

# Influence of Selection Criterion on the RBF Topology Selection for Crashworthiness Optimization

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## Abstract

*Meta-models are frequently used to offset high computational cost of crashworthiness optimization problems. Radial basis function based meta-models are gaining popularity among various meta-modeling techniques due to their ability to approximate non-linear responses with relatively low fitting cost. However, the performance of RBF networks is very sensitive to the choice of topology. In this paper, the influence of three selection criteria namely, PRESS, pointwise PRESS error ratio, and estimated variance of noise, over network topology is studied. The results are demonstrated for a few analytical functions and a crashworthiness simulation of a full NHTSA vehicle problem. The results showed that the PRESS-based method was the most reliable method to select network topology.*

## Introduction

Most engineering problems of practical significance are computationally expensive. This phenomenon is common in crashworthiness optimization due to the high cost of finite element simulations. To alleviate high computational cost, the use of meta-models is popular. In this approach, meta-models are developed using limited data and optimization is carried out using these computationally inexpensive meta-models. There are many meta-models available in literature with polynomial response surfaces being the most popular due to their simplicity. Radial basis functions (RBFs) have been gaining popularity for approximation because of their ability to model highly non-linear responses with low fitting cost.

There are numerous instances of using radial basis functions in engineering applications. A small representative sample of some engineering applications is given as follows. Kurdila and Peterson [1], Li et al., [2] and Young et al. [3] used radial basis functions to approximate control conditions of nonlinear systems applied to aircraft and rockets. Wheeler et al. [4] used radial basis functions to model high pressure oxidizer discharge temperature for space shuttle main engine. Papila et al. [5], Shyy et al. [6], Karakasis and Giannakoglou [7] used radial basis functions to design turbo-machinery and propulsion components. Meckesheimer et al. [8] used radial basis functions to approximate discrete/continuous responses in the design of a desk lamp. Rocha et al. [9] found RBFs to perform the best to approximate wing weight of a subsonic transport vehicle. Zhang et al. [10] used radial basis functions to optimize a microelectronic packaging system. Reddy and Ganguli [11] used radial basis functions to assess structural damage in helicopter rotor blades. Glaz et al. [12] used RBFs to approximate vibration loads while designing the helicopter rotor blades. Panda et al. [13] used RBFs to predict flank wear in drills. Lanzi et al. [14] used RBFs to approximate crash capabilities of composite absorbers. Fang et al. [15] found that RBFs approximate different responses in crashworthiness simulations very well.

Though RBFs have been gaining popularity, the quality of approximation highly depends on the topology of the network i.e., the number of radial basis functions, location of centers of neurons, radius of influence etc. Orr [16-20] and the references within discussed various issues in the selection of number and location of centers and the radius of influence of neurons. To date, there is no consensus on the best method of selecting network topology though it is agreed that network topology has a large bearing on the output.

The influence of different criteria on the selection of network topology is studied in this paper. Specifically, the most popular generalized cross-validation error (also known as PRESS) criterion is compared with other criteria like estimated variance of error, and integrated pointwise ratio of generalization error that is defined as PRESS-ratio in a subsequent section. A few analytical test examples and an engineering application problem from crash-worthiness simulations are used to compare different topology selection strategies.

The paper is arranged as follows. The theoretical model and stepwise procedure of RBF model construction is described in the next section. Test problems used to validate the proposed approach and performance metrics to appraise different criteria are described in the Section **Test Problems and Performance Metrics**. Next **Test Procedure and Numerical Setup** for each example is detailed. Results obtained for different examples are given in the Section **Results and Discussion**. Finally, the main conclusions derived from this study are summarized in the **Conclusions** Section.

## Radial Basis Function Theoretical Model

A response function  $f(\mathbf{x})$  is approximated using a metamodel of the response  $\hat{f}(\mathbf{x})$  as,

$$f(\mathbf{x}) = \hat{f}(\mathbf{x}) + \varepsilon, \quad (1)$$

where  $\varepsilon$  is the error in approximation.

### Regression Problem

Radial basis functions (RBFs) were introduced as approximation functions by Hardy [21] in 1971 for approximation of the topographical data. This is a non-parametric approximation technique because no global form of the approximation function is assumed *a priori*. Instead, the approximation  $\hat{f}(\mathbf{x})$  is represented as a linear combination of  $N_{RBF}$  radially symmetric functions (radial basis functions)  $h(\mathbf{x})$  as,

$$\hat{f}(\mathbf{x}) = w_0 + \sum_{i=1}^{N_{RBF}} w_i h_i(\mathbf{x}), \quad (2)$$

where  $w_i$  is the weight associated with the  $i^{th}$  radial basis function.

While many monotonically radially varying functions have been used as RBFs, the Gaussian function is the most commonly used radial basis function. A typical Gaussian function is given as follows

$$h(\mathbf{x}) = \exp(-\|\mathbf{x} - \mathbf{c}\|^2 / \delta_c^2) = \exp(-(r / \delta_c)^2); \quad \delta_c = s \times r_c, \quad (3)$$

where  $\mathbf{c}$  is the center of the radial basis function,  $r_c$  is the radius of the (radial basis function) neuron, and  $s$  is a spread constant. The behavior of a Gaussian function is shown in Figure 1. This is a radially decaying function i.e., the function value decays with increase in distance from the center. The Gaussian function assumes its peak value at the center and gradually decays to zero as  $r \rightarrow \infty$ . The rate of decay is controlled by  $\delta_c$ , often known as the radius of influence. If the radius of influence is large, the rate of decay is slow; and if the radius of influence is small, the rate of decay of the function is high.

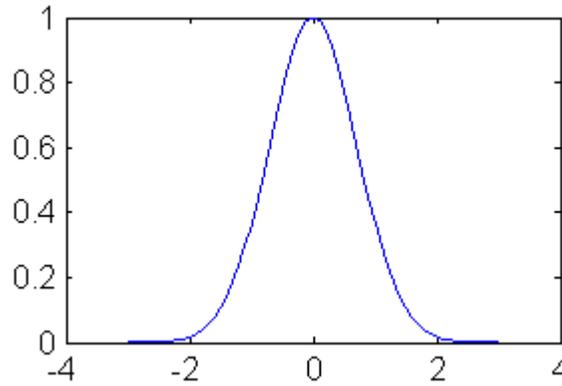


Figure 1: Gaussian radial basis function with center located at  $x=0$ .

Typically, a radial basis function approximation is a two-level optimization. Firstly, one needs to determine the topology of the network i.e., the number of radial basis functions, corresponding center locations, radii, and spread constant. Subsequently, the weights associated with each RBF are estimated. Mostly, weights are estimated by minimizing a quadratic loss function  $L$  that is the sum of square of errors in approximation.

$$L(\mathbf{w}) = \sum_{i=1}^{N_{pts}} (f(\mathbf{x}^{(i)}) - \hat{f}(\mathbf{x}^{(i)}))^2. \quad (4)$$

This choice of the quadratic loss function allows the use of linear regression to estimate weights vector. However, this may lead to overfitting of the data and may result into very large weights. Mullur and Messac [22] proposed the use of an extended RBF to avoid overfitting. However, a more conventional approach is to add a weight penalty to the loss function (Tikhonov and Arsenin, [23]),

$$L(\mathbf{w}) = \sum_{i=1}^{N_{pts}} (f(\mathbf{x}^{(i)}) - \hat{f}(\mathbf{x}^{(i)}))^2 + \sum_{i=0}^{N_{RBF}} \lambda_i w_i^2; \quad \lambda_i \geq 0, \quad (5)$$

where  $\lambda_i$  is the regularization parameter associated with the  $i^{\text{th}}$  weight. This formulation attempts to find parsimonious networks, reducing the sensitivity of the network to small changes.

Using ridge regression [18] to solve Equation (5), weights are estimated analytically as,

$$\hat{\mathbf{w}} = (H^T H + \Lambda)^{-1} H^T \mathbf{f}, \quad (6)$$

where  $\mathbf{f}$  is the vector of responses at design points,  $\Lambda$  is a diagonal matrix such that  $\Lambda_{ii} = \lambda_i$ ,  $i = 0, 1, \dots, N_{RBF}$ , and  $H$  is the design matrix constructed using the response of radial basis functions at design points such that

$$H_{i1} = 1, H_{ij+1} = h_j(\mathbf{x}^{(i)}), \quad i = 1, \dots, N_{pts}, j = 1, \dots, N_{RBF}.$$

The predicted response at any point is

$$\hat{f}(\mathbf{x}) = \hat{w}_0 + \sum_{i=1}^{N_{RBF}} \hat{w}_i h_i(\mathbf{x}). \quad (7)$$

It is obvious from the above description that the performance of the network depends on the choice of regularization parameters. Large  $\lambda_i$  might result into large deviation from the data and very small  $\lambda_i$  may lead to overfitting. To reduce computational complexity involved in finding optimal regularization parameters, often a single regularization parameter is used i.e.,  $\lambda_i = \lambda, i = 0, 1, \dots, N_{RBF}$ . The most common methods to select optimal value of  $\lambda$  are generalized cross-validation based method [24, 25], or expectation maximization method [20]. Nevertheless, the computational cost of determining optimal regularization parameters is high for even moderate size problems, and increases with the number of samples. So a computationally efficient iterative procedure is implemented to select a ‘good’ regularization parameter in this study [26].

### Error Metrics for RBFs

The quality of above approximation is assessed by using different error metrics. The most common error metrics are described as follows.

#### Estimated variance of noise (NoiseVar)

The error in approximation at design points is,

$$\mathbf{e} = \mathbf{f} - H(H^T H + \Lambda)^{-1} H^T \mathbf{f} = (I - H(H^T H + \Lambda)^{-1} H^T) \mathbf{f} = P \mathbf{f}. \quad (8)$$

where  $I$  is an identity matrix of size  $N_{pt}$  and  $P = I - H(H^T H + \Lambda)^{-1} H^T$ .  $P$  is known as projection matrix. The square root of estimated variance of noise [18] is,

$$\hat{\sigma} = \sqrt{(\mathbf{e}^T \mathbf{e}) / \text{trace}(P)}. \quad (9)$$

Predicted residual sum of squares (PRESS)

Leave-one-out cross-validation error or PRESS is another popular and effective error measure [27, 28]. To compute PRESS, the response is approximated using the data at  $N_{pt} - 1$  points and this approximation is used to compute the actual error at the left out point. This procedure is repeated for all  $N_{pt}$  points by leaving each point exactly once. The expression for PRESS is

$$PRESS = \sum_{i=1}^{N_{pt}} (e_i^{PRESS})^2 = \sum_{i=1}^{N_{pt}} (f(\mathbf{x}^{(i)}) - \hat{f}^{-i}(\mathbf{x}^{(i)}))^2, \quad (10)$$

where  $\hat{f}^{-i}(\mathbf{x}^{(i)})$  is the predicted response at design point  $\mathbf{x}^{(i)}$  which was not used to construct the approximation  $\hat{f}^{-i}$ . The need to fit many networks to estimate PRESS can be obviated by using the projection matrix [18] and the vector of cross-validation error is computed as follows.

$$\mathbf{e}^{PRESS} = (\text{diag}(P))^{-1} P\mathbf{f}. \quad (11)$$

The root mean square of the PRESS which is compared to other error measures is

$$\hat{\sigma}_{PRESS} = \sqrt{PRESS / N_{pt}}. \quad (12)$$

Mean point-wise cross-validation error ratio (PRESS-ratio)

While the leave-one-out cross-validation error is a good measure of actual error, it might be susceptible to the large magnitude of error values. To avoid contamination of prediction error, an error ratio based criterion is given as follows:

$$\hat{\sigma}_{ratio} = (1 / N_{pts}) \sum_{i=1}^{N_{pts}} \left| f(\mathbf{x}^{(i)}) / \hat{f}^{-i}(\mathbf{x}^{(i)}) - 1 \right|. \quad (13)$$

This criterion would scale the magnitude of the errors thus eliminating the influence of a few large errors on the predictions but this criterion might assign more importance to the errors in the prediction of small values.

**RBF Network Topology Selection**

As discussed earlier, RBF network selection is a two-level optimization. The theoretical model for the second step, that is, the selection of weights for a given topology is well developed but there is no computationally efficient method available for the optimal selection of network topology (first step). Consequently, trial and error procedure is used to select the suitable RBF network topology and optimal weights are selected for the best topology.

A stepwise procedure to construct a radial basis function network that is adopted in LS-OPT<sup>®</sup> [26] is given as follows.

1. Sample design points
2. Evaluate responses at design points

3. Select the criterion to select network topology
4. Identify the number of neurons
  - a. Determine the spread constant
    - i. Determine the location of centers and corresponding radii [26]
    - ii. Estimate the best regularization parameter(s) using chosen topology selection criterion
    - iii. Estimate different error measures
  - b. Repeat the loop over different spread constants
5. Estimate the best spread using chosen topology selection criterion
6. Repeat the loop (Step 3) for different number of neurons
7. Select the network topology that results in the best performance over the chosen topology selection criterion.

There are three optimization steps in the selection of RBF network topology, i) estimation of the regularization parameter, ii) estimation of the spread constant selection, and iii) choice of the number of neurons. While the choice of selection criterion can be different at each step, a consistent choice is maintained here. A different criterion can be used as objective function of the optimization process, e.g., minimization of the variance of error, PRESS error, or PRESS-ratio.

In this paper, the influence of above-mentioned three error criteria on the selection of network topology is studied. To isolate the influence of error criterion on the prediction performance, the location of centers and radii is fixed across all networks for chosen experimental design [26]. For the sake of simplicity, a single regularization parameter is used for all weights  $\lambda_i = \lambda, \forall i$ .

## Test Problems and Performance Metrics

The performance of different RBF networks obtained by using different topology selection criteria is studied using a suite of analytical and engineering test problems on a few error metrics. These examples and relevant error metrics are given as follows.

### Test Problems

Different analytical problems and engineering example from crashworthiness simulations used in this study are described as follows.

#### Branin-Hoo function [30]

$$f(x_1, x_2) = 10 + 10 \left( 1 - \frac{1}{8\pi} \right) \cos(x_1) + \left( x_2 - \frac{5.1}{4\pi^2} x_1^2 + \frac{5.0}{\pi} x_1 - 6 \right), \quad (15)$$

$-5 \leq x_1 \leq 10, 0 \leq x_2 \leq 15.$

Camelback function [30]

$$f(x_1, x_2) = \left( \frac{x_1^4}{3} - 2.1x_1^2 + 4 \right) x_1^2 + x_1x_2 + (4x_2^2 - 4)x_2^2, \tag{16}$$

$$-3 \leq x_1 \leq 3, \quad -2 \leq x_2 \leq 2.$$

Goldstein-Price [30]

$$f(x_1, x_2) = \left[ 1 + (x_1 + x_2 + 1)^2 (19 - 4x_1 + 3x_1^2 - 14x_2 + 6x_1x_2 + 3x_2^2) \right] \times \left[ 30 + (2x_1 - 3x_2)^2 (18 - 32x_1 + 12x_1^2 + 48x_2 - 36x_1x_2 + 27x_2^2) \right], \tag{17}$$

$$-2 \leq x_1 \leq 2, \quad -2 \leq x_2 \leq 2.$$

Table 1 – Parameters in Hartman problem with three design variables.

<i>i</i>	<i>a<sub>ij</sub></i>			<i>c<sub>i</sub></i>	<i>p<sub>ij</sub></i>		
1	3.0	10.0	30.0	1.0	0.3689	0.1170	0.2673
2	0.1	10.0	35.0	1.2	0.4699	0.4387	0.7470
3	3.0	10.0	30.0	3.0	0.1091	0.8732	0.5547
4	0.1	10.0	35.0	3.2	0.03815	0.5743	0.8828

Table 2 – Parameters in Hartman problem with six design variables.

<i>i</i>	<i>a<sub>ij</sub></i>						<i>c<sub>i</sub></i>
1	10.0	3.0	17.0	3.5	1.7	8.0	1.0
2	0.05	10.0	17.0	0.1	8.0	14.0	1.2
3	3.0	3.5	1.7	10.0	17.0	8.0	3.0
4	17.0	8.0	0.05	10.0	0.1	14.0	3.2
<i>i</i>	<i>p<sub>ij</sub></i>						
1	0.1312	0.1696	0.5569	0.0124	0.8283	0.5886	
2	0.2329	0.4135	0.8307	0.3736	0.1004	0.9991	
3	0.2348	0.1451	0.3522	0.2883	0.3047	0.6650	
4	0.4047	0.8828	0.8732	0.5743	0.1091	0.0381	

Hartman [30]

$$f(\mathbf{x}) = - \sum_{i=1}^4 c_i \exp \left( - \sum_{j=1}^{N_v} a_{ij} (x_j - p_{ij})^2 \right), \tag{18}$$

$$0 \leq x_j \leq 1, \quad j = 1, N_v.$$

1. Three variables:  $N_v = 3$ , The parameters are given in Table 1.
2. Six variables:  $N_v = 6$ , The parameters are given in Table 2. For this example, all variables were allowed to vary between 0 and 0.5.

Jin et al. [31] – two variables J2

$$f(x_1, x_2) = [30 + x_1 \sin(x_1)] [4 + \exp(-x_2^2)],$$

$$0 \leq x_1 \leq 10, 0 \leq x_2 \leq 6.$$
(19)

Table 3 – Parameters used in JIN-10 function.

	Value		Value
$t_1$	-6.089	$t_6$	-14.986
$t_2$	-17.164	$t_7$	-24.100
$t_3$	-34.054	$t_8$	-10.708
$t_4$	-5.914	$t_9$	-26.662
$t_5$	-24.721	$t_{10}$	-22.179

Jin et al. [31] – ten variables J10

$$f(\mathbf{x}) = \sum_{j=1}^{10} x_j \left( t_j + \ln \left( x_j / \sum_{i=1}^{10} x_i \right) \right),$$

$$0.5 \leq x_j \leq 1, j = 1, N_v.$$
(20)

The parameters used in this function are given in Table 3.

Giunta and Watson [32]

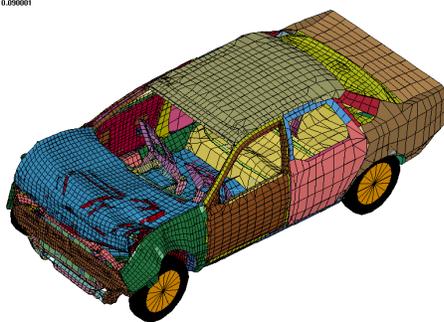
$$f(\mathbf{x}) = \sum_{j=1}^{10} \left( 0.3 + \sin \left( \frac{16}{15} x_j - 1 \right) + \sin^2 \left( \frac{16}{15} x_j - 1 \right) \right),$$

$$-1 \leq x_j \leq 1, j = 1, N_v.$$
(21)

This problem is studied for two instances of five and ten variables.

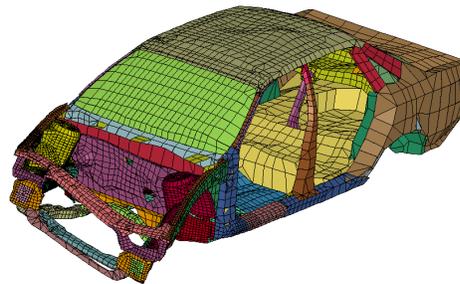
Multi-disciplinary analysis of a NHTSA vehicle undergoing full-frontal crash

FORD TAURUS MODEL  
Time = 0.000001



A) Crash simulation model

LS-DYNA eigenvalues at time 1.00000E-0  
Freq = 41.883



B) Body-in-white model for NVH simulation

Figure 2: Finite element models of a National Highway Transport and Safety Association vehicle.

Next, a multi-objective optimization problem of the crashworthiness simulation of a National Highway Transportation and Safety Association (NHTSA) vehicle undergoing full-frontal impact is considered. The goal of optimization is to simultaneously reduce mass and intrusion, while satisfying the constraints on the torsional frequency, maximum intrusion, and different stage pulses [33]. For this multi-disciplinary analysis, the finite element model, containing approximately 30000 elements, is obtained from the National Crash Analysis Center (NCAC website) [34]. A modal analysis of the vehicle is conducted on a so-called ‘body-in-white’ model with approximately 18000 elements. The crash and vibration finite element models are shown in Figure 2.



Figure 3: Exploded view of structural components influenced by design variables.

The design variables are the gauges of different structural members that are affected. These members include aprons, outer and inner rails, inner and outer shotguns, cradle rail, and cradle cross-members (Figure 3). The description and ranges of these seven design variables is given in Table 4. The mathematical formulation of the optimization problem is as follows:

Minimize

Mass  
Intrusion (xcrash)

Subject to:

Maximum intrusion  $\leq 551.27$  mm  
 Stage 1 pulse  $\geq 14.512$ g  
 Stage 2 pulse  $\geq 17.586$ g  
 Stage 3 pulse  $\geq 20.745$ g  
 $41.385$  Hz  $\leq$  Torsional mode frequency  $\leq 42.38$  Hz

The stage pulses are calculated from the SAE filtered (60 Hz) acceleration  $\ddot{x}$  and displacement  $x$  of a left rear sill node as

$$\text{Stage } j \text{ pulse} = -\frac{k}{(d_2 - d_1)} \int_{d_1}^{d_2} \ddot{x} dx; k = 0.5 \text{ for } j = 1, k = 1.0 \text{ otherwise} \quad (22)$$

The minus sign is used to convert acceleration to deceleration. The limits on the integration for different stage pulse are (0:184) for  $i=1$ , (184:334) for  $i=2$ , and (334: maximum displacement) for  $i=3$ . LS-DYNA [35] is used in explicit and implicit mode to simulate different designs.

Table 4 – Design variables used for crashworthiness simulation of the National Highway Transport and Safety Association (NHTSA) vehicle.

Variable Name	Lower Bound	Baseline Design	Upper Bound
Rail inner	1.0	2.0	3.0
Rail outer	1.0	1.5	3.0
Cradle rails	1.0	1.93	3.0
Apron	1.0	1.3	2.5
Shotgun inner	1.0	1.3	2.5
Shotgun outer	1.0	1.3	2.5
Cradle cross member	1.0	1.93	3.0

### Performance Metrics

The performance of the predictions was compared using the following three metrics

#### Correlation between predicted and observed responses

The correlation coefficient is calculated as

$$R(f, \hat{f}) = \frac{1}{V(\sigma(f)\sigma(\hat{f}))} \int_V (f - \bar{f})(\hat{f} - \bar{\hat{f}}) dV, \tag{23}$$

where  $\bar{f}$  and  $\sigma(f)$  are the mean and standard deviation of actual responses,  $\bar{\hat{f}}$  and  $\sigma(\hat{f})$  are the mean and standard deviation of predicted responses, and  $V$  is the volume of the domain. The mean and standard deviations are computed as,

$$\bar{f} = \frac{1}{V} \int_V f dV; \quad \sigma(f) = \sqrt{\frac{1}{V} \int_V (f - \bar{f})^2 dV}. \tag{24}$$

High correlation coefficient is desired for a good quality of approximation.

The above equations are numerically evaluated using the data at test points by implementing quadrature for integration [36] as follows,

$$\bar{f} = \frac{\sum_{i=1}^{N_{test}} \gamma_i f_i}{\sum_{i=1}^{N_{test}} \gamma_i}; \quad \sigma(f) = \sqrt{\frac{\sum_{i=1}^{N_{test}} \gamma_i (f_i - \bar{f})^2}{\sum_{i=1}^{N_{test}} \gamma_i}}. \tag{25}$$

$$\frac{1}{V} \int_V \hat{f} dV = \sum_{i=1}^{N_{test}} \gamma_i f_i \hat{f}_i / \sum_{i=1}^{N_{test}} \gamma_i. \quad (26)$$

In the above equations,  $\gamma_i$  represents the weight associated with the  $i^{th}$  test point, as determined by the quadrature for integration. For uniform grid of points, the Simpson's integration rule is used whereas for non-uniform grids Monte-Carlo integration method is used.

The correlation coefficient captures the prediction trends but yields no information about the actual errors in approximation, which can be high despite a high correlation. So the approximation errors are quantified using two error-based criteria.

#### Root mean square error in the predictions

The root mean square error at test points is given as,

$$RMSE = \sqrt{\frac{1}{V} \int_V (f - \hat{f})^2 dV}. \quad (27)$$

Using the quadrature, the RMSE is estimated as,

$$RMSE = \sqrt{\sum_{i=1}^{N_{test}} \gamma_i (f_i - \hat{f}_i)^2 / \sum_{i=1}^{N_{test}} \gamma_i}. \quad (28)$$

#### Maximum absolute error in the predictions

Another measure of the quality of any approximation is the maximum absolute error.

A good approximation yields low errors and high correlation.

## **Test Procedure and Numerical Setup**

### **Test Procedure**

For each test example, the stepwise test procedure to identify the best topology selection criterion is outlined as follows:

1. Identify an experimental design.
2. Evaluate response at the design points.
3. Identify different RBF network topologies using the following criteria
  - a. Minimize square root of the estimated variance of noise
  - b. Minimize root mean square of the PRESS error
  - c. Minimize mean PRESS-ratio.
4. For each RBF network, estimate predicted response and error at test points.
5. For each network, compute test metrics.
6. Repeat procedure starting from Step 1, 1000 times for analytical examples and 100 times for engineering example to minimize the influence of experimental designs.
7. Summarize the results using mean and coefficient of variation of test metrics.

## Numerical Setup

The numerical setup used to analyze different examples is summarized in Table 5. The number of sampling points is taken such that reasonable approximation of the underlying function can be obtained. For all analytical examples, the experimental designs were selected in two steps. Firstly, a large set with  $N_{LHS}$  points is generated using a Latin hypercube sampling (LHS)<sup>1</sup> criterion. This set is used as the basis set to select  $N_S$  points using D-optimality criterion [37]. 1000 experimental designs were used to minimize the influence to experimental designs. To compare different approximations,  $N_{test}$  independent test points, selected using Latin hypercube sampling criterion, were used. For the crashworthiness example, 4800+ designs were analyzed during a multi-objective optimization using genetic algorithms. This data set is used as basis set to select  $N_S$  experimental designs using D-optimality criterion. 100 experimental designs were used to study the influence of experimental designs. All points were used as test points.

Table 5 – Numerical setup for different example problems.  $N_v$  is the number of variables,  $N_{pts}$  is the number of samples used for approximation,  $N_{LHS}$  is the number of basis points used for D-optimality criterion, and  $N_{test}$  is the number of test points.

Problem	$N_v$	$N_{pts}$	$N_{LHS}$	$N_{test}$
<b>Branin-Hoo</b>	2	20	100	150
<b>Camelback</b>	2	30	150	150
<b>Goldstein-Price</b>	2	42	200	150
<b>Jin-2</b>	2	30	150	150
<b>Hartman-3</b>	3	70	250	500
<b>GW5</b>	5	80	300	2000
<b>Hartman-6</b>	6	56	200	2000
<b>Jin-10</b>	10	150	500	5000
<b>GW10</b>	10	100	350	5000
<b>NHTSA</b>	7	250	4847	4847

## Results and Discussion

In this section, the results of comparison among different criterion for network selection are summarized. Results for analytical examples and crash-worthiness simulation are summarized in Figure 4 and Figure 5, respectively.

### Correlation Coefficient

While no single criterion performed the best for all examples, the PRESS error and the estimated noise variance criteria performed quite well for most analytical examples. The RBF networks selected using PRESS criterion performed consistently well for all examples. The networks selected using PRESS-ratio resulted in the worst performance among all topology-selection

<sup>1</sup> Matlab routine 'lhsdesign' with 'maximin' criterion that maximizes the minimum distance between points is used to generate LHS designs. 500 iterations were used to find an optimum design.

criteria for analytical examples. The RBF network topologies selected using the estimated noise variance criterion was good, particularly for high dimension analytical examples.

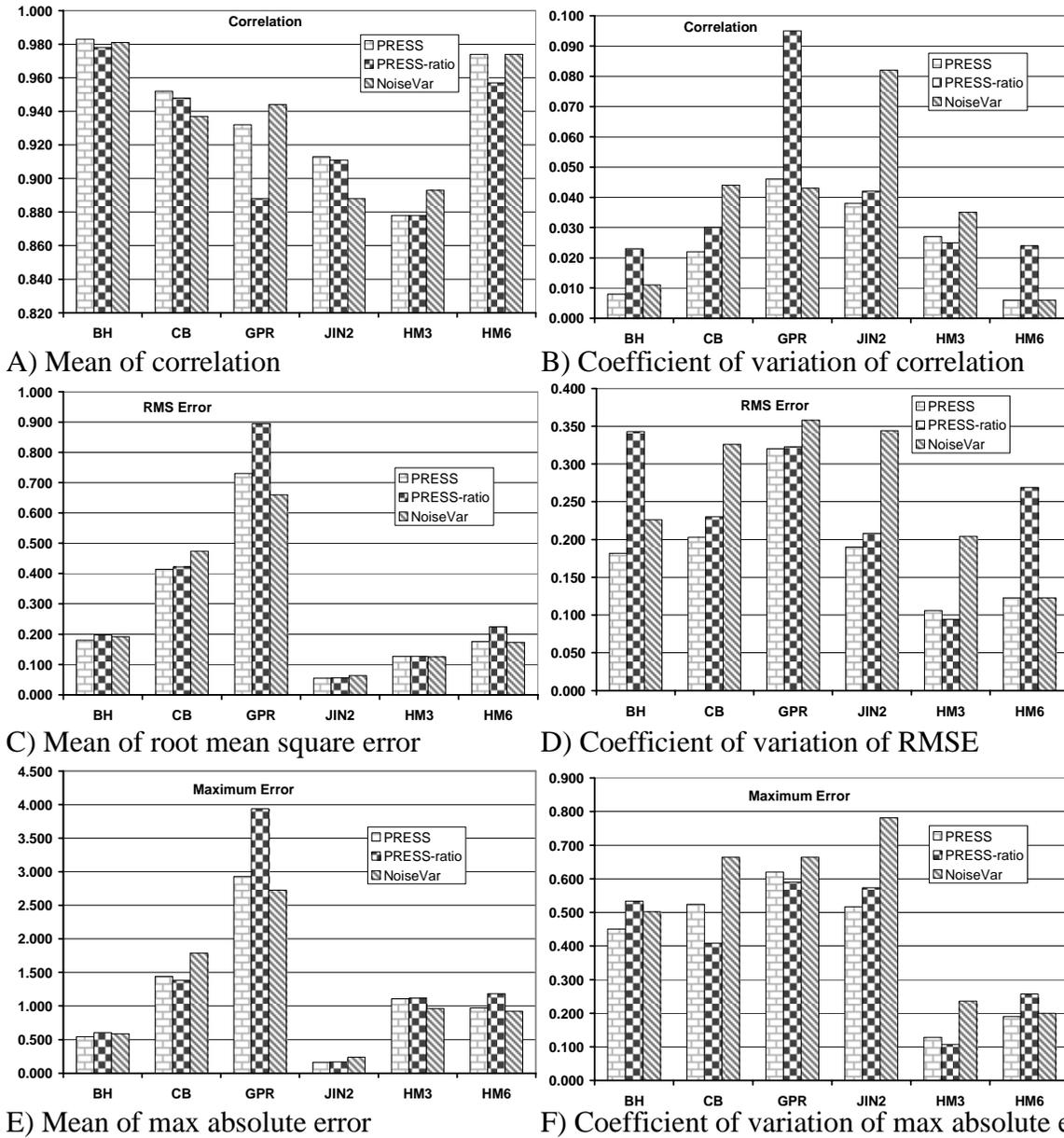


Figure 4: Comparison of different RBF network topology selection criteria (PRESS: predicted residual sum of squares, PRESS-ratio: averaged pointwise ratio of PRESS errors, NoiseVar: estimated variance of noise) for analytical examples (based on 1000 DOEs). BH – Branin-Hoo, CB – Camelback, GPR – Goldstein-Price, JIN2 – Jin et al. problem with two variables, HM3 – Hartman problem with three variables, HM6 – Hartman problem with six variables.

However, as is evidenced in Figure 5, RBF network topology selection using PRESS and PRESS-ratio based criteria significantly outperformed estimated noise variance based criterion for approximation of responses in crash-worthiness simulation example. The estimated noise variance based criterion to select network topology had a high sensitivity to the choice of experimental designs (high coefficient of variation) and the problem. On the other hand, both the

PRESS based topology selection criterion and the PRESS-ratio based criterion performed comparably.

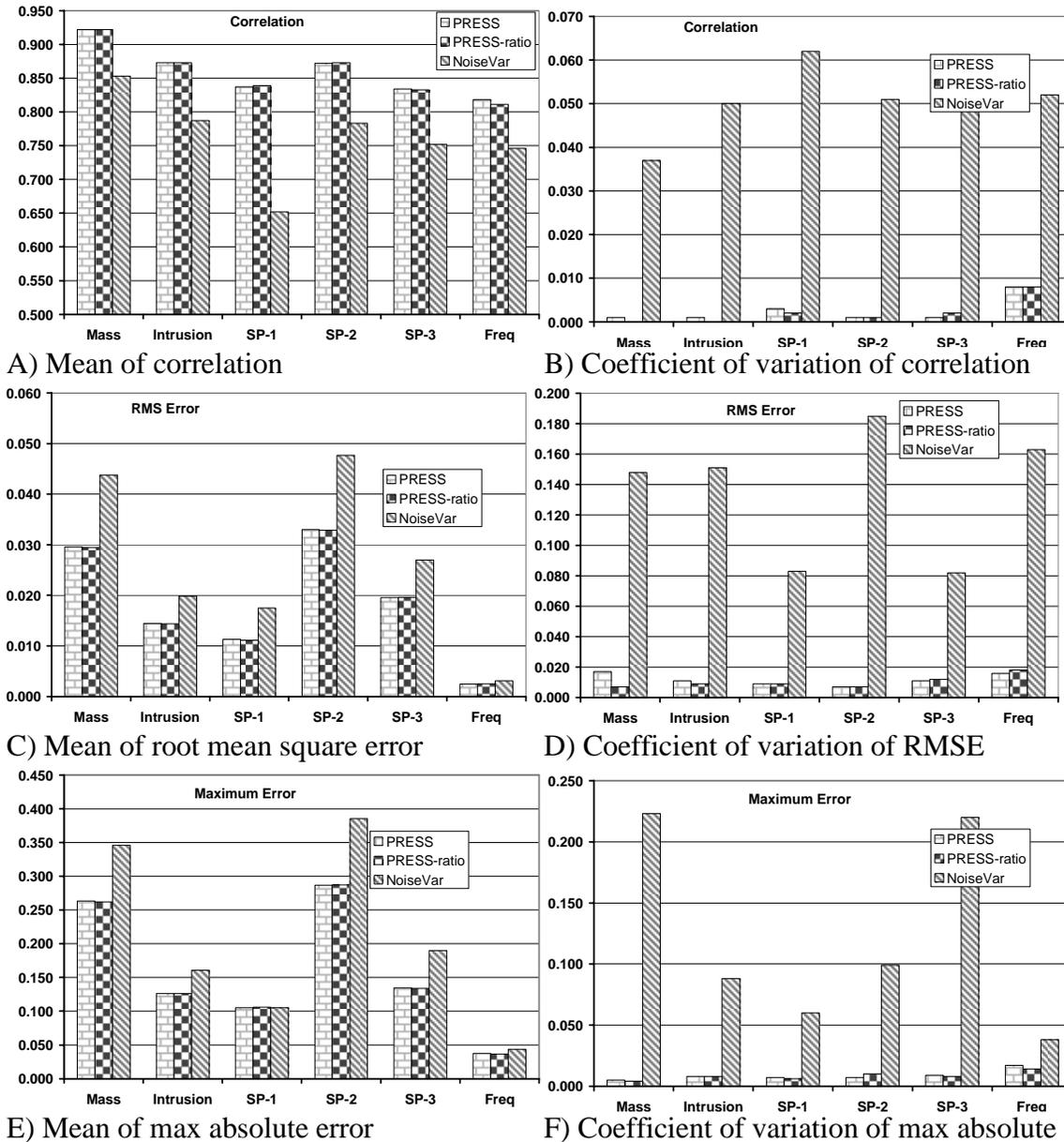


Figure 5: Comparison of different RBF network topology selection criteria (PRESS: predicted residual sum of squares, PRESS-ratio: averaged pointwise ratio of PRESS errors, NoiseVar: estimated variance of noise) for approximation of responses in crashworthiness simulations (based on 100 DOEs). SP-1 indicates Stage 1 pulse, SP-2 is Stage 2 pulse and SP-3 is Stage 3 pulse.

### Root Mean Square Error

It was observed that the network selected using the PRESS error based criterion consistently resulted in low RMS errors for both analytical examples and the crashworthiness simulation. The performance of the PRESS-ratio based criterion was good for crashworthiness simulation

example and the estimated noise variance based criterion yielded good performance for analytical examples only. The RBF network topology selection using the PRESS-ratio based criterion resulted in poor approximation of analytical examples. The network topologies selected using estimated noise variance based criterion approximated the responses in crashworthiness simulation very poorly. The estimated noise variance criterion based topology selection also resulted in high variability with the experimental designs.

### Maximum Absolute Error

The results obtained for root mean square errors in approximation were valid for maximum absolute error test metric. Using the PRESS criterion to select network topology yielded robust performance for all analytical and crash-simulation performances, whereas the estimated noise variance based criterion was good only for analytical problems and the PRESS-ratio based criterion resulted in good approximations only for crashworthiness simulations.

## Conclusions

The results indicated that the choice of best network topology selection criterion depends on the problem and experimental design. However, the PRESS-based criterion to select RBF network topology results in robust performance for all examples and experimental designs. For analytical examples, the estimated noise variance based RBF network topology selection criterion was significantly better than other criteria, particularly for high dimension problems. On the other hand, the PRESS-ratio based criterion yielded good RBF approximations for crashworthiness simulations. The results for estimated noise variance based criterion were more sensitive to the choice of experimental designs.

## References

1. Kurdila AJ, Peterson JL, "Adaptation of Centers of Approximation for Nonlinear Tracking Control", *Journal of Guidance Control, and Dynamics*, 19(2), 1996, pp. 363-369.
2. Li Y, Sundarajan N, Saratchandran P, "Stable Neuro-Flight Controller Using Fully Tuned Radial Basis Function Neural Networks", *Journal of Guidance, Control and Dynamics*, 24(4), 2001.
3. Young A, Cao C, Patel V, Hovakimyan N, Lavertsky E, "Adaptive Control Design Methodology for Nonlinear-in-Control Systems in Aircraft Application", *Journal of Guidance, Control and Dynamics*, 30(6), 2007.
4. Wheeler KR, Dhawan AP, Meyer CM, "Space Shuttle Main Engine Sensor Modeling using Radial Basis Function Neural Networks", *Journal of Spacecraft and Rockets*, 31(6), 1994, pp. 1054-1060.
5. Papila N, Shyy W, Griffin L, Dorney DJ, "Shape Optimization of Supersonic Turbines using Global Approximation Methods", *Journal of Propulsion and Power*, 18(3), 2002, pp. 509-518.
6. Shyy W, Papila N, Vaidyanathan R, Tucker K, "Global Design Optimization for Aerodynamics and Rocket Propulsion Components", *Progress in Aerospace Sciences*, 37(1), 2001, pp. 59-118.
7. Karakasis MK, Giannakoglou KC, "On the use of Metamodel Assisted Multi-objective Evolutionary Algorithms", *Engineering Optimization*, 38(8), 2006, pp. 941-957.
8. Meckesheimer M, Barton RR, Simpson T, Limayen F, Yannou B, "Metamodeling of Discrete/Continuous Responses", *AIAA Journal*, 39(10), 2001, pp. 1950-1959.
9. Rocha H, Li W, Hahn A, "Principal Component Regression for Fitting Wing Weight Data of Subsonic Transports", *Journal of Aircraft*, 43(6), 2006, pp. 1925-1936.
10. Zhang T, Choi KK, Rahman S, Cho K, Baker P, Shakil M, Heitkamp D, "A Hybrid Surrogate and Pattern Search Optimization Method and Application to Microelectronics", *Structural and Multi-disciplinary Optimization*, 32(4), 2006, pp. 327-345.

11. Reddy RRK, Ganguli R, "Structural Damage Detection in a Helicopter Rotor Blade using Radial Basis Function Neural Networks", *Smart Materials and Structures*, 12, 2003, pp. 232-241.
12. Glaz B, Friedmann PP, Liu L, "Surrogate based Optimization of Helicopter Rotor Blades for Vibration Reduction in Forward Flight", *Structural and Multi-disciplinary Optimization*, in press.
13. Panda SS, Chakraborty D, Pal SK, "Flank Wear Prediction in Drilling using Back Propagation Neural Networks and Radial Basis Function Network", *Applied Soft Computing*, 2007, in press.
14. Lanzi L, Castelletti LML, Anghileri M, "Multi-objective Optimization of Composite Absorber Shape under Crashworthiness Requirements", *Composite Structures*, 65(3-4), 2004, pp. 433-441.
15. Fang H, Rais-Rohani M, Liu A, Horstemeyer MF, "A Comparative Study of MetaModeling Methods for Multi-objective Crashworthiness Optimization", *Computers and Structures*, 83(25-26), 2005, pp. 2121-2136.
16. Orr MJL, "Local Smoothing of Radial Basis Function Networks", Center for Cognitive Science, University of Edinburgh, 1995.
17. Orr MJL, "Regularization in the Selection of Radial Basis Function Centers", Center for Cognitive Science, University of Edinburgh, 1995.
18. Orr MJL, "Introduction to Radial Basis Function Networks", Center for Cognitive Science, University of Edinburgh, 1996.
19. Orr MJL, "Optimizing the Widths of Radial Basis Functions", Center for Cognitive Science, University of Edinburgh, 1998.
20. Orr MJL, "Recent Advances in Radial Basis Function Networks", Institute of Adaptive and Neural Computation, University of Edinburgh, 1999.
21. Hardy RL, "Multiquadrics Equations of Topography and Other Irregular Surfaces", *Journal of Geophysical Research*, 76, 1991, pp. 1905-1915.
22. Mullur AA, Messac A, "Extended Radial Basis Functions: More Flexible and Effective Metamodeling", *AIAA Journal*, 43(6), 2005, pp 1306-1315.
23. Tikhonov AN, Arsenin VY, *Solutions to Ill-posed Problems*, Wiley, New York, 1977.
24. Golub G, Heath M, Wahba G, "Generalized Cross-Validation as a Method for Choosing a Good Ridge Parameter", *Technometrics*, 21(2), 1979, pp. 215-223.
25. Golub GH, von Matt U, "Generalized Cross-Validation for Large Scale Problems", *Journal of Computational and Graphical Statistics*, 6(1), 1997, pp. 1-34.
26. Livermore Software Technology Corporation, "LS-OPT Manual v 3.3", Livermore CA, 2007.
27. Goel T, Haftka RT, Shyy W, Queipo NV, "Ensemble of Surrogates", *Structural and Multidisciplinary Optimization*, 33, 2007, pp. 199-216.
28. Goel T, Haftka RT, Shyy W, "Error Measures on Surrogate Approximation Based on Noise-free Data", In *Proceedings of 46th AIA Aerospace Sciences Meeting and Exhibit*, Reno NV, 2008, AIAA-2008-0901.
29. Deb K, *Multi-Objective Optimization Using Evolutionary Algorithms*, Wiley Chichester, 2001.
30. Dixon LCW, Szego GP, *Towards Global Optimization 2*, North Holland, Amsterdam, 1978.
31. Jin R, Chen W, Simpson T, "Comparative Studies of Metamodeling Techniques under Multiple Modeling Criteria", *Structural and Multidisciplinary Optimization*, 23(1), 2001, pp. 385-398.
32. Giunta AA, Watson LT, "A Comparison of Approximation Modeling Techniques: Polynomial versus Interpolating Models", In *Proceedings of 7th AIAA/UAF/NASA/ISSMO Symposium on Multidisciplinary Analysis and Optimization*, St. Louis MO, 1998, AIAA-98-4758.
33. Craig KJ, Stander N, Dooge DA, Varadappa S, "Automotive Crashworthiness Design Using Response Surface-Based Variable Screening and Optimization", *Engineering Optimization*, 22(1), 2005, pp. 38-61.
34. National Crash Analysis Center (NCAC), Public Finite Element Model Archive, [www.ncac.gmu.edu/archives/model/index.html](http://www.ncac.gmu.edu/archives/model/index.html), 2001
35. Livermore Software Technology Corporation, "LS-Dyna Manual v 971", Livermore CA, 2007.
36. Ueberhuber CW, *Numerical Computation 2: Methods, Software, and Analysis*, Springer, New York, p 71.
37. Goel T, Haftka RT, Shyy W, Watson LT, "Pitfalls of Using a Single Criterion for Selecting Experimental Designs", *International Journal of Numerical Methods in Engineering*, 2008, in press.