d -dimensional design $\{\mathbf{x}_i, i = 1, \dots, n\} = \{(x_{i,1}, \dots, x_{i,d}), i = 1, \dots, n\}$ around $0 \in \mathbb{R}^d$ and we define a functional design $\{x_i, i = 1, \dots, n\}$ verifying

$$x_i := x_0 + \sum_{j=1}^d x_{i,j} \varphi_j.$$

The advantage of such a method is its flexibility: all multivariate designs and all basis of \mathbb{H} can be used. Then, by choosing an appropriate design and an appropriate basis, we can generate designs satisfying some constraints defined by the context.

Choice of basis. The choice of the basis has a significant influence on the quality of design. According to the context, it is possible to use a fixed basis such as Fourier basis, spline basis, wavelet basis, histogram basis...

However, if we have a training sample $\{(X_i, Y_i), i = 1, \dots, n\}$, it may be relevant to use the information of this sample to find a suitable basis. The data-driven bases existing in the literature are.

- The PCA basis (Dauxois et al., 1982; Mas and Ruymgaart, 2015) which is the basis of \mathbb{H} verifying

$$\frac{1}{n} \sum_{i=1}^n \|X_i - \widehat{\Pi}_d X_i\|^2 = \min_{\Pi_d} \left\{ \frac{1}{n} \sum_{i=1}^n \|X_i - \Pi_d X_i\|^2 \right\},$$

where $\widehat{\Pi}_d$ is the orthogonal projector on $\text{span}\{\varphi_1, \dots, \varphi_d\}$, $\|\cdot\|$ is a norm on the space \mathbb{H} (which has to be a Hilbert space here) and the minimum on the right-hand side is taken over all orthogonal projectors Π_d on d -dimensional subspaces of \mathbb{H} .

- The PLS basis (Wold, 1975; Preda and Saporta, 2005) which permits to take into account the interaction between X and Y . It is computed iteratively by the procedure described in Delaigle and Hall (2012). For theoretical results on the PLS basis in a functional context see Delaigle and Hall (2012) and references therein.

2.2. Least-squares estimation and design properties. In this section we focus on least-squares estimation for first and second-order models. We first define first and second-order models in functional data contexts. Then, we prove that the properties of orthogonality, rotatability and alphabetic optimality can be extended to our context.

We focus here on first-order and second-order designs but the same reasoning may apply to other models and other kind of optimality properties related to the model considered.

First-order model. We define first-order models in the following form

$$y := \alpha + \langle \beta, x \rangle + \varepsilon,$$

with $\alpha \in \mathbb{R}$, $\beta \in \mathbb{H}$ and $\varepsilon \sim \mathcal{N}(0, \sigma^2)$. This model is known as functional linear model (Ramsay and Dalzell, 1991; Cardot et al., 1999) and has been widely studied (see Cardot and Sarda 2011 for a recent overview or Brunel and Roche 2014 for a recent work on this subject).

Now recall that, for all $i = 1, \dots, n$, $x_i = x_0 + \sum_{j=1}^d x_{i,j} \varphi_j$, then the first-order model can be rewritten

$$(3) \quad y_i := \beta_0 + \langle \beta, x_0 \rangle + \sum_{j=1}^d x_{i,j} \langle \beta, \varphi_j \rangle + \varepsilon_i, \text{ for } i = 1, \dots, n.$$

With our choice of design points, this model is nothing more than a first-order multivariate model and can be written

$$(4) \quad \mathbf{Y} = \mathbf{X}\boldsymbol{\beta} + \boldsymbol{\varepsilon}$$

with design matrix

$$\mathbf{X} = \begin{pmatrix} 1 & x_{1,1} & \dots & x_{1,d} \\ 1 & x_{2,1} & & x_{2,d} \\ \vdots & \vdots & \ddots & \vdots \\ 1 & x_{n,1} & \dots & x_{n,d} \end{pmatrix}$$

and coefficients $\boldsymbol{\beta} = (\beta_0 + \langle \beta, x_0 \rangle, \langle \beta, \varphi_1 \rangle, \dots, \langle \beta, \varphi_d \rangle)^t$. Then least-squares estimates of the model parameters can be obtained directly and, since the design matrix \mathbf{X} is exactly the same, it is easily seen that all first-order properties of the multivariate design $\{\mathbf{x}_i, i = 1, \dots, d\}$ are also verified by the functional design.

Second-order model. Now we can see that a similar conclusion holds for the second-order model, which can be written here

$$(5) \quad y := \beta_0 + \langle \beta, x \rangle + \frac{1}{2} \langle Hx, x \rangle + \varepsilon,$$

where $\beta_0 \in \mathbb{R}$, $\beta \in \mathbb{H}$ and $H : \mathbb{H} \rightarrow \mathbb{H}$ is a linear self-adjoint operator. Then, by definition of $x_i = x_0 + \sum_{j=1}^d x_{i,j} \varphi_j$ we have

$$y_i = \beta_0 + \langle \beta, x_0 \rangle + \frac{1}{2} \langle Hx_0, x_0 \rangle + \sum_{j=1}^d x_{i,j} (\langle \beta, \varphi_j \rangle + \langle Hx_0, \varphi_j \rangle) + \frac{1}{2} \sum_{j,k=1}^d x_{i,j} x_{i,k} \langle H\varphi_j, \varphi_k \rangle + \varepsilon_i.$$

This model is a second-order linear model for the data $\{(\mathbf{x}_i, y_i), i = 1, \dots, n\}$, can also be written in the form (4) with the same design matrix as in the model (2). Hence, all second-order properties of $\{\mathbf{x}_i, i = 1, \dots, n\}$ apply to the functional design $\{x_i, i = 1, \dots, n\}$.

3. APPLICATION TO NUCLEAR SAFETY

3.1. Data and objectives. An hypothetical cause of nuclear accident is the loss of coolant accident (LOCA). This is caused by a breach on the primary circuit. In order to avoid reactor meltdown, the safety procedure consists in incorporating cold water in the primary circuit. This can cause a pressurised thermal shock on the nuclear vessel inner wall which increases the risk of failure of the vessel.

The parameters influencing the probability of failure are the evolution over time of temperature, pressure and heat transfer. Obviously, the behavior of the reactor vessel during the accident can be hardly explored by physical experimentation and numerical codes have been developed, for instance by the CEA¹, reproducing the mechanical behavior of the vessel given the three mentioned parameters (temperature, pressure, heat transfer). Figure 1 represents different evolution of each parameter during the procedure depending on the value of several input parameters.

The aim is to find the temperature transient which minimizes the risk of failure. We have access here to the margin factor (MF) which decreases when the risk of failure increases. Hence, the aim is to maximise the MF.

¹French Alternative Energies and Atomic Energy Commission (Commissariat l'énergie atomique et aux énergies alternatives), government-funded technological research organisation. <http://www.cea.fr/>

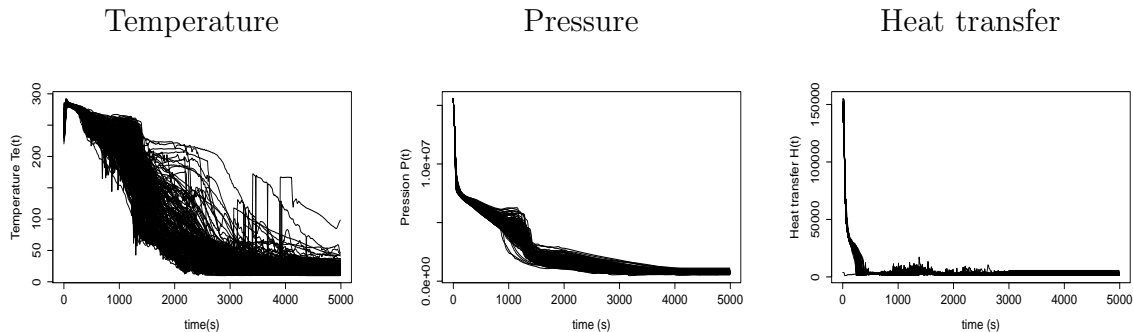


FIGURE 1. Evolution of temperature, pressure and heat transfer. Source: CEA.

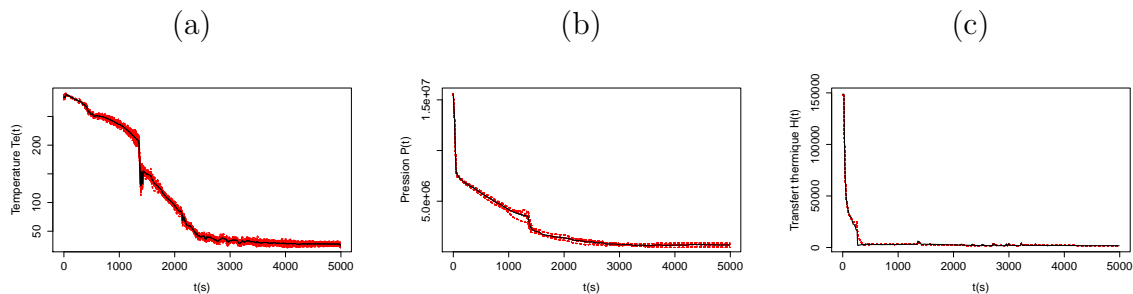


FIGURE 2. Functional design around the initial curves.

3.2. Generation of design. The aim of this section is to generate a factorial design for the temperature, pressure and heat transfer transient given in Figure 1. Since the PLS basis has given good results in simulations, we focus on this basis.

Then, for each quantity considered (temperature, pressure, heat transfer) we define the starting point of the algorithm. We choose the element for which the margin factor is maximal.

We generate a functional design based on a minimum aberration 2^{10-5} fractional design for the temperature, a 2^{3-2} design for the pressure and the heat transfer. As some design points of the functional design around the initial heat transfer curve took negative values (which can not correspond to the physic since the heat transfer is always positive), we remove it and keep only the design points which are always positive. The design points are plotted in Figure 2. The resulting design, which is a combination of all curves of the three designs obtained (for temperature, pressure and heat penetration) counts 128 design points.

3.3. Results. We compute an estimation of the gradient with the results of the experiments on the design points given in Figure 2. The results are given in Figure 3. We take $\alpha_0 = 200$. The final estimates of the optimal curves are given in Figure 4.

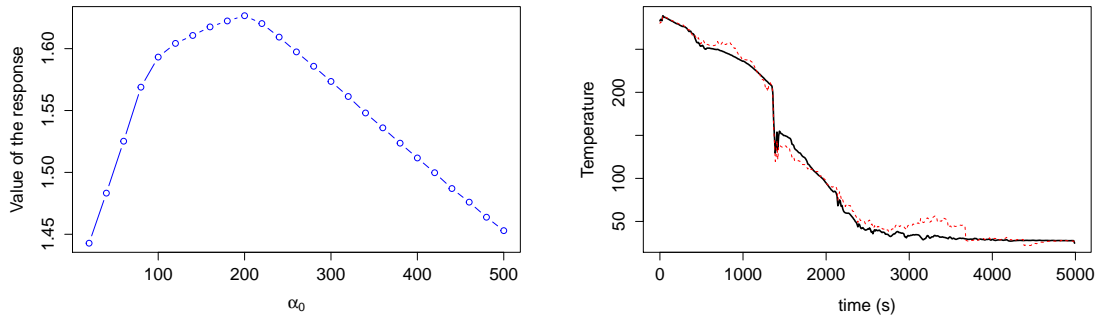


FIGURE 3. Left: value of the response on the estimated steepest ascent direction. Right: solid line initial temperature point, dotted line: optimal temperature transient estimated.

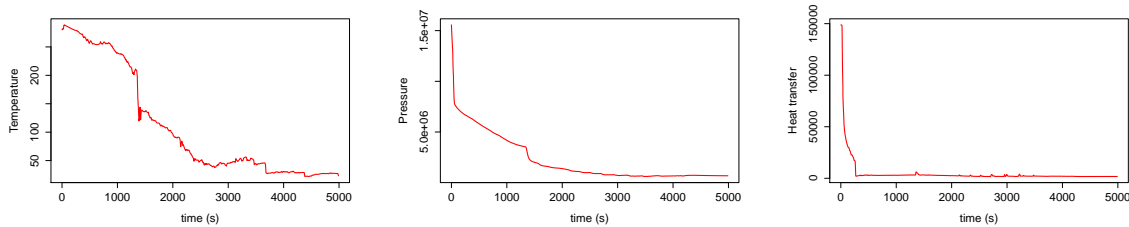


FIGURE 4. Point of the estimated steepest ascent direction maximizing the response.

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