Introductory Course: Using LS-OPT® on the TRACC Cluster

January 20-21, 2010

By:

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Hubert Ley, PhD

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Layout of the workshop

Day 1

1. Welcome to TRACC (Ron Kulak)
2. Introduction to Response Surface Methodology (Cezary Bojanowski)
3. Introduction to Optimization Theory (Vadim Sokolov)

Lunch break 12:30 PM – 1:30 PM

4. Introduction to LS-OPT GUI (Cezary Bojanowski)
5. Running LS-OPT on TRACC cluster (Cezary Bojanowski)
6. Design Optimization (Cezary Bojanowski)

Layout of the workshop

Day 2

1. Best Practices on TRACC Cluster (Hubert Ley)
2. User defined solver – Perl or OCTAVE (Cezary Bojanowski)
3. Multiobjective Optimization (Cezary Bojanowski)
4. Parameter Identification (Cezary Bojanowski)

Lunch break 12:30 PM – 1:30 PM

5. Probabilistic Analysis (Ron Kulak)
6. Reliability Based Design Optimization (Cezary Bojanowski)

Introductory Course: Using LS-OPT® on the TRACC Cluster

1.2a - Introduction to Response Surface Methodology

By: Cezary Bojanowski, PhD

Outline of the Presentation

- Introduction
- Steps in Constructing Response Surface
- Other Metamodels
- Strategies for Metamodel-Based Optimization
- Design of Experiments
- Analysis of Metamodeling Errors
- Sensitivity Study
- Summary

Introduction

- Response surface methodology (RSM) is a collection of statistical and mathematical techniques useful for developing, improving and optimizing processes.

- The underlying true response is driven by some unknown physical mechanism. In most practical situations it is only know for finite number of discrete sets of input variables.

- In the response surface methodology an approximate response is built based on polynomial approximations.

Advantages

- Response surface smoothes the design response, thus it stabilizes the solution.
- Response surfaces spanned over small regions allow for accurate designs.
- For the optimization process response surface methodology does not require analytical derivatives of the true response. Derivatives of the approximate response based on polynomials are easy to compute.
- Most applicable to the cases where multiple input variables (design variables) potentially influence some performance measure or quality characteristic of a product or a process (response).

RSM – linear regression models

- The observed data are used to approximate the real response by some empirical model.

- The unknown response is a function of design variables:

$$y = \eta(x)$$

- If it is dependent on two design variables, it can be approximated by first-order response surface model:

$$y = \beta_0 + \beta_1 x_1 + \beta_2 x_2 + \varepsilon$$

- In general the response y can be related to k regressor variables and can be approximated by a multiple linear regression model as:

$$y = \beta_0 + \beta_1 x_1 + \beta_2 x_2 + \ldots + \beta_k x_k + \varepsilon$$

RSM – linear regression models

- Linear model with interaction term yields nonlinear response surface

$$y = \beta_0 + \beta_1 x_1 + \beta_2 x_2 + \beta_{12} x_1 x_2 + \varepsilon$$

- Second order response surface model in two variables:

$$y = \beta_0 + \beta_1 x_1 + \beta_2 x_2 + \beta_{11} x_1^2 + \beta_{22} x_2^2 + \beta_{12} x_1 x_2 + \varepsilon$$

- Any regression model that is linear in the parameters is a linear regression model regardless of the shape of the response surface it generates.

$$x_3 = x_1^2, x_4 = x_2^2, x_5 = x_1 x_2 \qquad \beta_3 = \beta_{11}, \beta_4 = \beta_{22}, \beta_5 = \beta_{12}$$

$$y = \beta_0 + \beta_1 x_1 + \beta_2 x_2 + \beta_3 x_3 + \beta_4 x_4 + \beta_5 x_5 + \varepsilon$$

Estimation of the Parameters in Linear Regression Models

- If the response is known at *n* points, the model equation can be written as:

$$y_i = \beta_0 + \beta_1 x_{i1} + \beta_2 x_{i2} + \ldots + \beta_k x_{ik} + \varepsilon_i$$

$$y_i = \beta_0 + \sum_{j=1}^{k} \beta_j x_{ij} + \varepsilon_i$$

$$i = 1,2\ldots n \qquad n > k+1$$

- The least squares function is:

$$L = \sum_{i=1}^{n} \varepsilon_i^2 = \sum_{i=1}^{n} \left(y_i - \beta_0 - \sum_{j=1}^{k} \beta_j x_{ij} \right)^2$$

Estimation of the Parameters in Linear Regression Models

- In matrix notation the model equation is given as:

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

- The function of least squares:

$$L = \sum_{i=1}^{n} \varepsilon_i^2 = \boldsymbol{\varepsilon}'\boldsymbol{\varepsilon} = (\mathbf{y} - \mathbf{X}\boldsymbol{\beta})'(\mathbf{y} - \mathbf{X}\boldsymbol{\beta})$$

$$L = \mathbf{y}'\mathbf{y} - 2\boldsymbol{\beta}'\mathbf{X}'\mathbf{y} + \boldsymbol{\beta}'\mathbf{X}'\mathbf{X}\boldsymbol{\beta}$$

- To minimize the L function, the least square estimators must satisfy:

$$\left.\frac{\partial L}{\partial \boldsymbol{\beta}}\right|_{\mathbf{b}} = -2\mathbf{X}'\mathbf{y} + 2\mathbf{X}'\mathbf{X}\mathbf{b} = 0$$

Estimation of the Parameters in Linear Regression Models

- ... which simplifies to the least squares normal equations in matrix form:

$$\mathbf{X}'\mathbf{X}\mathbf{b} = \mathbf{X}'\mathbf{y}$$

- Thus, the least squares estimator of $\boldsymbol{\beta}$ is:

$$\mathbf{b} = \left(\mathbf{X}'\mathbf{X}\right)^{-1}\mathbf{X}'\mathbf{y}$$

- And the fitted regression model is:

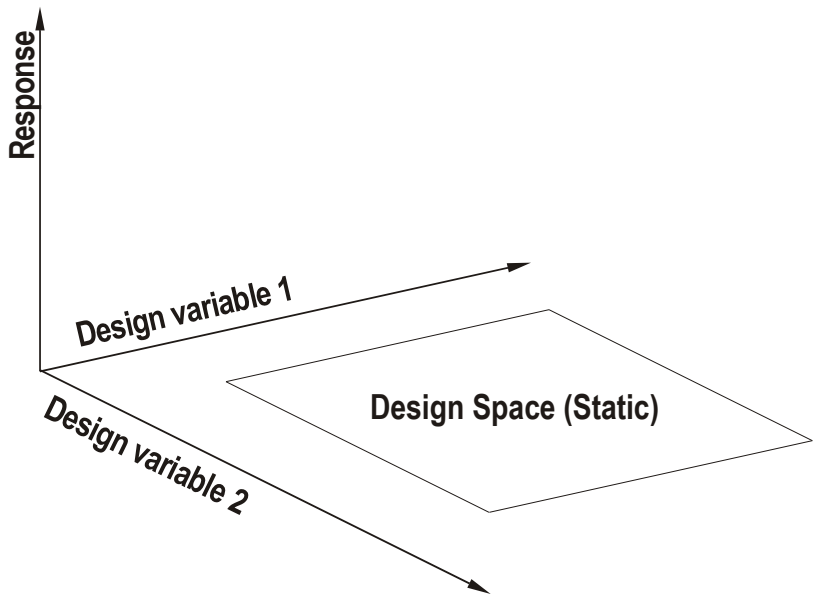
$$\hat{\mathbf{y}} = \mathbf{X}\mathbf{b}$$

- The difference between the observation and the fitted value is a residual:

$$\mathbf{e} = \mathbf{y} - \hat{\mathbf{y}}$$

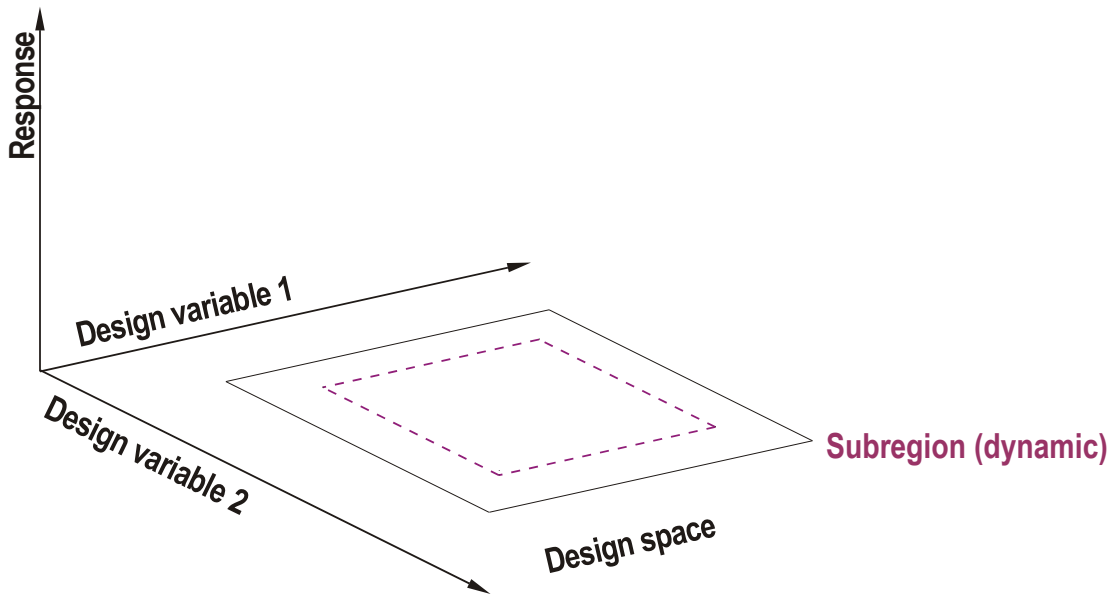
Response Surface Methodology - Design Cycle

Step 1: Define design space



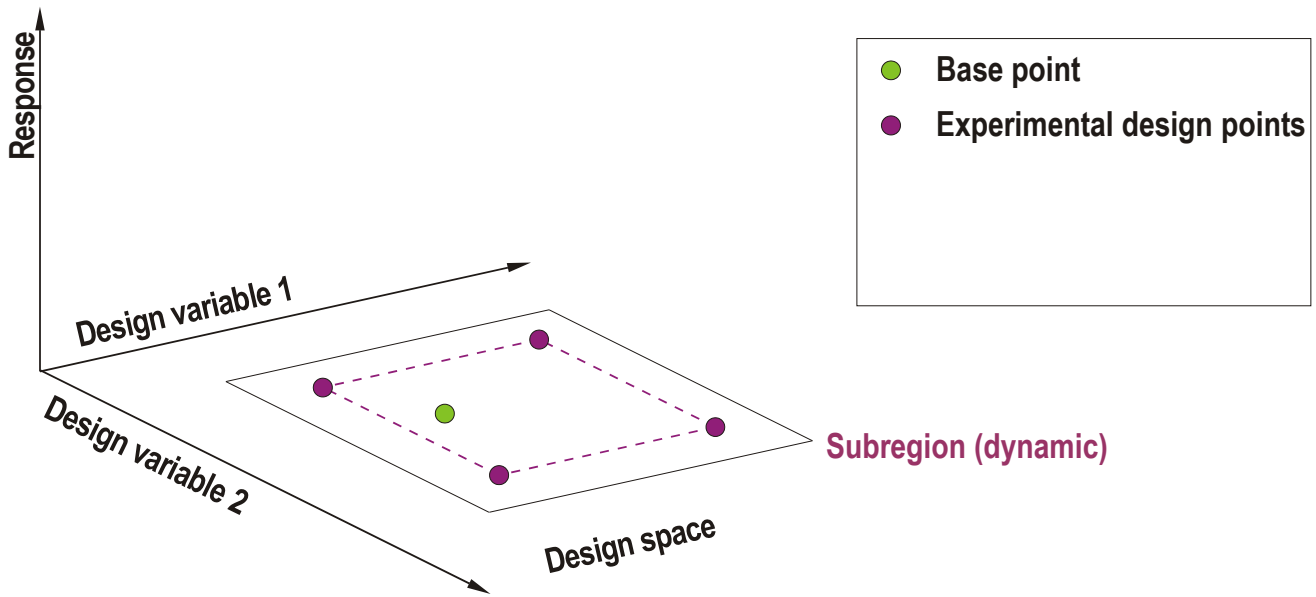
Response Surface Methodology - Design Cycle

Step 2: Define initial region of interest



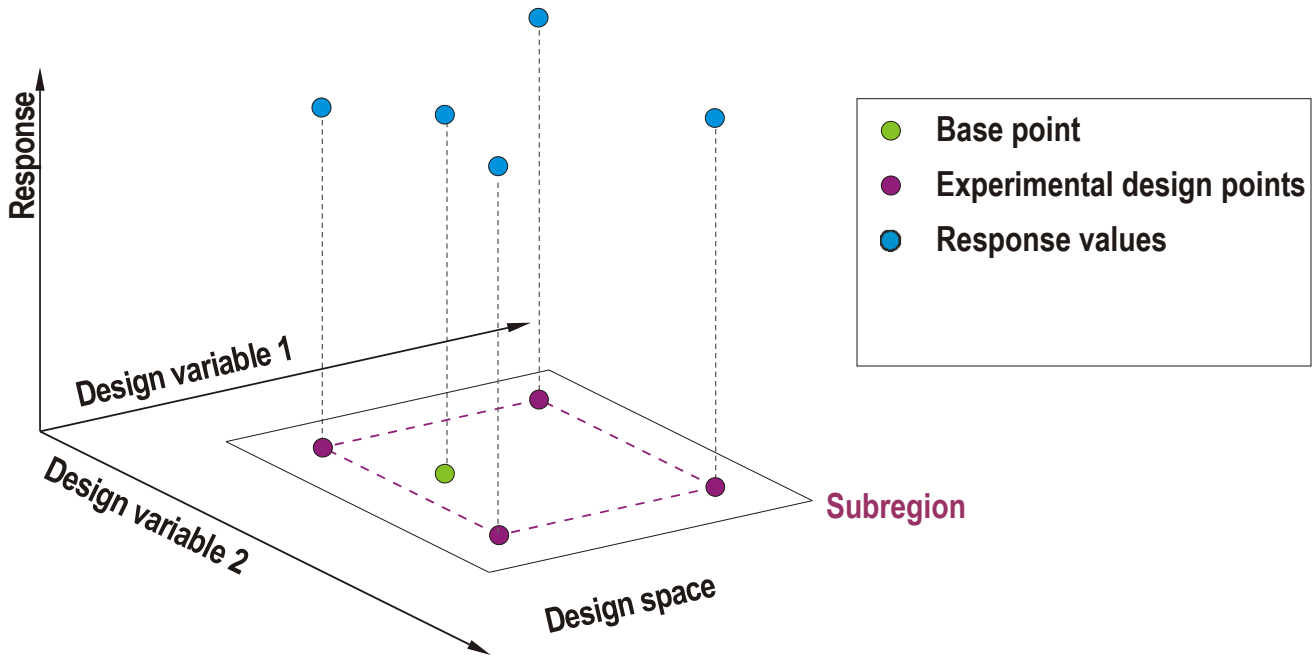
Response Surface Methodology - Design Cycle

Step 3: Perform Design of Experiments



Response Surface Methodology - Design Cycle

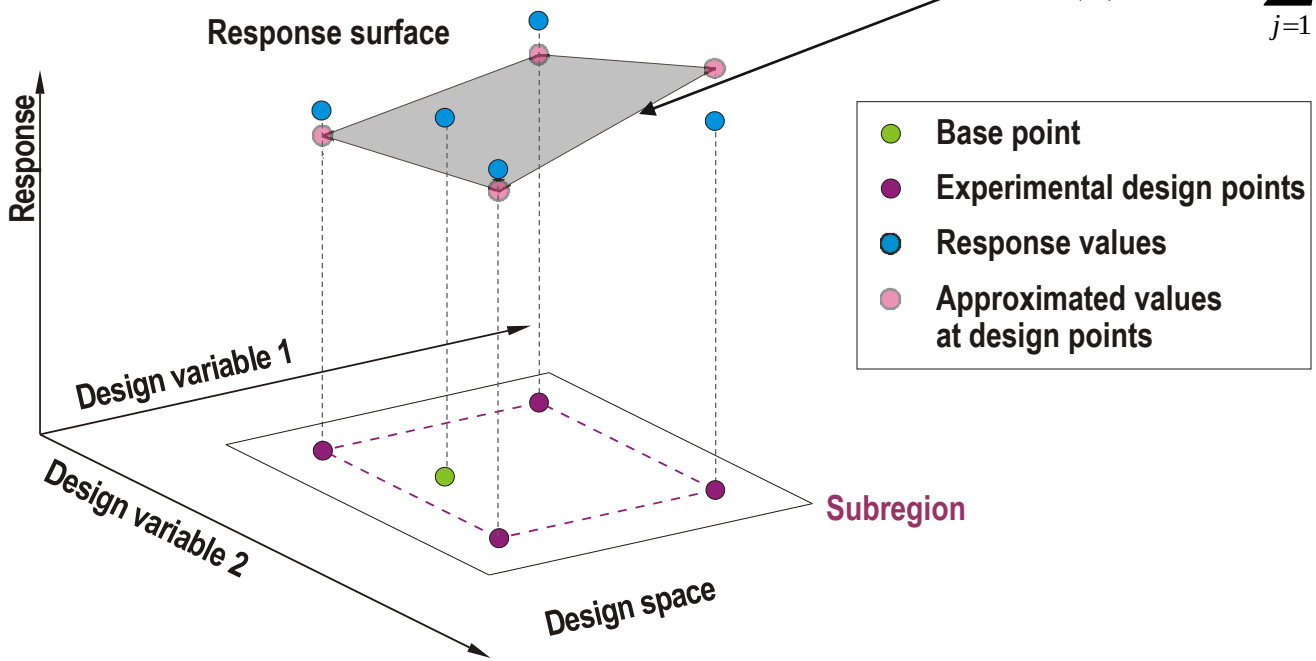
Step 4: Compute response – LS-DYNA simulations



Response Surface Methodology - Design Cycle

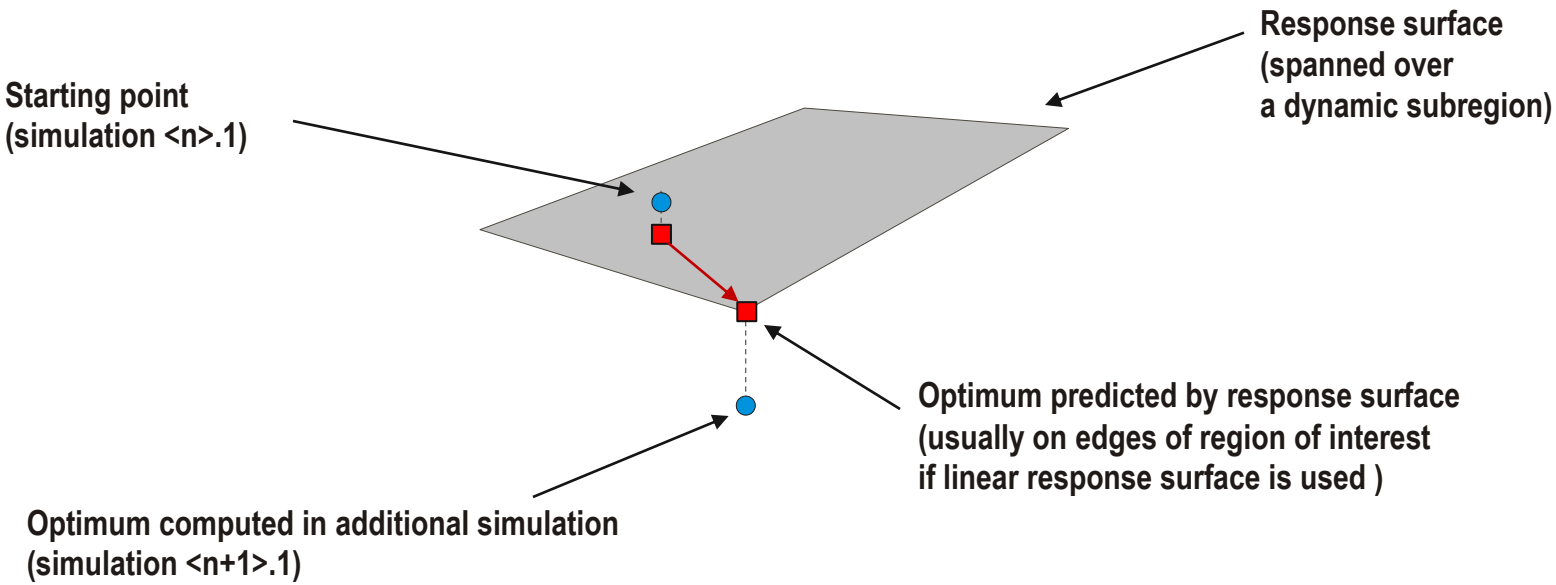
Step 5: Build response surface

$$f(x) = \beta_0 + \sum_{j=1}^{k} \beta_j \phi_j(x)$$



Response Surface Methodology - Design Cycle

Step 6: Optimize



RSM Linear vs. Quadratic Approximation

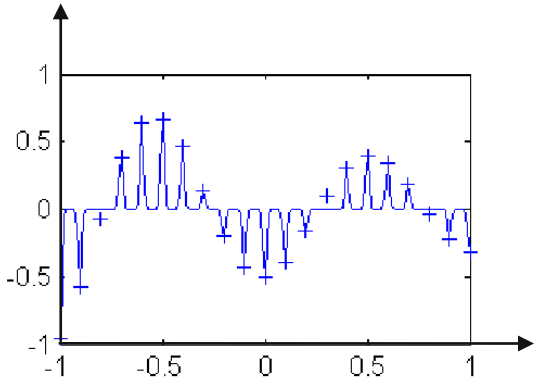
- First order polynomials
  - The most basic approximation
  - The most inexpensive one
  - Often oscillations occur when used for SRSM
  - Nonetheless, are recommended for sequential approximations for optimization
  - Cost is proportional to number of design variables (n)

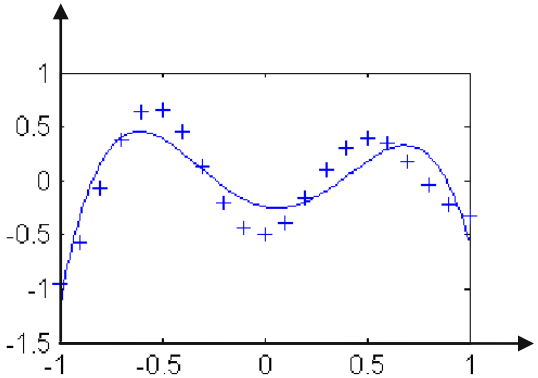
- Second order polynomials
  - More accurate
  - More expensive – cost is proportional to n^2

- Both good only for local approximations

Radial Basis Function Networks for Global Approximations

- Accuracy of polynomial models may be not enough for global approximations
- Networks based metamodels can be built for any number of simulation runs
- Network based metamodels can be locally refined maintaining global relevance
- NN's and RBFN's can have high accuracy but overfitting may occur





Response Surface Methodology vs. Networks

Response Surface	Networks
regression model	network
estimation	learning
approximation	generalization
observations	training set
parameters	weights
independent variables	inputs
dependent variables	outputs

Radial Basis Function Network

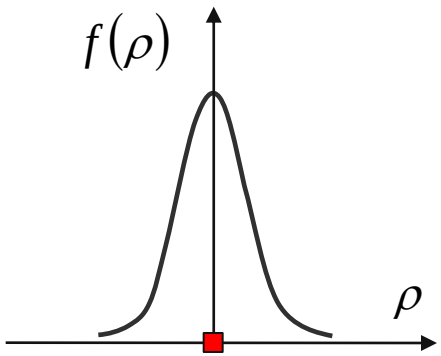
- Linear output layer:

Number of basis functions

$$y(x,a) = a_0 + \sum_{h=1}^{H} a_h \cdot f(\rho_h)$$

bias weights

- Hidden layer (basis function):



$$f(\rho_h) = e^{-\rho_h}$$

$$\rho_h = \frac{\sum_{k=1}^{K} (x_k - X_{hk})^2}{2\sigma_h^2}$$

- Center:

$$\boldsymbol{X}_h = (X_{h1}, \ldots, X_{hk})$$

Center location in K dimensional space

Radial Basis Function Network

- Linear output layer:

Number of basis functions

$$y(x,a) = a_0 + \sum_{h=1}^{H} a_h \cdot f(\rho_h)$$

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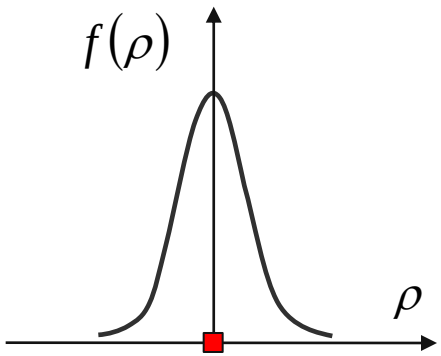
- Hidden layer (basis function):



$$f(x) = ae^{-\frac{(x-b)^2}{2c^2}}$$

a – Height of the peak

b – Position of center

c – Controls the width of the “bell”

- Center:

$$\boldsymbol{X}_h = (X_{h1}, \ldots, X_{hk})$$

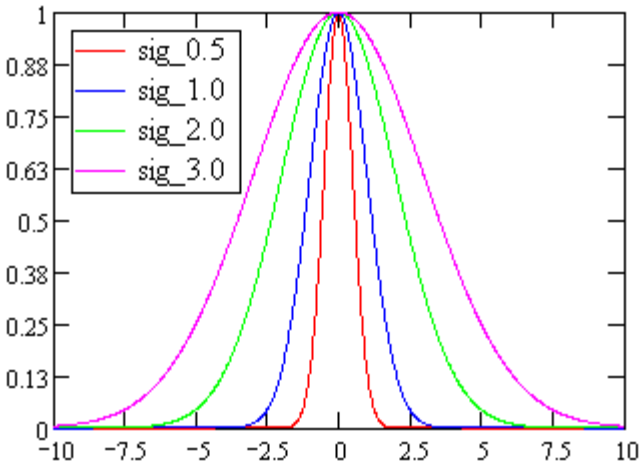
Center location in K dimensional space

Radial Basis Function Network - Basis Functions

Gaussian function:

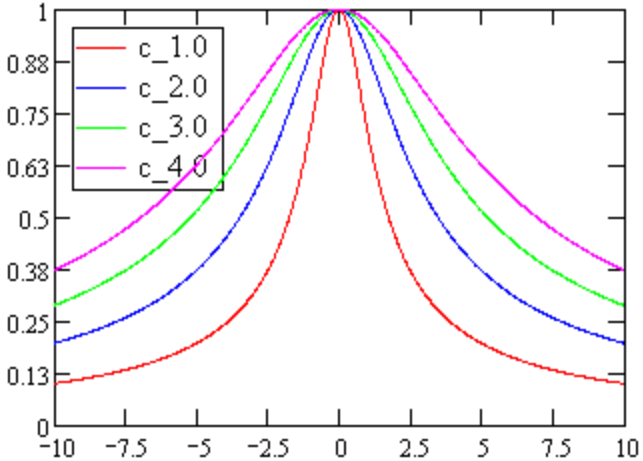
$$f(\rho_h) = e^{-\rho_h} \qquad \rho_h = \frac{\sum_{k=1}^{K}(x_k - X_{hk})^2}{2\sigma_h^2}$$

$$\phi(r) = e^{-\frac{r^2}{2\sigma^2}} \qquad \sigma > 0 \qquad r = \sum_{k=1}^{K}(x_k - X_{hk})^2$$



Inverse multiquadratic function:

$$\phi(r) = \frac{c}{\sqrt{r^2 + c^2}} \qquad c > 0$$



Radial Basis Function Network - Learning

- Polynomial based response surface:

$$\sum_{i=1}^{P}\left\{\left[y_i(x)-f_i(x)\right]^2\right\}=\sum_{i=1}^{P}\left\{\left[y_i(x)-\sum_{j=1}^{L}b_j\phi_j(x)\right]^2\right\}$$

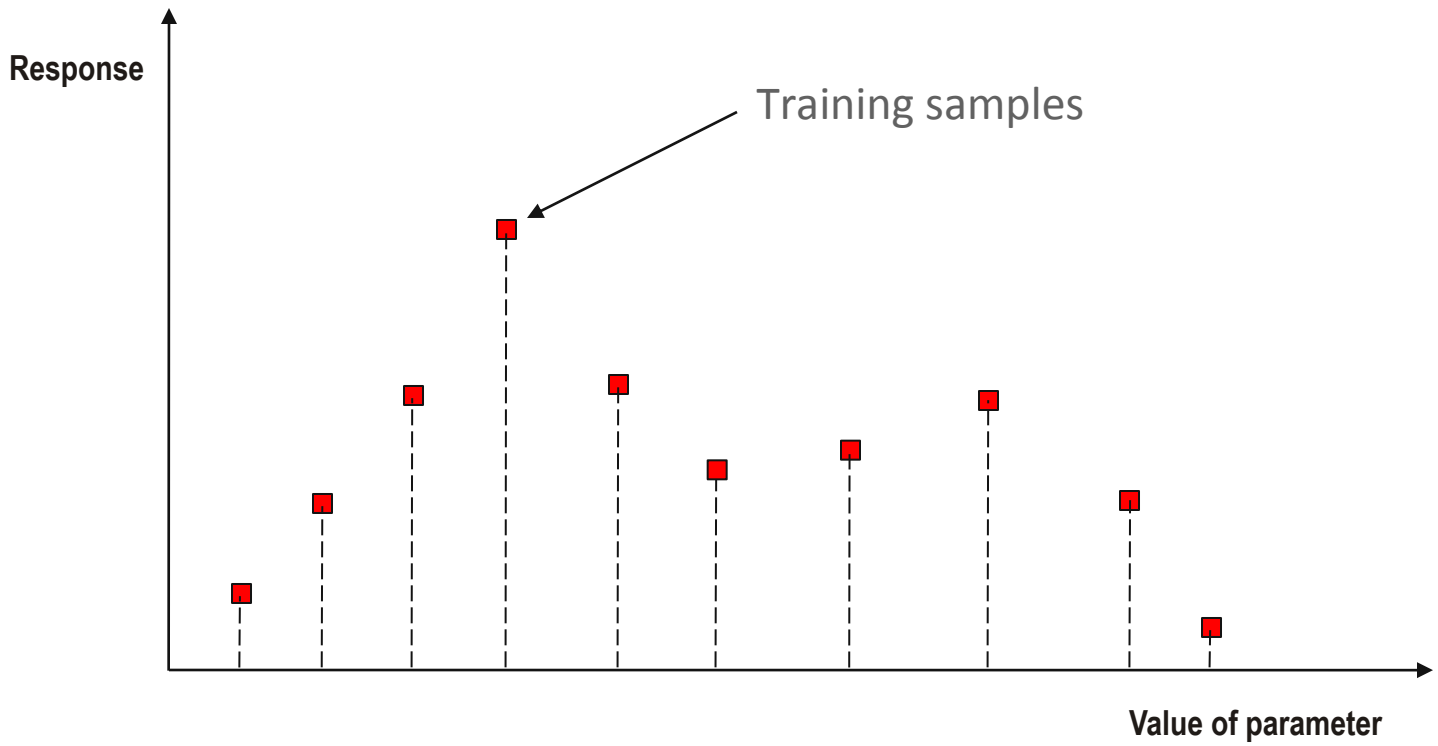
Minimize error to get approximate values of b

- Radial basis function network:

$$\sum_{i=1}^{P}\left\{\left[y_i(x)-f_i(x)\right]^2\right\}=\sum_{i=1}^{P}\left\{\left[y_i(x)-\left(a_0+\sum_{h=1}^{H}a_h\cdot f(\rho_h)\right)\right]^2\right\}$$

Minimize error to get approximate values of a

Construction of Radial Basis Function Network

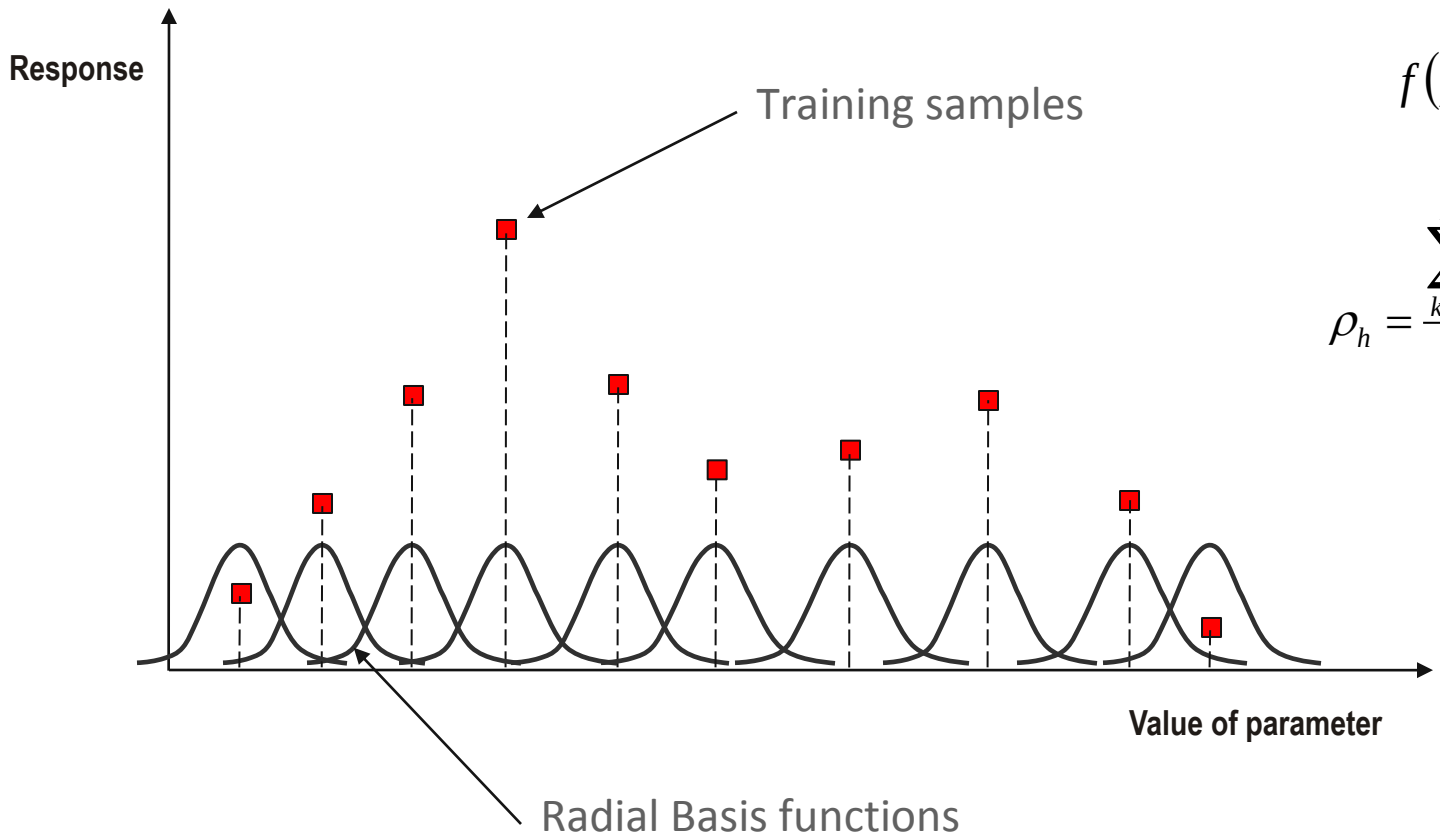


Construction of Radial Basis Function Network

$$y(x,a) = a_0 + \sum_{h=1}^{H} a_h \cdot f(\rho_h)$$

$$f(\rho) = e^{-\rho}$$

$$\rho_h = \frac{\sum_{k=1}^{K} (x_k - X_{hk})^2}{2\sigma_h^2}$$



Construction of Radial Basis Function Network

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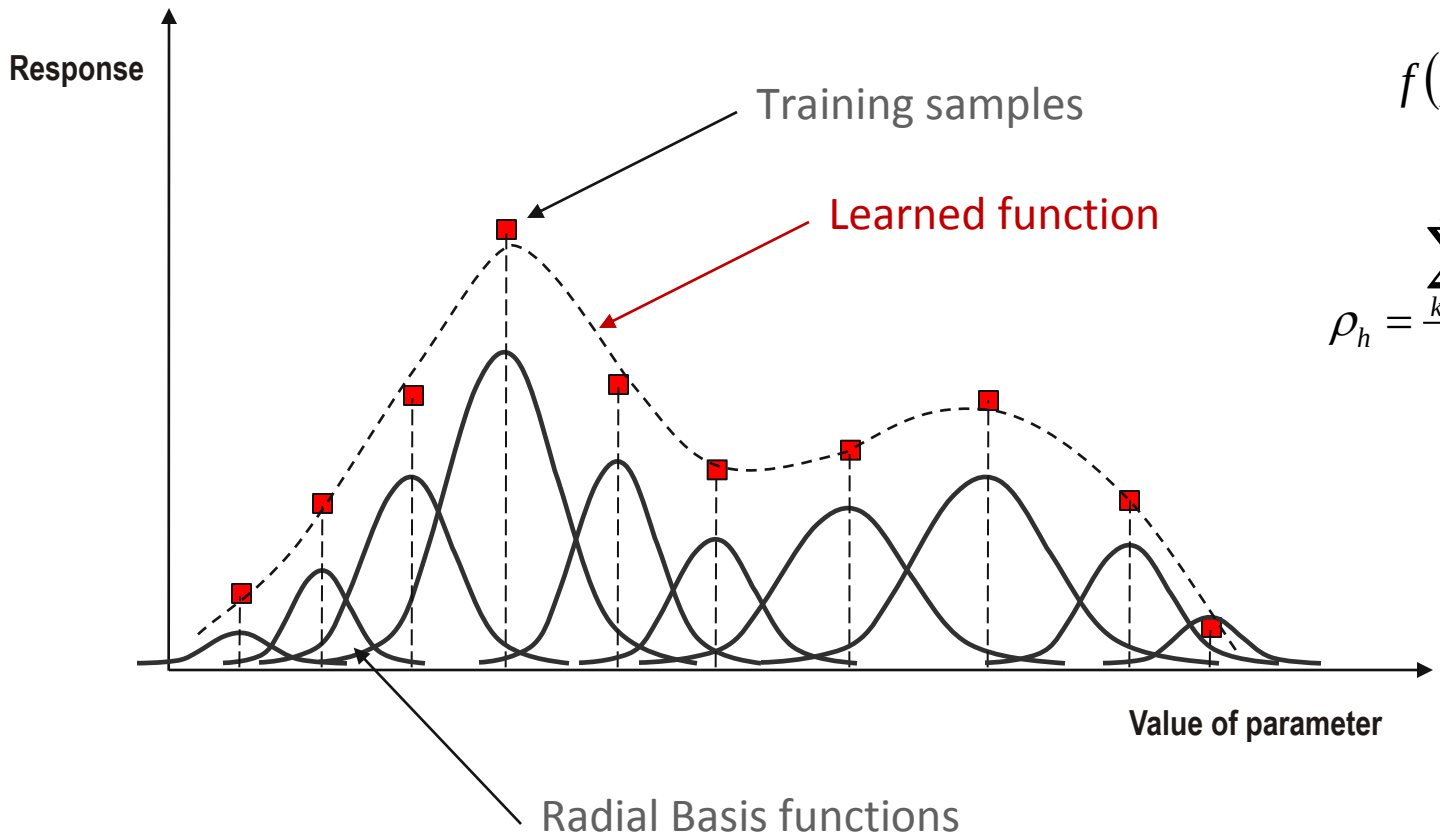
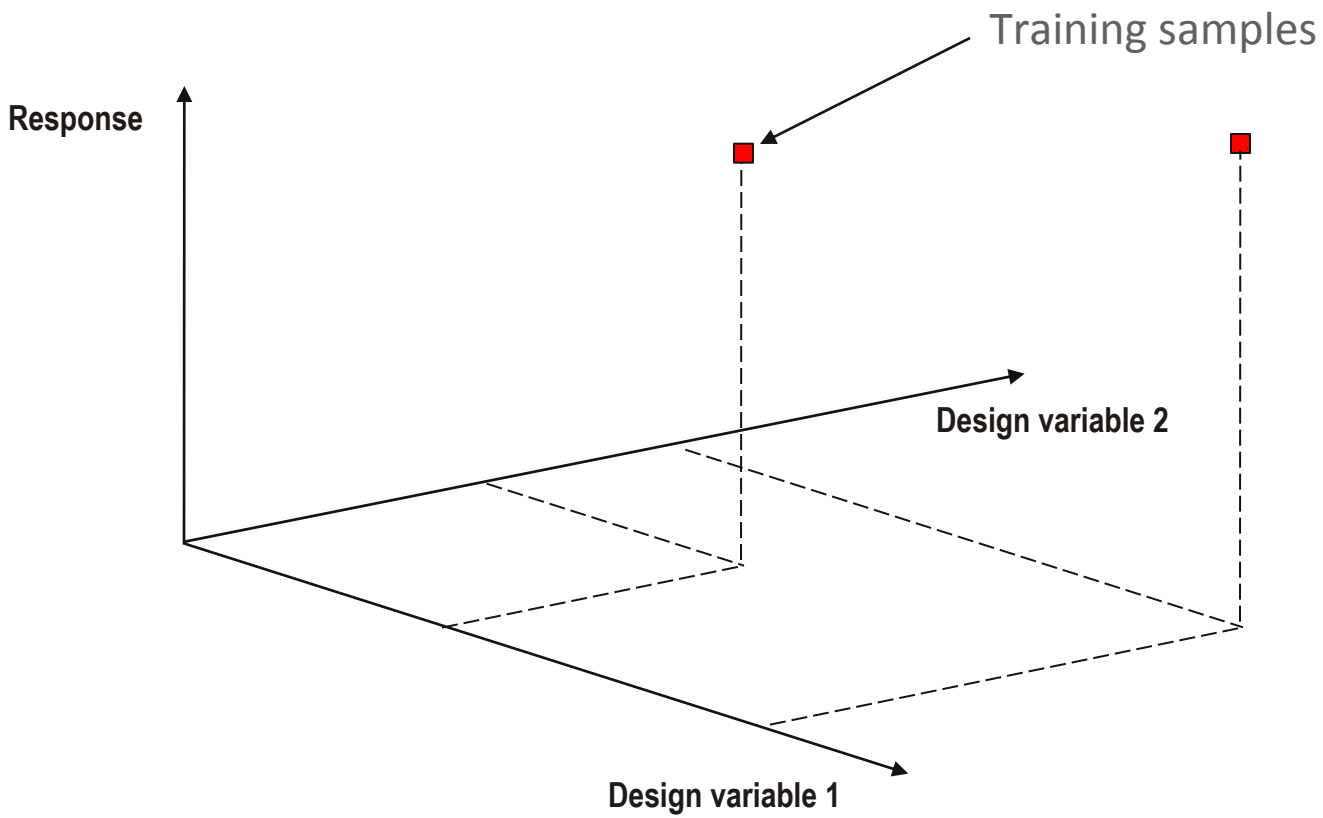
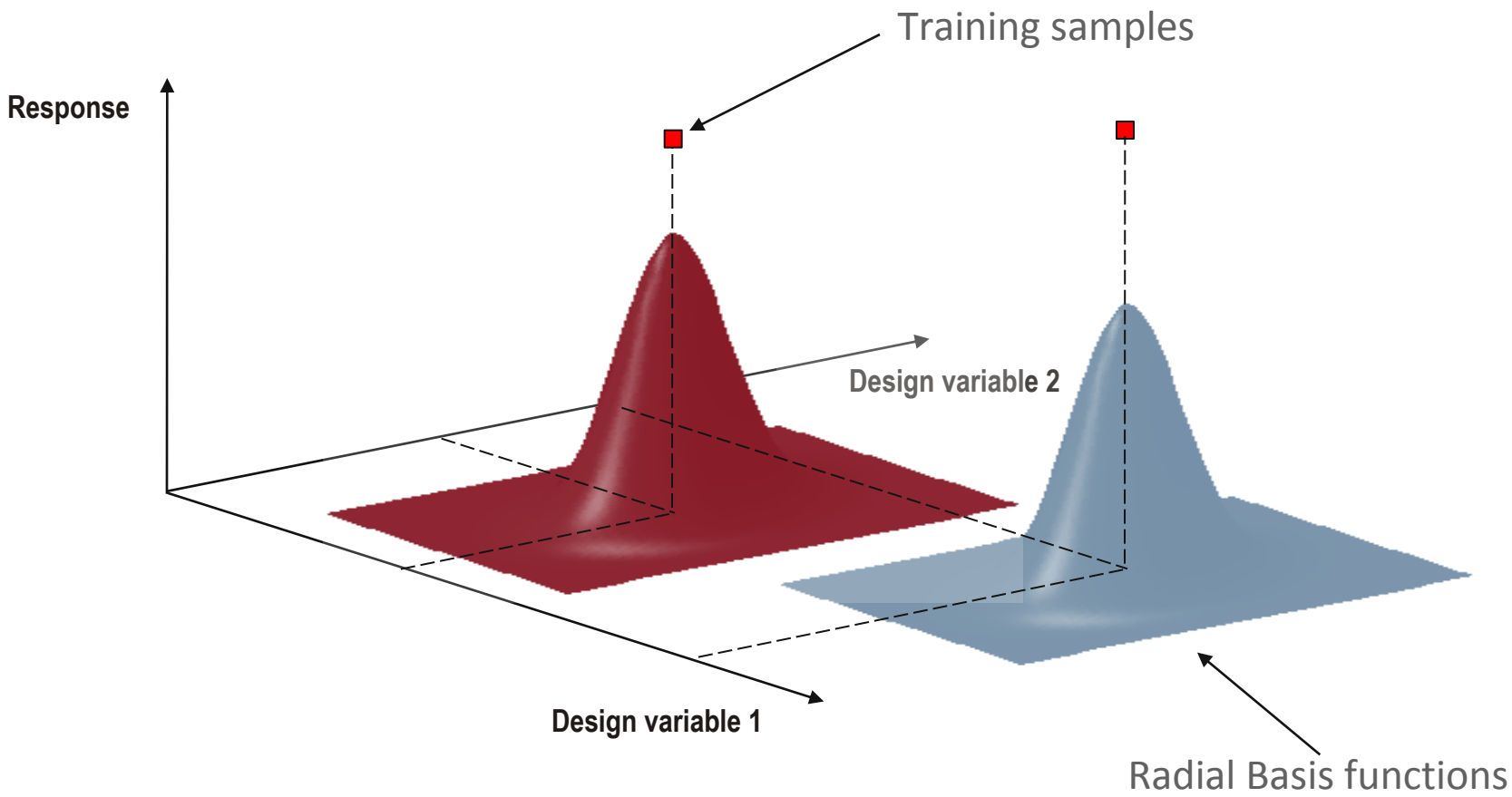


Construction of Radial Basis Function Network

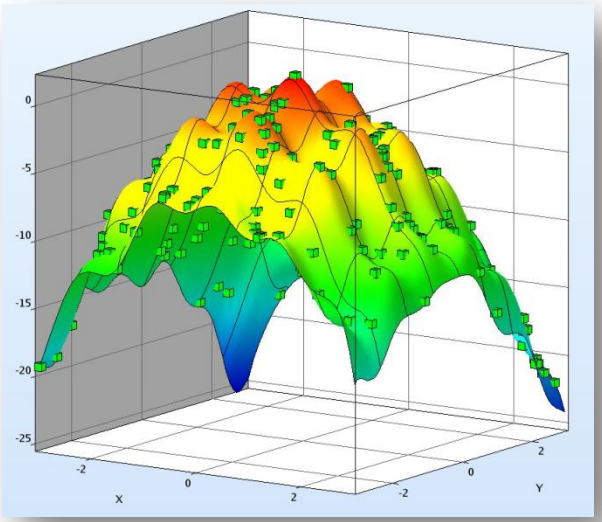


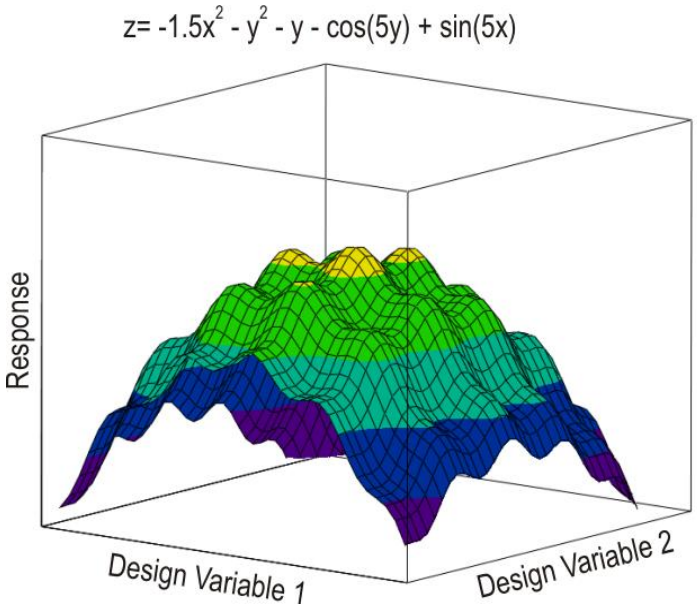
Construction of Radial Basis Function Network



Radial Basis Function Network - Example

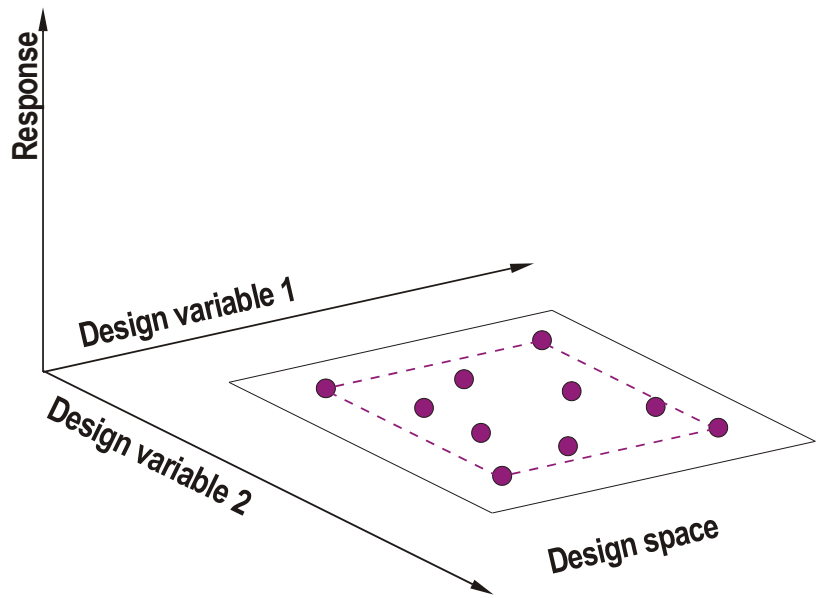
- RBFN is an universal approximation technique if enough training points are provided





Strategies for Metamodel-Based Optimization

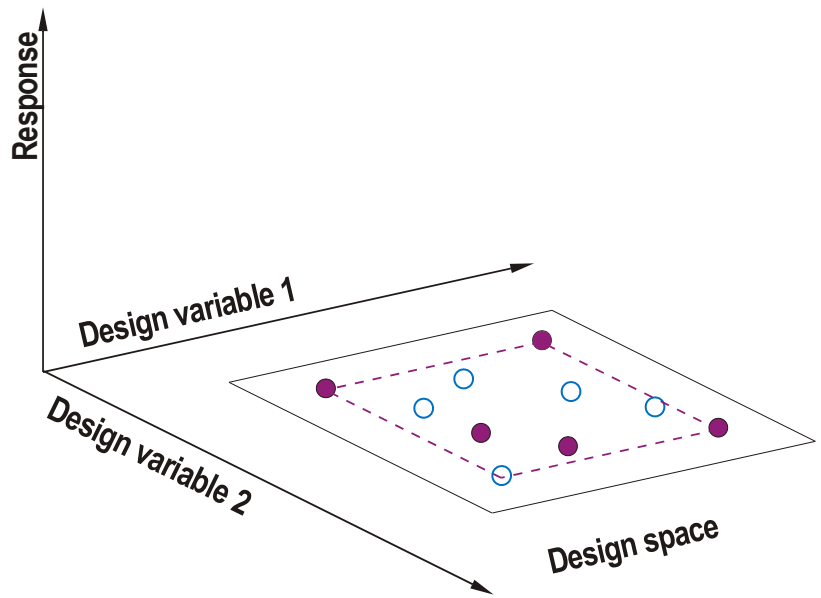
- Single stage
  - The experimental design for choosing the sampling points is done only once
  - A typical application would be to choose a large number of points (as much as can be afforded) to build metamodels such as, RBF networks using the Space Filling sampling method.
  - Suitable for global design exploration.



- Stage 1

Strategies for Metamodel-Based Optimization

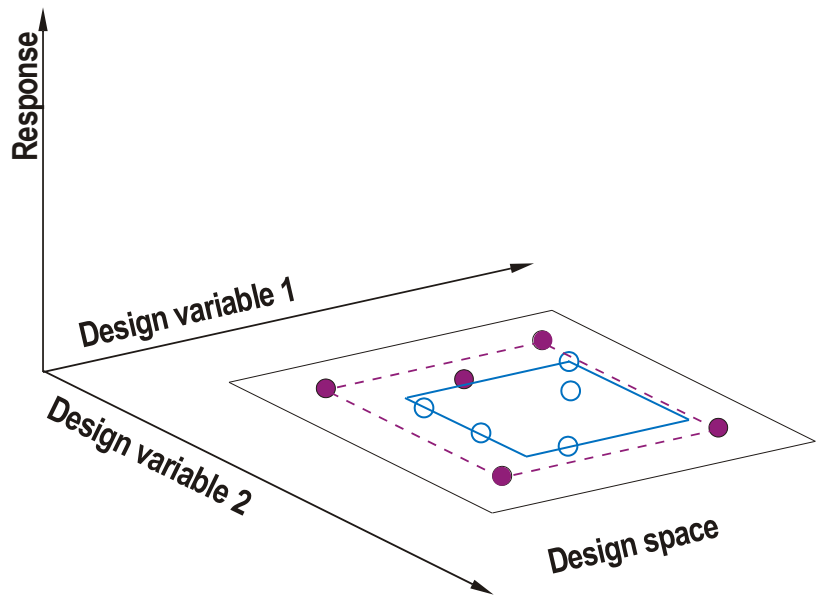
- Sequential strategy
  - Small number of points is chosen for each iteration – Sampling is done sequentially in multiple iterations
  - Can be stopped as soon as the metamodel or optimum points have sufficient accuracy.
  - Suitable for global design exploration.
  - Both work better with metamodels other than polynomials because of flexibility of metamodels to adjust to an arbitrary number of points.



- Stage 1
- Stage 2

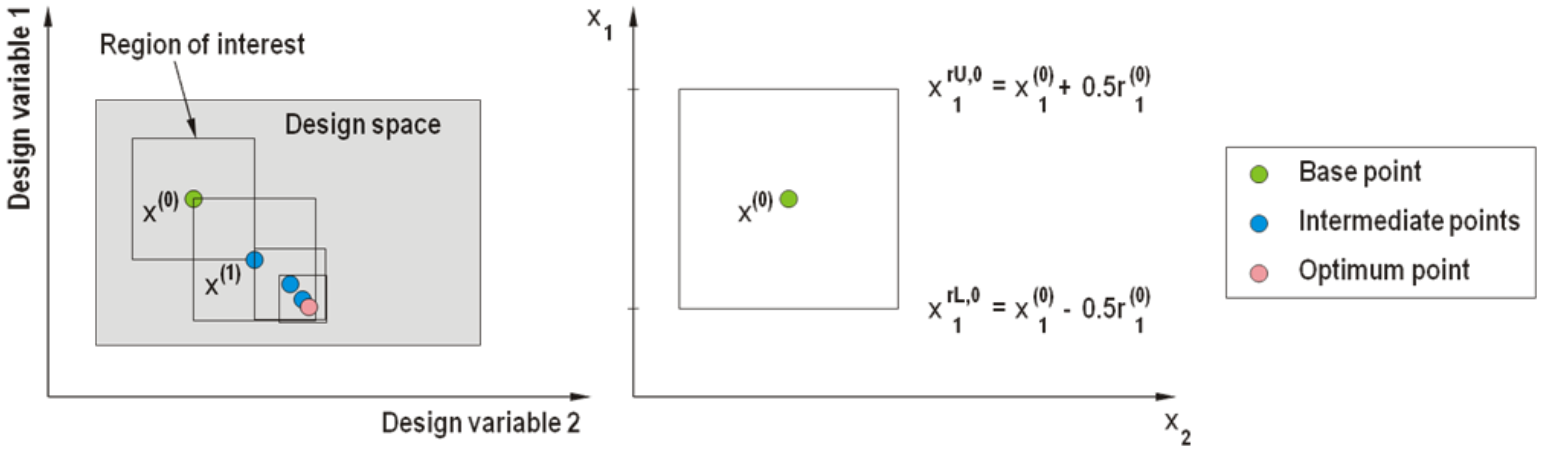
Strategies for Metamodel-Based Optimization

- Sequential strategy with domain reduction
  - Sampling is performed in every iteration.
  - Subregions are used to bound new design points.
- Two approaches possible:
  - Sequential Adaptive Metamodeling (SAM) – global
  - Sequential Response Surface Method (SRSM) – local
    - Previous points are ignored
    - The only one suitable for polynomial metamodels



- ● Stage 1, subregion 1
- ○ Stage 2, subregion 2

Sequential Response Surface with Domain Reduction



Contraction rate:

$$\lambda_i = \eta + \left|d_i^{(k)}\right|(\gamma - \eta)$$

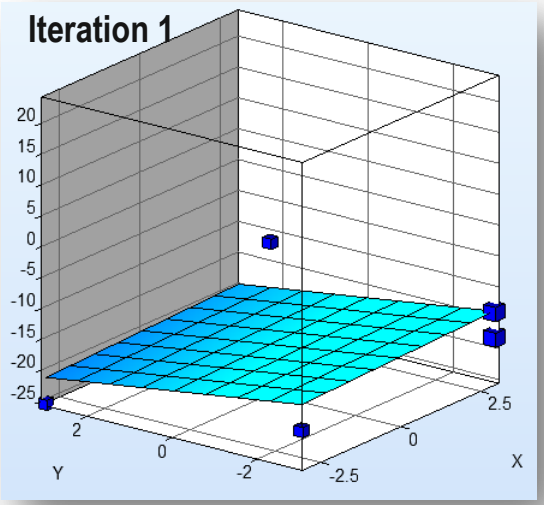
$$\gamma = \frac{\gamma_{pan}(1+\hat{c}) + \gamma_{osc}(1-\hat{c})}{2}$$

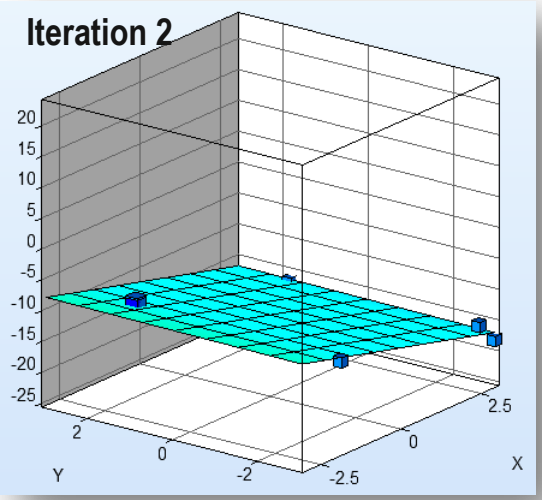
$\gamma -$ contraction parameter

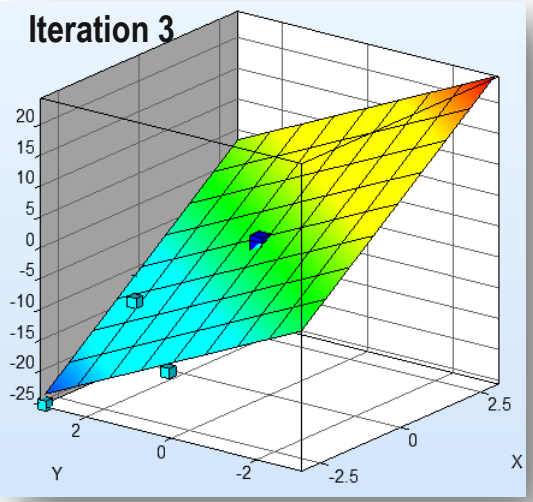
$\eta -$ zooming parameter

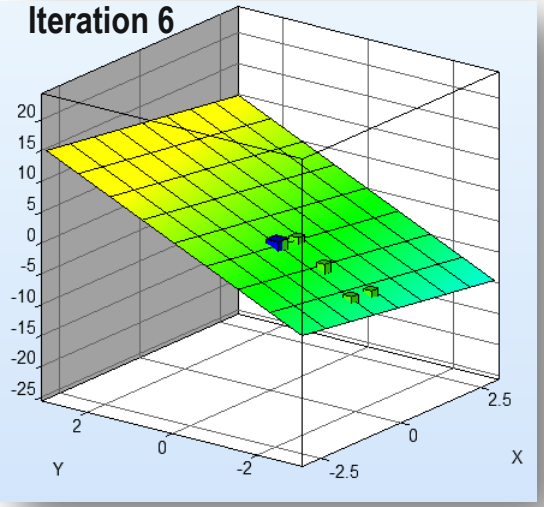
$\hat{c} -$ contraction indicator

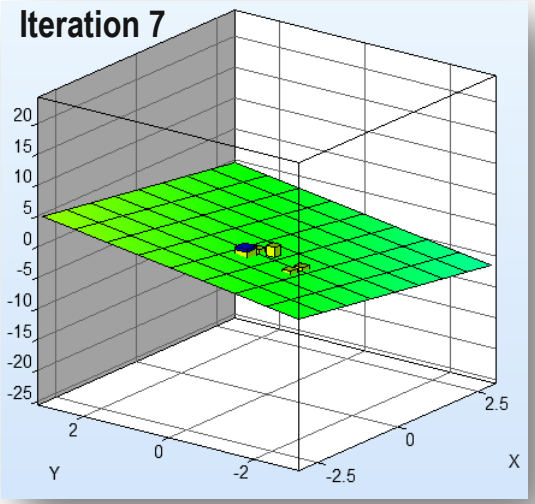
SRSM with Domain Reduction - Linear Surface

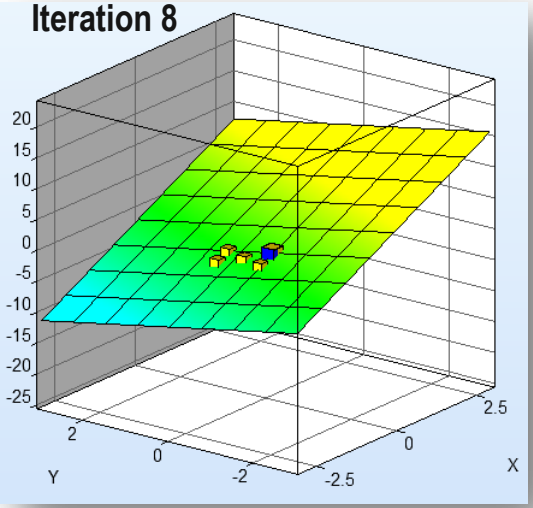




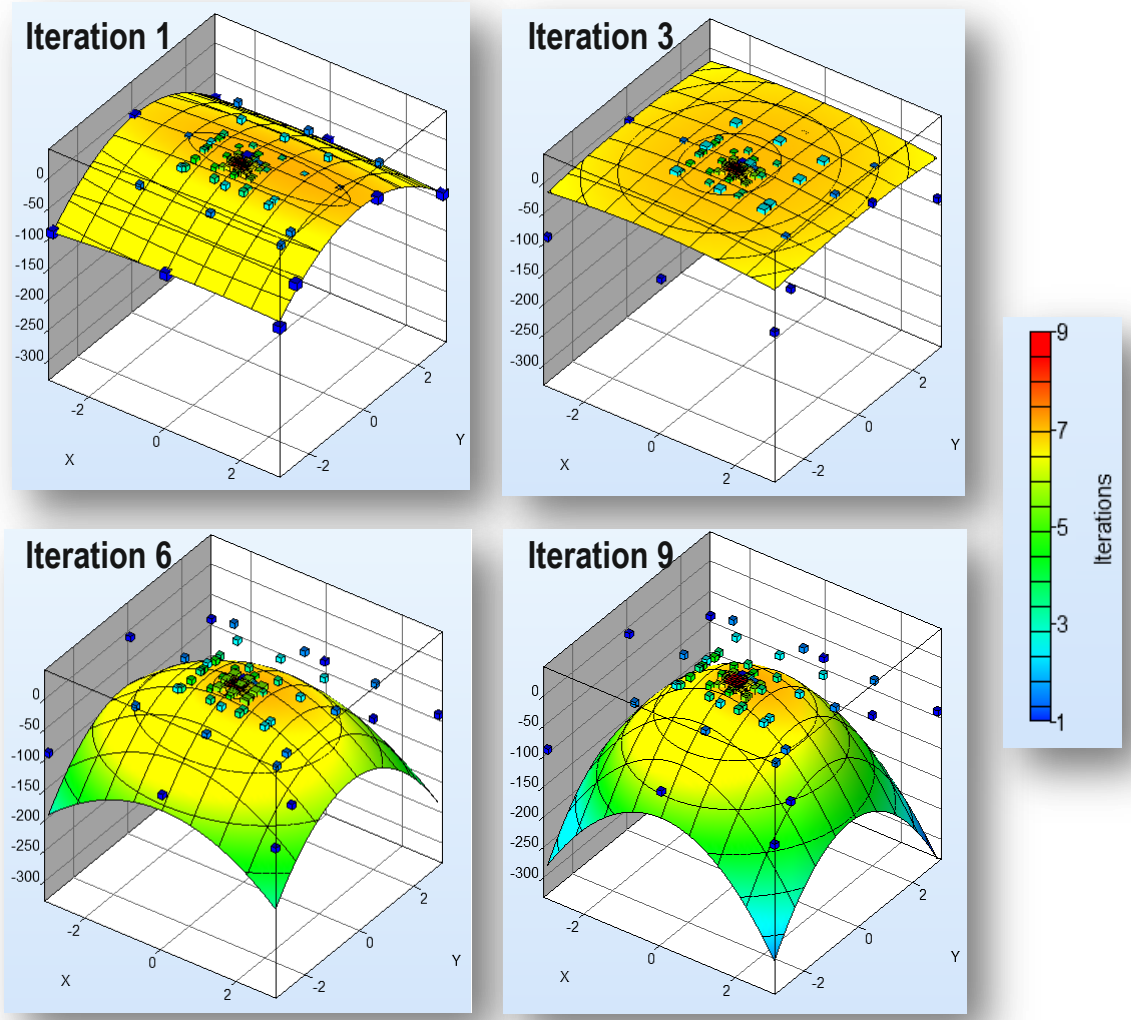








SRSM with Domain Reduction – Quadratic Surface



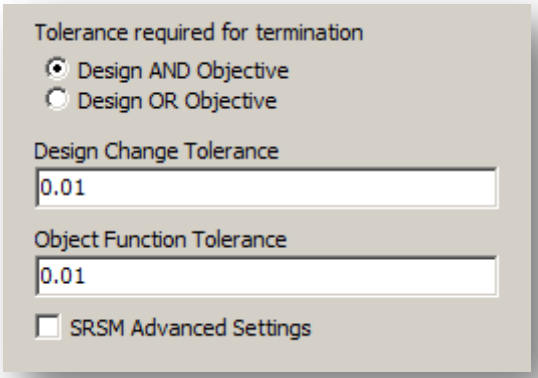
Convergence Criteria in LS-OPT

- Objective function convergence

$$\varepsilon_f > \frac{\left\| f^{(k)} - f^{(k-1)} \right\|}{\left\| f^{(k)} \right\|}$$

- Error norm of design variables

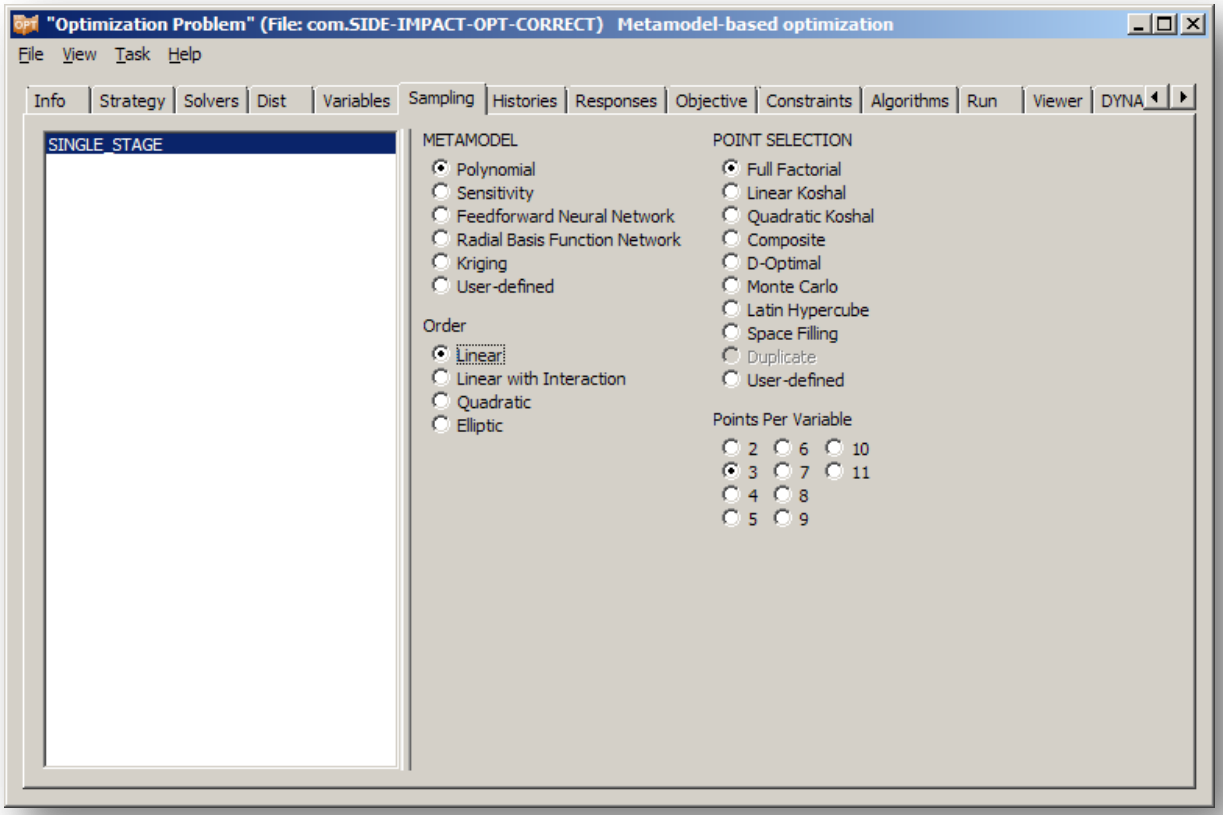
$$\varepsilon_x > \frac{\left\| x^{(k)} - x^{(k-1)} \right\|}{\left\| d \right\|}$$



$x -$	refers to the vector of design variables
$d -$	size of the design space
$f -$	denotes the value of the objective function
$(k),(k-1) -$	refer to two successive iteration numbers

Questions?

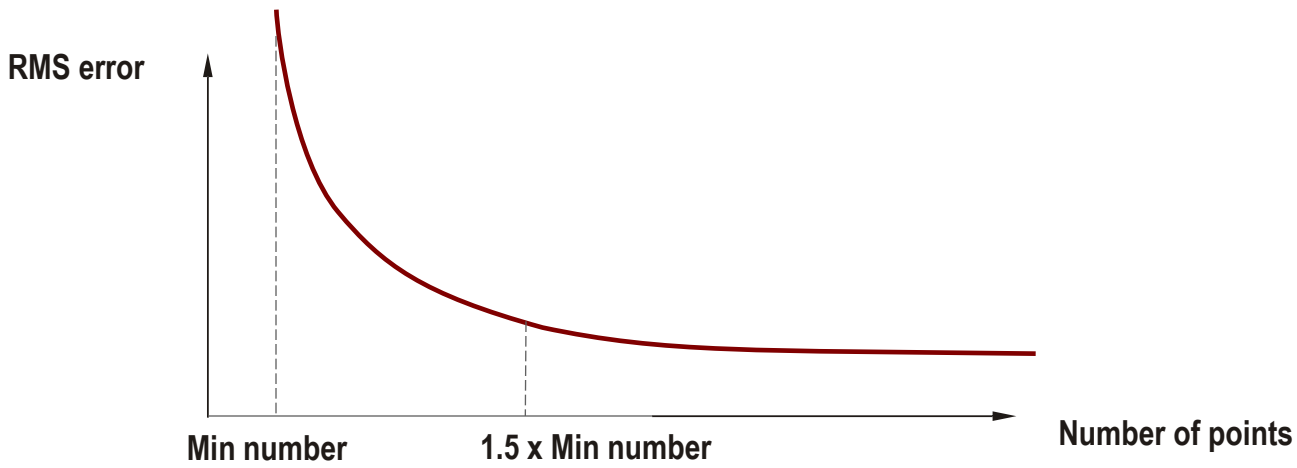
- How to select best points to construct the response surface model?
  - How many of them?
  - What should be their distribution over the design space?



Factors influencing the accuracy

- Size of the region of interest - the smaller the size the more accurate the model. To the point when only the noise is dominating.

- Number of experimental points and their distribution increases the predictive capability of the model.



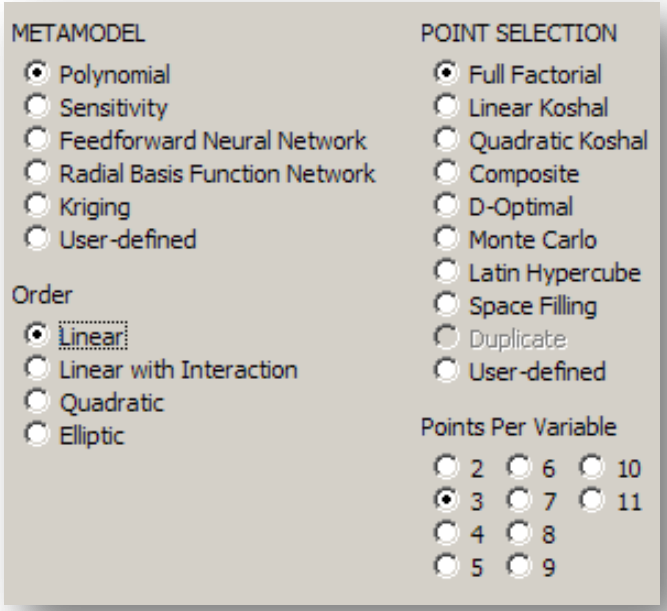
- Order and type of the approximating function. The higher the order the more accuracy model has. But to the point when overfitting can occur.

Design of Experiments

- Design of Experiments (DoE) is a process of selection of most representative points in the design space for which the response will be calculated.

- The selection of these points considerably influences the approximation accuracy and the cost of response surface construction.

- The points selected in the DoE process are intended to:
  - give minimum number of approximation points for spanning the response surface with good quality,
  - find improved or optimal simulation settings,
  - troubleshoot simulation problems
  - make a model more robust.



Two-level Factorial Designs

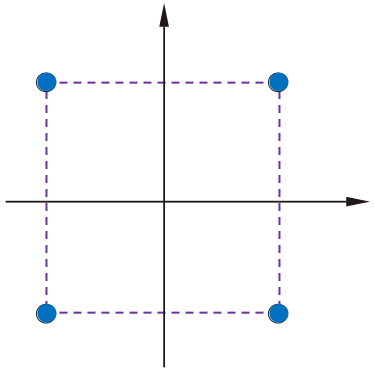
- The factorial design uses a set of l^k designs where l is a number of levels (grid points in one direction) and k is a number of factors (which determines the dimension of the space).

- For example 2^2 design with two levels and two factors, would mean that there are two design variables and two values can be assigned to them in a given design.

- This design option is efficient for the screening purposes and is a basis for other more advanced design methods.

- 2^k designs are used commonly to fit first order response surface models

2^2

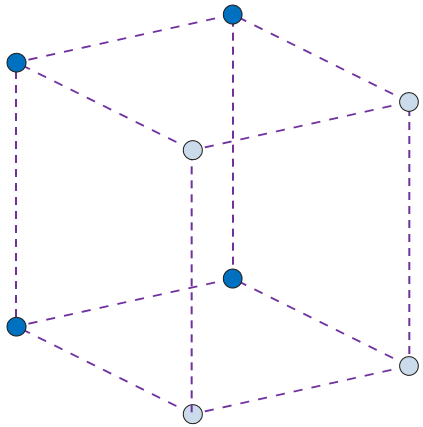


$$\begin{array}{cc} x_1 & x_2 \\ \end{array}$$
$$\begin{bmatrix} -1 & -1 \\ -1 & 1 \\ 1 & -1 \\ 1 & 1 \end{bmatrix}$$

Factorial Design

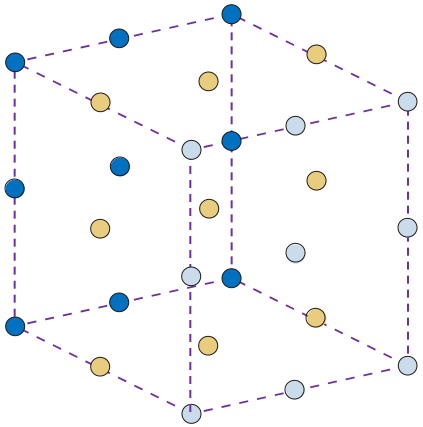
- three factors at two levels
  - good for linear surface

2^3



- three factors at three levels
  - good for quadratic surface

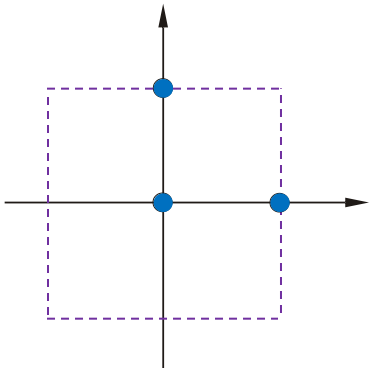
3^3



Koshal Design

- The Koshal design uses the minimum number of the design points required to construct surface of given order.
- The approach leads to the saturated design which is characterized by the same number of points as the number of coefficients of the approximation function.
- It influences the accuracy of the surface approximation.
- If simulation fails in one of the points – the surface can not be constructed

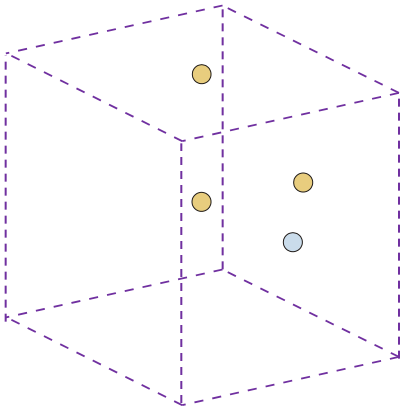
- first order n=2 design



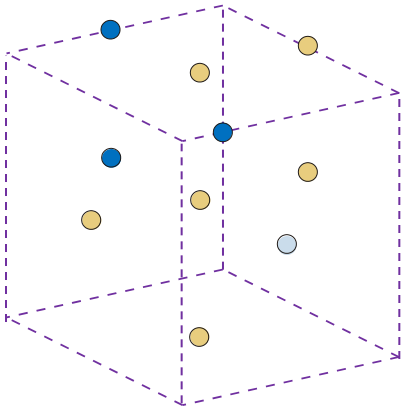
$$\begin{array}{cc} x_1 & x_2 \\ \end{array}$$
$$\begin{bmatrix} 0 & 0 \\ 1 & 0 \\ 0 & 1 \end{bmatrix}$$

Koshal Design

- first order n=3 design
  - good for linear model
- second order n=3 design
  - good for quadratic model



$$\begin{array}{ccc} x_1 & x_2 & x_3 \end{array}$$
$$\begin{bmatrix} 0 & 0 & 0 \\ 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \end{bmatrix}$$

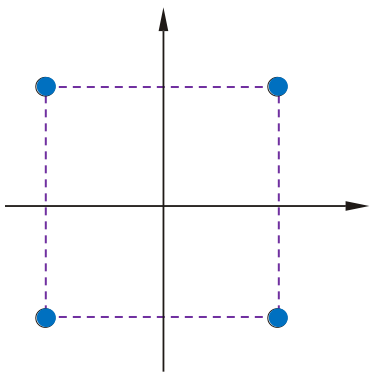


$$\begin{array}{ccc} x_1 & x_2 & x_3 \end{array}$$
$$\begin{bmatrix} 0 & 0 & 0 \\ 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \\ -1 & 0 & 0 \\ 0 & -1 & 0 \\ 0 & 0 & -1 \\ 1 & 1 & 0 \\ 1 & 0 & 1 \\ 0 & 1 & 1 \end{bmatrix}$$

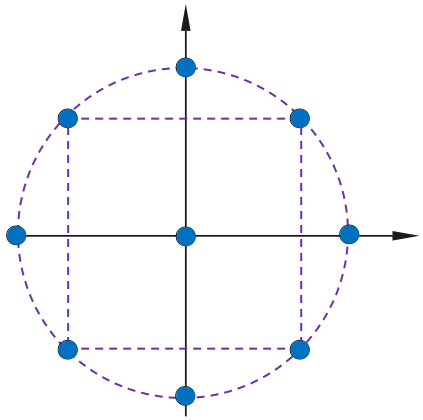
Central Composite Design

- For two variables the design consist of 8 equally spaced points on the perimeter of a circle with radius $\sqrt{2}$ and central point
- As a basis factorial design is used
- Four axial points and central point are added

- factorial (for linear)



- CCD (for quadratic)

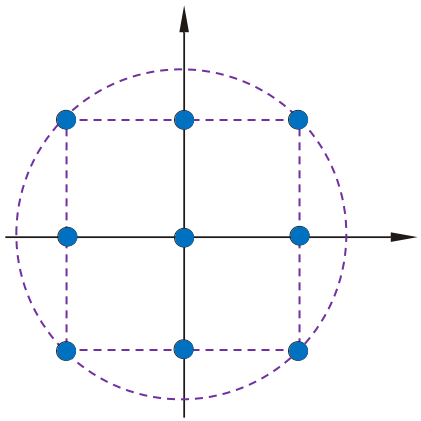


$$\begin{array}{cc} x_1 & x_2 \end{array}$$
$$\begin{bmatrix} 1 & 1 \\ -1 & 1 \\ 1 & -1 \\ -1 & -1 \\ 0 & \sqrt{2} \\ \sqrt{2} & 0 \\ 0 & -\sqrt{2} \\ -\sqrt{2} & 0 \\ 0 & 0 \end{bmatrix}$$

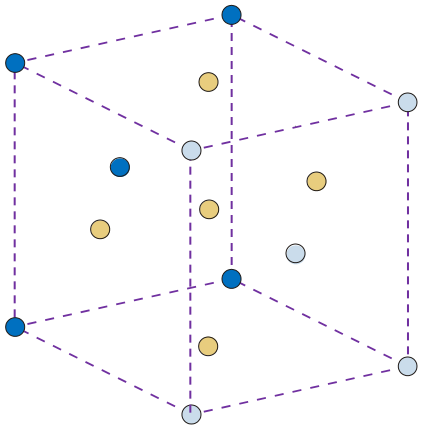
Central Composite Design

- Axial distance generally can vary from 1.0 (face center points) to $\sqrt{n}$ on common sphere
- With n variables the design requires $P = 2^n + 2n + 1$ points

$n = 2$



$n = 3$



D-optimal Design

- Optimal design theory developed for best choice of points.
- D-optimal was proven to be one of the best of optimal designs.
- It uses points that are solution to the sub-problem:

$$\max\left|\boldsymbol{X}^T\boldsymbol{X}\right| \qquad \boldsymbol{X}=\left[X_{ij}\right]=\left[\phi_j\left(x_i\right)\right]=\begin{bmatrix}\phi_1\left(x_1\right) & \dots & \phi_j\left(x_1\right)\\ \vdots & \ddots & \vdots\\ \phi_1\left(x_i\right) & \dots & \phi_j\left(x_i\right)\end{bmatrix}$$

- This criterion assures best estimation of parameters (low bounds for confidence regions on regression coefficients).

D-optimal Design

- Usually subset from the grid of factorial designs is taken as a candidate for D-optimal design.
- The advantage of D-optimal design is that it allows for approximation of irregular shapes, with any number of experimental points
- The D-optimal design can be also useful for constrained design space, where standard factorial method would fail
- Experimental points from previous iterations can be easily incorporated in subsequent ones to increase the accuracy of a new experimental design.

$$X_a(x_p) = \begin{bmatrix} X \\ A(x_p) \end{bmatrix}$$

$$\max\left|X_a^T X_a\right| = \max\left|X^T X + A^T A\right|$$

D-optimal Design

- Based on the D-optimal method of point's selection, for n number of the design points in the linear approximation the number of simulations needed to be performed is equal to:

$$\mathrm{int}\left(1.5\left(n+1\right)+1\right)$$

- The number of simulations in the quadratic approximation:

$$\mathrm{int}\left(0.75\left(n+1\right)\left(n+2\right)+1\right)$$

- 50% +1 points more than would be required by saturated design.

- Oversampling guaranties that the surface will be created even if LS-DYNA (solver) fails at some points.

Number of Design Points

Number of Variables n	Linear approximation			Quadratic approximation			Central Composite
	Koshal	*D*-optimal	Factorial	Koshal	*D*-optimal	Factorial	
1	2	4	2	3	5	3	3
2	3	5	4	6	10	9	9
3	4	7	8	10	16	27	15
4	5	8	16	15	23	81	25
5	6	10	32	21	32	243	43
6	7	11	64	28	43	729	77
7	8	13	128	36	55	2187	143
8	9	14	256	45	68	6561	273
9	10	16	512	55	83	19683	531
10	11	17	1024	66	100	59049	1045

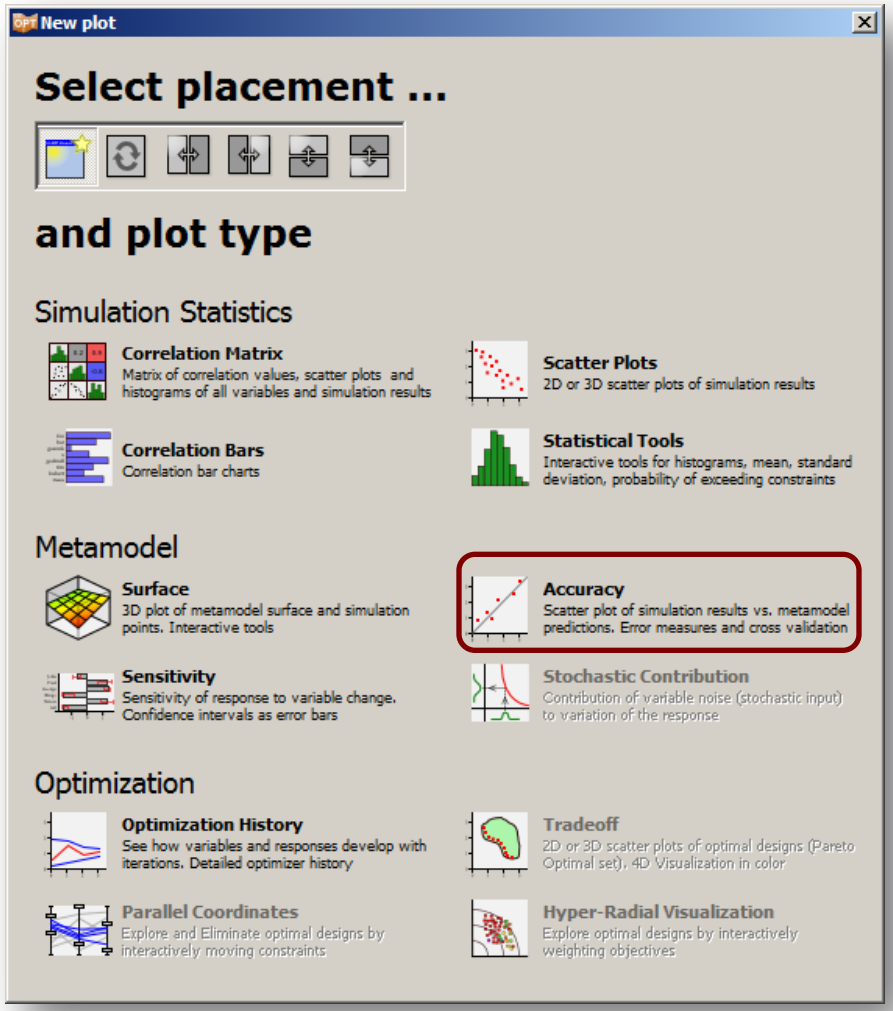
LS-OPT manual, LSTC, April, 2009

Point Selection in LS-OPT

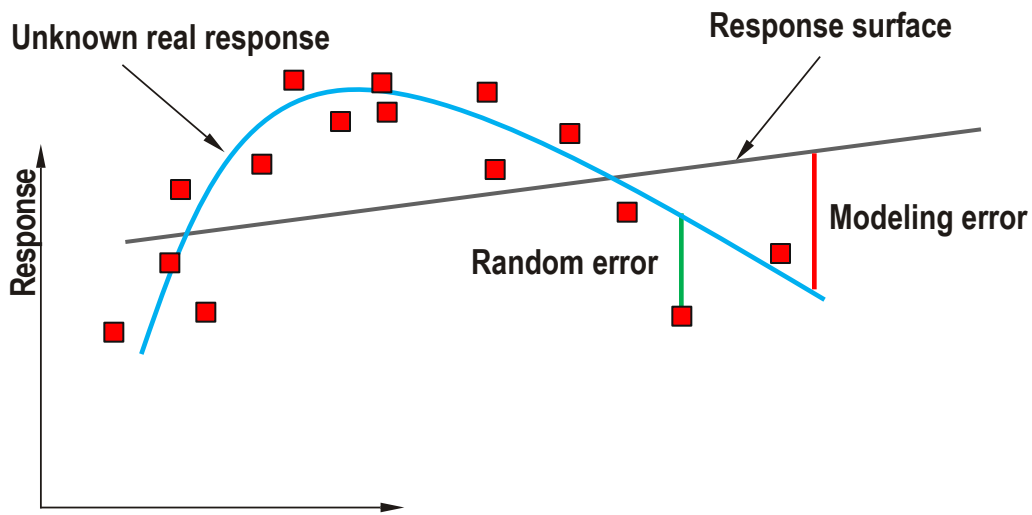
- Factorial
- Koshal
- Composite
- D-Optimal
- Monte Carlo
- Latin Hypercube
- Space Filling
- User Defined

Questions?

- Is the model a good approximation of the real, physical process?
- What is the error of the metamodel?
- How to quantify and how to minimize it?
- What are prediction capabilities of the model?



Error Analysis



- Two sources of errors are present in surrogate model based design:
  - Random error (noise)
  - Modeling error (difference between real and predicted response)

- Adequacy of the surrogate model and its capability of predicting accurate response <u>must be checked</u>

Error Analysis

- Total sum of squares can be partitioned to:

$$SS_y = SS_R + SS_E$$

modeling error

sum of squares of the residuals

- ... and it is defined as:

$$S_{yy} = \sum_{i=1}^{n} y_i^2 - \frac{\left(\sum_{i=1}^{n} y_i\right)^2}{n}$$

Residuals and Regression Sum of Squares

- The sum of squares of the residuals:

$$SS_E = \sum_{i=1}^{n} (y_i - \hat{y}_i)^2 = \sum_{i=1}^{n} e_i^{\,2} \qquad\qquad SS_E = \mathbf{e'e}$$

- Recalling that $\mathbf{e} = \mathbf{y} - \hat{\mathbf{y}}$ and $\hat{\mathbf{y}} = \mathbf{Xb}$ it can be transformed to:

$$SS_E = \mathbf{y'y} - \mathbf{b'X'y}$$

- The regression sum of squares is:

$$SS_R = \mathbf{b'X'y} - \frac{\left(\sum_{i=1}^{n} y_i\right)^2}{n}$$

Metamodeling Errors in LS-OPT

- Root mean square error (RMS)
  - summarizes overall model error
  - used for saturated model will give zero value

$$\varepsilon_{RMS} = \sqrt{\frac{SS_E}{n}} = \sqrt{\frac{1}{n}\sum_{i=1}^{n}\left(y_i - \hat{y}_i\right)^2}$$

n – number of design points

$\hat{y}_i$ – predicted response

y_i – the actual (computed) response

- Maximum error

$$\varepsilon_{\max} = \max\left|y_i - \hat{y}_i\right|$$

Coefficient of Multiple Determination

- Indicates how much better the function predicts the response than just using the mean value of that response.
- Or if the model is able to detect variability in the response.
- A fraction of the variation in the data explained by the model

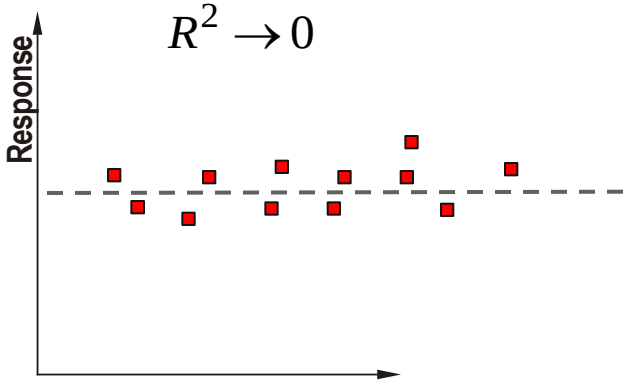
$$R^2 = \frac{SS_R}{SS_y} = 1 - \frac{SS_E}{SS_y}$$

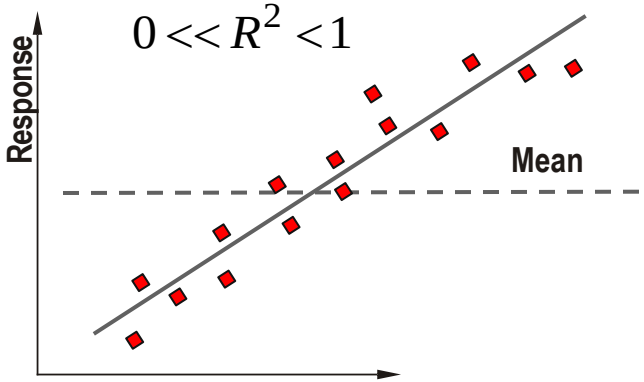
$$R^2 = \frac{\sum_{i=1}^{n}\left(\hat{y}_i - \bar{y}\right)^2}{\sum_{i=1}^{n}\left(y_i - \bar{y}\right)^2}$$

- Takes values: $0 \le R^2 \le 1$

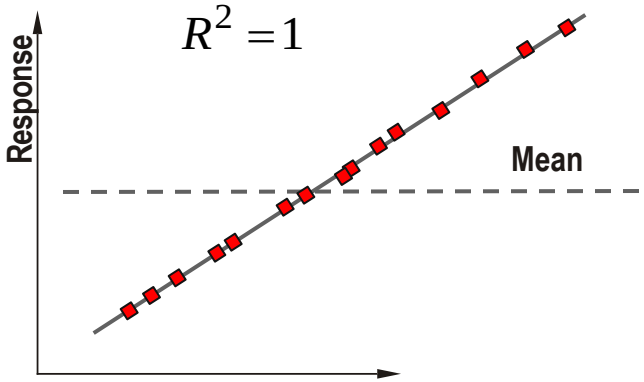
- Adding a variable to the model always increases the coefficient of multiple determination

Coefficient of Multiple Determination





$$R^2 = \frac{\sum_{i=1}^{n}\left(\hat{y}_i - \bar{y}\right)^2}{\sum_{i=1}^{n}\left(y_i - \bar{y}\right)^2}$$



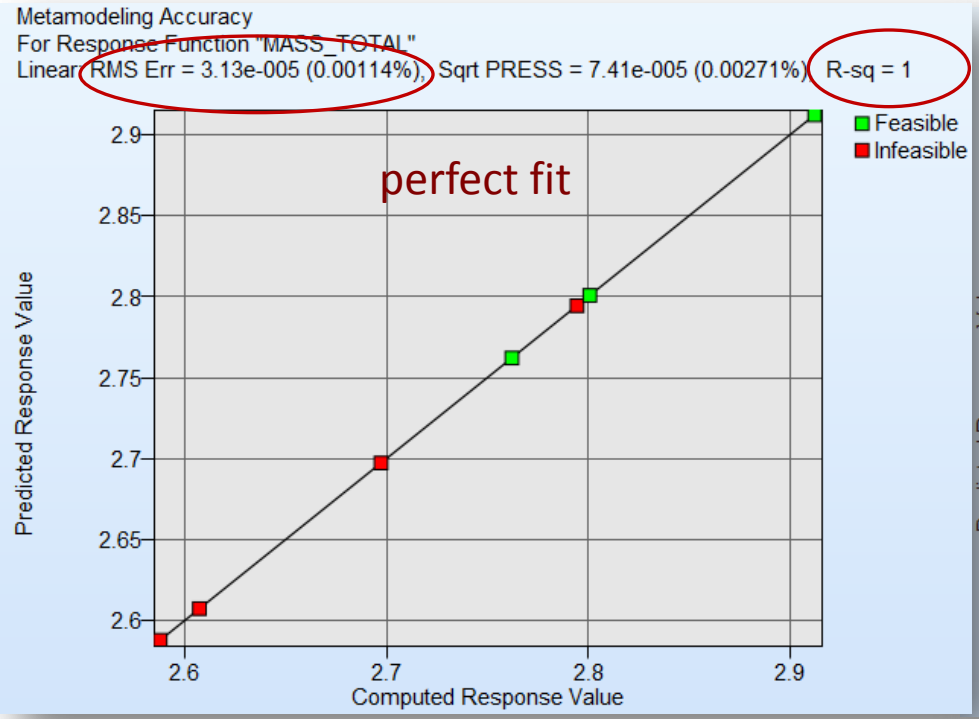
Error Analysis

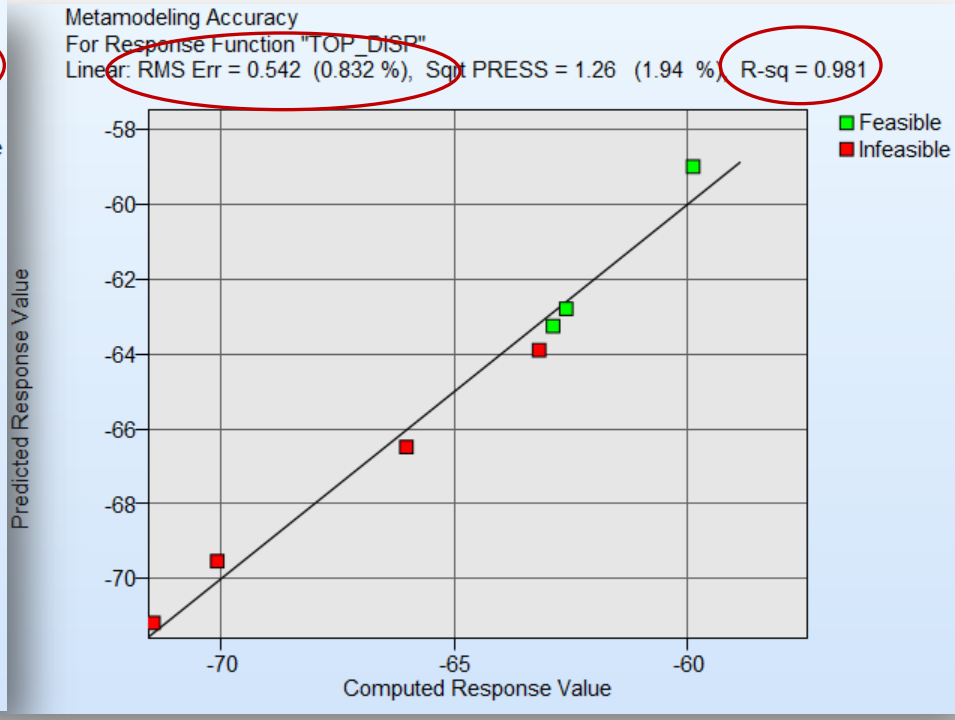
RMS	R^2	
small	~ 1	low noise, good fit, high variability detection
small	~ 0	low noise, good fit, small gradient
large	~ 1	Large noise in the model, high variability detection
large	~ 0	Lack of fit, must refine model or shrink bounds

- In the iterative scheme with shrinking region the R-sq tends to be small at the beginning, then goes to unity when the region shrinks – improves the modeling ability.
- It may reduce again when the noise starts to dominate the response causing variability to be indistinguishable.

RMS & Coefficient of Multiple Determination

- predicted vs. computed response in LS-OPT viewer





Prediction Sum of Squares (PRESS) Error

Leave-one-out:

- Select an observation, for example i.
- Fit the model to the remaining $n-1$ observations
- Use model equation to predict the withheld observation y_i
- Repeat the procedure for each variable
- Compute the sum of squares

$$PRESS = \sum_{i=1}^{n} \left(\frac{y_i - \hat{y}_i}{1 - h_{ii}} \right)^2$$

Prediction Sum of Squares (PRESS) Error

- In fact PRESS does not need to compute n regression models.

$$PRESS = \sum_{i=1}^{n} \left(\frac{y_i - \hat{y}_i}{1 - h_{ii}} \right)^2$$

- where “hat” matrix:

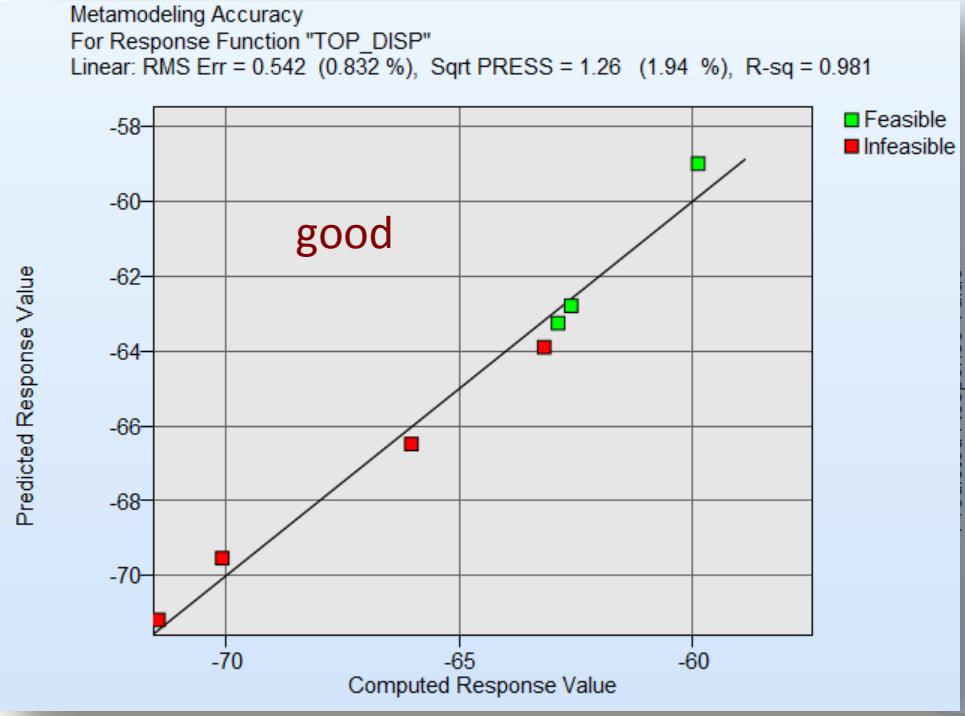
$$\mathbf{H} = \mathbf{X}\left(\mathbf{X}^T \mathbf{X}\right)^{-1} \mathbf{X}^T$$

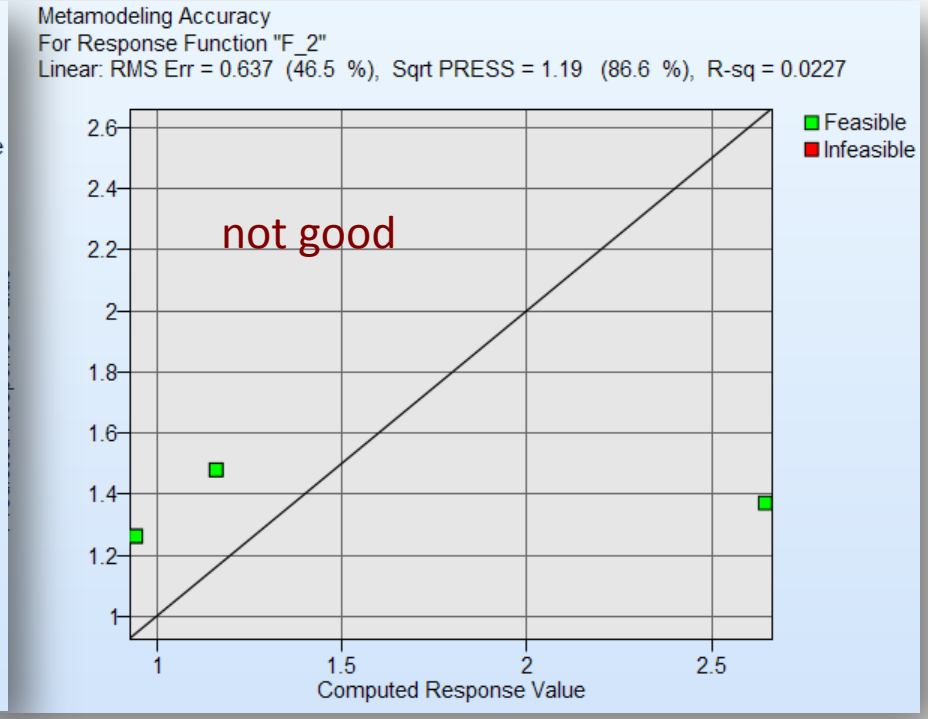
- maps observed response to the fitted response:

$$\hat{\mathbf{y}} = \mathbf{H}\mathbf{y}$$

Prediction Sum of Squares (PRESS) Error

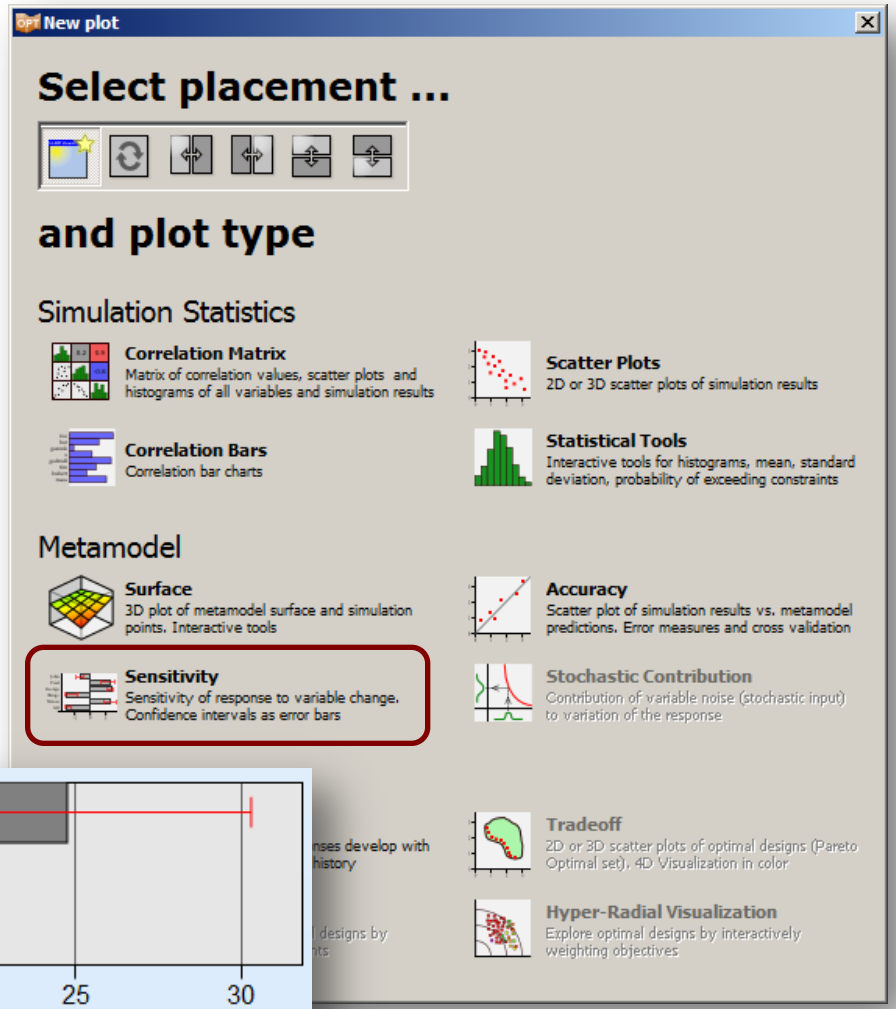
- Large discrepancy between SPRESS and residual sum of squares indicates high influence of one variable on the response – model performs badly without it.
- In LS-OPT SPRESS error is computed: $SPRESS = \sqrt{PRESS}$

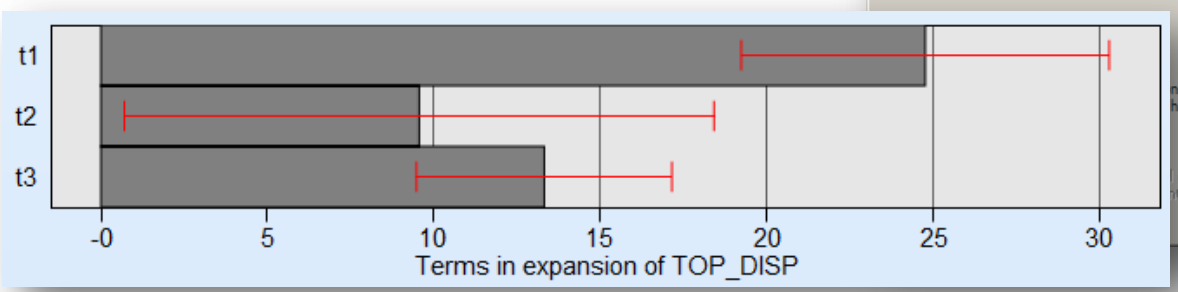




Questions?

- Are the variables used in the model important for the response
- Which of them are most crucial for the response?





Confidence Intervals in Multiple Regression

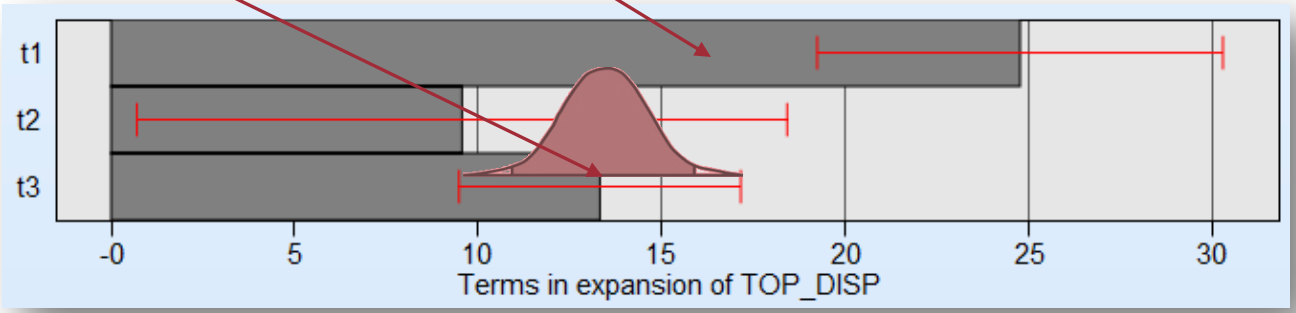
- recall that : $\mathbf{y} = \mathbf{X}\boldsymbol{\beta} + \boldsymbol{\varepsilon}$ and $\hat{\mathbf{y}} = \mathbf{X}\mathbf{b}$

- b_j is normally distributed with mean vector β_j

$$b_j - t_{\alpha/2,n-p}\sqrt{\hat{\sigma}^2 C_{jj}} \le \beta_j \le b_j + t_{\alpha/2,n-p}\sqrt{\hat{\sigma}^2 C_{jj}}$$

$2t_{\alpha/2,n-p}\sqrt{\hat{\sigma}^2 C_{jj}}$

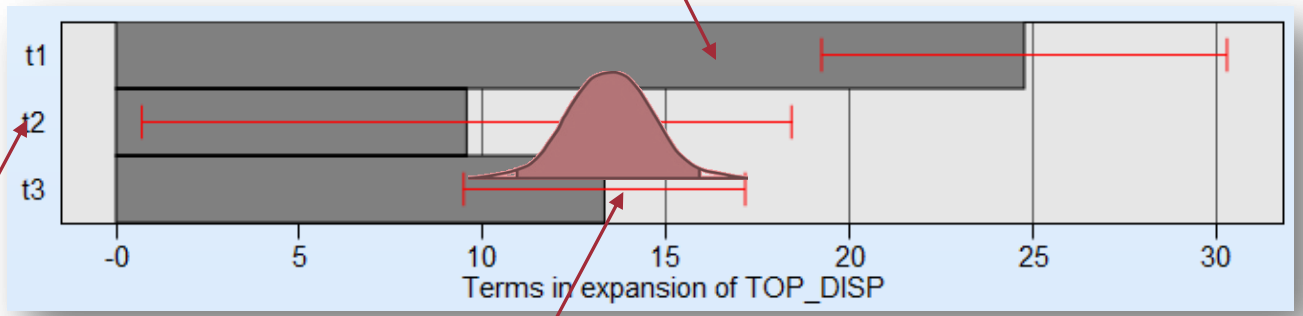
b_j



- where C_{jj} is the diagonal element of $(\mathbf{X}'\mathbf{X})^{-1}$ corresponding to b_j

Confidence Intervals in Multiple Regression

Significance of the variable normalized with respect to design space
(df/dx) * (xUpper - xLower)



Insignificant variable

Uncertainty of variable distributed as *t*

- Used for screening of variables with small contribution to the response
- Allows to lower the number of simulation runs

Metamodel Based Optimization Process - Summary

Item	Input data	Output data
Design of Experiments	• Location and size of the subregion in the design space, • The experimental design desired, • An approximation order, • An affordable number of points.	• Location of the experimental points.
Simulation	• Location of the experimental points, • Analysis programs to be scheduled.	• Responses at the experimental points.
Build response surface	• Location of the experimental points, • Responses at the experimental points, • Function types to be fitted.	• The response surface,
Check adequacy	• The approximate functions (response surfaces), • The location of the check points, • The responses at the check points.	• The goodness-of-fit of the approximate functions at the check points.
Optimization	• The approximate functions (response surfaces), • Bounds on the responses and variables.	• The approximate optimal design, • The approximate responses at the optimal design, • Pareto optimal curve data.

References

- R. H. Myers, D.C. Montgomery, “Response Surface Methodology. Process and Product Optimization Using Designed Experiments”, John Wiley & Sons, INC., 1995
- N. Stander et al., “LS-OPT® User’s Manual, A Design Optimization and Probabilistic Analysis Tool for the Engineering Analyst”, LSTC, 2009
- N. Stander, T. Goel, “LS-OPT® Training Class. Optimization Theory ”, LSTC, 2009