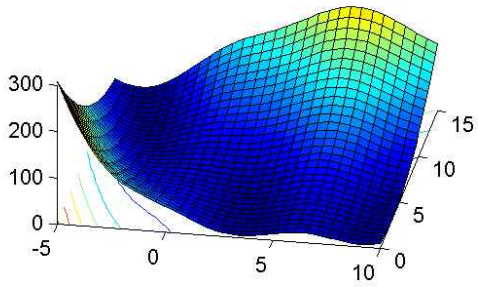
# CHAPTER 7. SURROGATE MODELING (OR RESPONSE SURFACE METHODOLOGY)

## 7.1 Introduction

Response surface methodology (RSM) is a collection of statistical and mathematical techniques useful for developing, improving, and optimizing processes. The most extensive applications of RSM are in the industrial world, particularly in situations where several input variables potentially influence some responses (e.g., performance measure or quality characteristic of the product or process). The input variables are called "independent variables", and they are subject to the control of the engineer or scientist, at least for purposes of a test or an experiment.



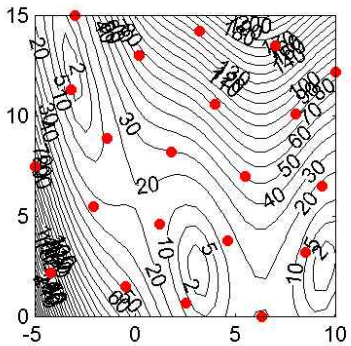




Figure in the side shows graphically the relationship between the response ($y$) and the two design variables (or independent control variables). To construct the response surface, there must be a systematic way of gathering response data in the design space. Two primary procedures are involved with collecting the response information: (1) Design of Experiment (DOE) and (2) Response Approximation (or Surrogate Modeling). The general procedure can be summarized as

Step 1. Choose design variables and response model(s) to be considered.
Step 2. Plan "Design of Experiments (DOE)" over a design space.
Step 3. Perform "experiments" or "simulation" at the DOE points.
Step 4. Construct a response surface over the design space.
Step 5. Determine a confidence interval of the response surface.
Step 6. Check the model adequacy over the design space.
Step 7. If not adequate, then go to step 1 and refine the model.

## 7.2 Design of Experiments (DOEs)

Design of experiments is the design of all information-gathering exercises where variation is present, whether under the full control of the experimenter or not. Often the experimenter is interested in the effect of some product or process parameters on some relevant responses, which may be product performances or process quality attributes. Design of experiments is thus a discipline that has very broad application across all the natural and social sciences, and various engineering.

In basic, it is concerned about how to gather the information as effective as possible. Thus, the objective of the DOE is to collect the information with minimal experimental cost and maximum model accuracy. The existing DOEs include:

1. (Two-level) Full factorial designs
2. (Two-level) Fractional factorial designs

3. Orthogonal designs (or arrays)
   3.a Box-Behnken designs
   3.b Koshal design
   3.c Hybrid design
   3.d Design optimality

7.3 Response Surface Methods (RSMs)

In general, suppose that the scientist or engineer is concerned with a product, process, or system involving a response $y$ that depends on the controllable input variables ($x_1$, $x_2$, ···,$x_n$). The relationship is

$$\hat{g} = f\left(x_1, x_2, \cdots, x_n\right) + \varepsilon\left(x_1, x_2, \cdots, x_n\right) \tag{88}$$

where the form of the true response function $f$ is unknown and perhaps very complicated, and $\varepsilon$ is a term that represents other sources of variability not accounted for in $f$. Thus, $\varepsilon$ includes errors in measurement, regression (or interpolation), numerical noise, etc.

7.3.1 Least Squares (LS) Method

The LS approximation can be formulated as

$$\hat{g}(\mathbf{x}) = \sum_{i=1}^{NB} h_i(\mathbf{x}) a_i \equiv \mathbf{h}^T(\mathbf{x})\mathbf{a}, \quad \mathbf{x} \in R^{ND} \tag{89}$$

where $NB$ is the number of terms in the basis, $ND$ is the number of elements in the union set of both design and random parameters, $\mathbf{h}$ is the basis functions, and $\mathbf{a}$ is the LS coefficient vector. Mutually independent functions must be used in a basis.

A global LS approximation at $\mathbf{x}_I$ can be expressed as

$$\hat{g}(\mathbf{x}_I) = \sum_{i=1}^{NB} h_i(\mathbf{x}_I) a_i = \mathbf{h}^T(\mathbf{x}_I)\mathbf{a}, \quad I = 1, \cdots, NS \tag{90}$$

where $NS$ is the number of sample points and $\mathbf{x}_I$ is a given sample point. The coefficients $a_i$ are obtained by performing a least squares fit for the global approximation, which is obtained by minimizing the difference between the global approximation and exact response at the set of given sample points. This yields the quadratic form

$$\begin{aligned} E &= \sum_{I=1}^{NS} \left[\hat{g}(\mathbf{x}_I) - g(\mathbf{x}_I)\right]^2 \\ &= \sum_{I=1}^{NS} \left[\sum_{i=1}^{NB} h_i(\mathbf{x}_I) a_i - g(\mathbf{x}_I)\right]^2 \end{aligned} \tag{91}$$

Equation above can be rewritten in a matrix form as

$$E = \left[\mathbf{H}\mathbf{a} - \mathbf{g}\right]^T \left[\mathbf{H}\mathbf{a} - \mathbf{g}\right] \tag{92}$$

where

$$\mathbf{g} = \begin{bmatrix} g(\mathbf{x}_1) & g(\mathbf{x}_2) & \cdots & g(\mathbf{x}_{NS}) \end{bmatrix}^T,$$
$$\mathbf{a} = \begin{bmatrix} a_1 & a_2 & \cdots & a_{NS} \end{bmatrix}^T, \text{ and} \tag{93}$$
$$\mathbf{H} = \begin{bmatrix} h_1(\mathbf{x}_1) & h_2(\mathbf{x}_1) & \cdots & h_{NB}(\mathbf{x}_1) \\ h_1(\mathbf{x}_2) & h_2(\mathbf{x}_2) & \cdots & h_{NB}(\mathbf{x}_2) \\ \vdots & \vdots & \ddots & \vdots \\ h_1(\mathbf{x}_{NS}) & h_2(\mathbf{x}_{NS}) & \cdots & h_{NB}(\mathbf{x}_{NS}) \end{bmatrix}$$

To find the coefficients **a**, the extreme of the square error $E(\mathbf{x})$ can be obtained by

$$\frac{\partial E}{\partial \mathbf{a}} = \mathbf{H}^T\mathbf{H}\mathbf{a} - \mathbf{H}^T\mathbf{g} = 0 \tag{94}$$

where **H** is referred to as the basis matrix. The coefficient vector in Eq. (89) is represented by

$$\mathbf{a} = \left(\mathbf{H}^T\mathbf{H}\right)^{-1}\mathbf{H}^T\mathbf{g} \tag{95}$$

By substituting Eq. (95) into Eq. (89), the approximation $\hat{g}(\mathbf{x})$ can then be expressed as

$$\begin{aligned} \hat{g}(\mathbf{x}) &= \mathbf{h}^T(\mathbf{x})\mathbf{a} \\ &= \mathbf{h}^T(\mathbf{x})\left(\mathbf{H}^T\mathbf{H}\right)^{-1}\mathbf{H}^T\mathbf{g} \end{aligned} \tag{96}$$

Read Chapter 2 in the reference book, Response Surface Methodology, written by Raymond H. Myers and Douglas C. Montgomery.

### 7.3.2 Moving Least Squares (MLS) Method

The MLS approximation can be formulated as

$$\hat{g}(\mathbf{x}) = \sum_{i=1}^{NB} h_i(\mathbf{x})a_i(\mathbf{x}) \equiv \mathbf{h}^T(\mathbf{x})\mathbf{a}(\mathbf{x}), \quad \mathbf{x} \in R^{ND} \tag{97}$$

where *NB* is the number of terms in the basis, *ND* is the number of elements in the union set of both design and random parameters, **h** is the basis functions, and **a**(**x**) is the MLS coefficient vector, which as indicated, is a function of the design parameter **x**. Mutually independent functions must be used in a basis. Any function included in the basis can be exactly reproduced using MLS approximation, which is characterized as a consistency.

Lancaster and Salkauskas (1986) defined a local approximation at $\mathbf{x}_I$ by

$$\hat{g}(\mathbf{x}, \mathbf{x}_I) = \sum_{i=1}^{NB} h_i(\mathbf{x}_I)a_i(\mathbf{x}) = \mathbf{h}^T(\mathbf{x}_I)\mathbf{a}(\mathbf{x}), \quad I = 1, \cdots, NS \tag{98}$$

where *NS* is the number of sample points and $\mathbf{d}_I$ is a given sample point. The coefficients $a_i(\mathbf{x})$ are obtained by performing a weighted least squares fit for the local approximation, which is obtained by minimizing the difference between the local approximation and exact response at the set of given sample points. This yields the quadratic form

$$E(\mathbf{x}) = \sum_{I=1}^{NS} w(\mathbf{x}-\mathbf{x}_I)\left[\hat{g}(\mathbf{x},\mathbf{x}_I) - g(\mathbf{x}_I)\right]^2 = \sum_{I=1}^{NS} w(\mathbf{x}-\mathbf{x}_I)\left[\sum_{i=1}^{NB} h_i(\mathbf{x}_I)a_i(\mathbf{x}) - g(\mathbf{x}_I)\right]^2 \tag{99}$$

where $w(\mathbf{x}-\mathbf{x}_I)$ is a weight function with a compact support. An appropriate support size for the weight function at any data point $\mathbf{x}_I$ must be selected so that a large enough number of neighboring data points is included to avoid a singularity. A variable weight over the compact support furnishes a local averaging property of the response.

Equation (99) can be rewritten in a matrix form as

$$E(\mathbf{x}) = \left[\mathbf{H}\mathbf{a}(\mathbf{x}) - \mathbf{g}\right]^T \mathbf{W}(\mathbf{x})\left[\mathbf{H}\mathbf{a}(\mathbf{x}) - \mathbf{g}\right] \tag{100}$$

where

$$\mathbf{g} = \begin{bmatrix} g(\mathbf{x}_1) & g(\mathbf{x}_2) & \cdots & g(\mathbf{x}_{NS}) \end{bmatrix}^T,$$
$$\mathbf{a}(\mathbf{x}) = \begin{bmatrix} a_1 & a_2 & \cdots & a_{NS} \end{bmatrix}^T, \quad \text{and} \tag{101}$$
$$\mathbf{H} = \begin{bmatrix} h_1(\mathbf{x}_1) & h_2(\mathbf{x}_1) & \cdots & h_{NB}(\mathbf{x}_1) \\ h_1(\mathbf{x}_2) & h_2(\mathbf{x}_2) & \cdots & h_{NB}(\mathbf{x}_2) \\ \vdots & \vdots & \ddots & \vdots \\ h_1(\mathbf{x}_{NS}) & h_2(\mathbf{x}_{NS}) & \cdots & h_{NB}(\mathbf{x}_{NS}) \end{bmatrix}$$

and

$$\mathbf{W}(\mathbf{x}) = \begin{bmatrix} w(D_1 = |\mathbf{x}-\mathbf{x}_1|) & 0 & \cdots & 0 \\ 0 & w(D_2 = |\mathbf{x}-\mathbf{x}_2|) & \cdots & 0 \\ \vdots & \vdots & \ddots & \vdots \\ 0 & 0 & \cdots & w(D_{NS} = |\mathbf{x}-\mathbf{x}_{NS}|) \end{bmatrix} \tag{102}$$

To find the coefficients $\mathbf{a}(\mathbf{d})$, the extreme of the weighted square error $E(\mathbf{x})$ can be obtained by

$$\frac{\partial E(\mathbf{x})}{\partial \mathbf{a}(\mathbf{x})} = \mathbf{M}(\mathbf{x})\mathbf{a}(\mathbf{x}) - \mathbf{B}(\mathbf{x})\mathbf{g} = 0 \tag{103}$$

where $\mathbf{M}(\mathbf{x})$ is referred to as the moment matrix, and is given by

$$\mathbf{M}(\mathbf{x}) = \mathbf{H}^T\mathbf{W}(\mathbf{x})\mathbf{H} \quad \text{and} \quad \mathbf{B}(\mathbf{x}) = \mathbf{H}^T\mathbf{W}(\mathbf{x}) \tag{104}$$

The coefficient vector in Eq. (97) is represented by

$$\mathbf{a}(\mathbf{x}) = \mathbf{M}^{-1}(\mathbf{x})\mathbf{B}(\mathbf{x})\mathbf{g} \tag{105}$$

By substituting Eq. (105) into Eq. (97), the approximation $\hat{g}(\mathbf{x})$ can then be expressed as

$$\begin{aligned}\widehat{g}(\mathbf{x}) &= \mathbf{h}^T(\mathbf{x})\mathbf{a}(\mathbf{x}) \\ &= \mathbf{h}^T(\mathbf{x})\mathbf{M}^{-1}(\mathbf{x})\mathbf{B}(\mathbf{x})\mathbf{g}\end{aligned} \tag{106}$$

In this study, the modified form of the original **exponential weight function**, $w(D_I) = e^{-\alpha D_I^2}/2$, is proposed to yield the form

$$w(D_I(\mathbf{x})) = \begin{cases} \dfrac{1}{2}\dfrac{\left(e^{-\alpha D_I^2} - e^{-\alpha}\right)^2}{1-e^{-\alpha}} & \text{for } D_I \le 1 \\ 0 & \text{for } D_I > 1 \end{cases}$$
$$D_I(\mathbf{x}) = \left|\mathbf{x} - \mathbf{x}_I\right|$$

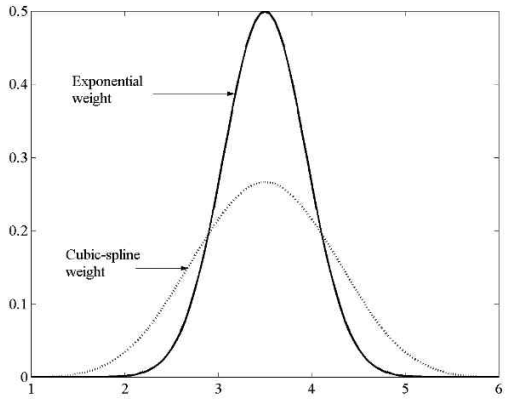
in order to possess $C^1$ continuity. The parameter $\alpha$ determines the localizing magnitude of the weight function. As parameter $\alpha$ decreases, exponential weighting possesses more localizing characteristics, since it approaches the Dirac delta function with an unchanged support. The appropriate localizing parameter is selectively suggested in the range $\alpha$=8~12.

The **cubic-spline weight function**, which is a $C^2$-function, is expressed in the form

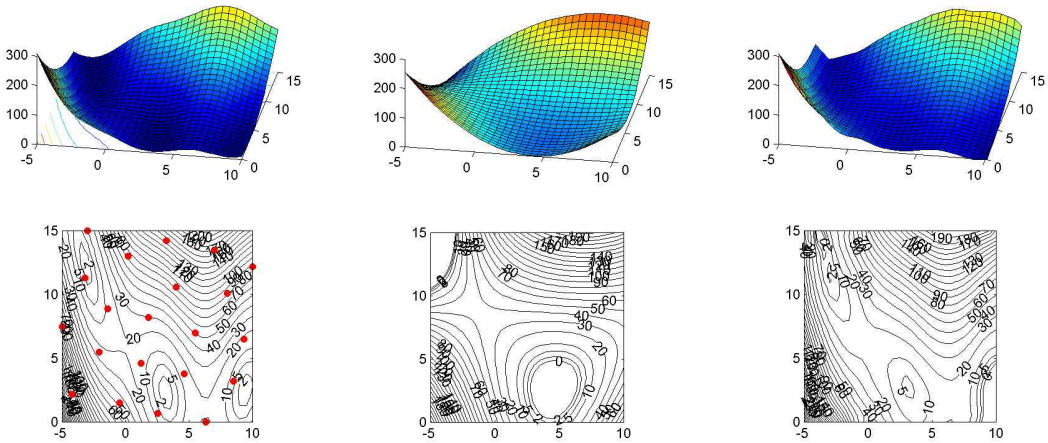
$$w(D_I) = \begin{cases} \frac{2}{3} - 4D_I^2 + 4D_I^3 & \text{for } 0 \le D_I \le \frac{1}{2} \\ \frac{4}{3} - 4D_I + 4D_I^2 - \frac{4}{3}D_I^3 & \text{for } 0 \le D_I \le \frac{1}{2} \\ 0 & \text{for } D_I \ge 1 \end{cases}$$
$$D_I(\mathbf{x}) = \left|\mathbf{x} - \mathbf{x}_I\right|$$

Exponential and cubic-spline weight functions are comparatively plotted in Figure below. In comparison, the cubic-spline function possesses less localizing and greater averaging features over the compactly supported subdomain. Hence, the approximation is evenly accurate.

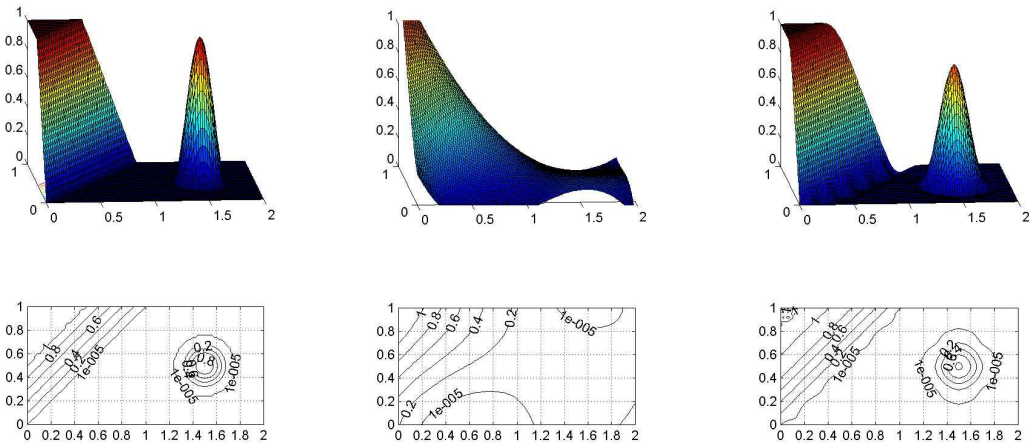



Exponential Weight ($\alpha$=8) and Cubic-Spline Weight (s=2.5) Functions



( a ) Exact Response ( b ) Using LS Method ( c ) Using MLS Method

Response Surface Approximation for Branin Response



( a ) Exact Response ( b ) Using LS Method ( c ) Using MLS Method

Response Surface Approximation for Severe Response

### 7.3.3 Kriging Method

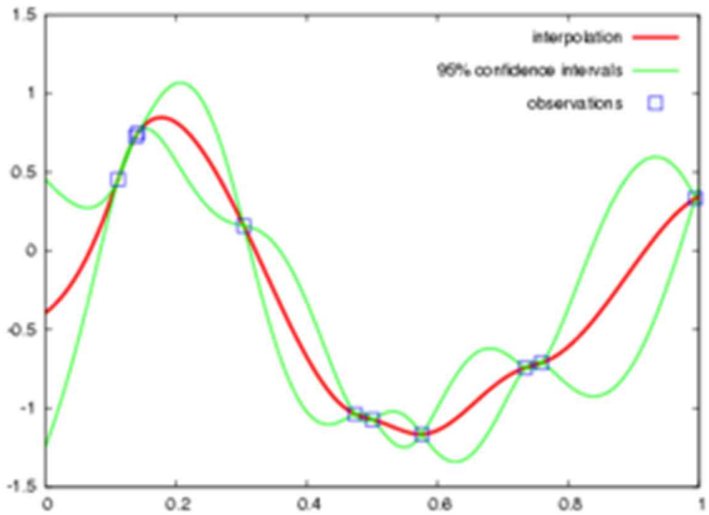
Kriging belongs to the family of nonlinear least squares estimation algorithms. As illustrated in Figure below, the aim of kriging is to estimate the value of an unknown real-valued function, $g$, at a point, $\mathbf{x}^*$, given the values of the function at some other points, $x_1$, ..., $x_{NS}$. A kriging estimator is said to be *linear* because the predicted value $\hat{g}(\mathbf{x})$ is a linear combination that may be written as

$$\hat{g}(\mathbf{x}) = \sum_{I=1}^{NS} w(D_I(\mathbf{x}))g(\mathbf{x}_I) \quad \text{where } D_I(\mathbf{x}) = \|\mathbf{x} - \mathbf{x}_I\|$$

The weights $w_i(D)$ are solutions of a system of linear equations which is obtained by assuming that $g$ is a sample-path of a *random process* $G(\mathbf{x})$, and that the error of prediction

$$\varepsilon(\mathbf{x}) = G(\mathbf{x}) - \sum_{I=1}^{NS} w(D_I(\mathbf{x}))g(\mathbf{x}_I)$$

is to be minimized in some sense. For instance, the so-called *simple kriging* assumption is that the mean and the covariance of $G(\mathbf{x})$ is known and then, the kriging predictor is the one that minimizes the variance of the prediction error.




Other advanced RSM techniques include “radial basis function”, “support vector machine”, “relevance vector machine”, “polynomial chaos expansion”, “stochastic collocation method”, etc.

Advantages of RSM:

1. Sensitivity (or derivative) of system performances with respect to design variables can be obtained based on the approximate responses.

2. No need to construct an interface between design optimization and engineering analysis.
3. Graphical method can be used for design optimization.

Disadvantages of RSM:

1. A curse of dimensionality
2. Accuracy of an approximate response surface and its derivative is of greatest concern.
3. It may lead to a wrong solution although it is more convenient.