MODELLING AND ANALYSIS OF SIMPLE PENDULUM COMPUTER EXPERIMENTS USING A SUPPORT VECTOR REGRESSION MODEL WITH B-SPLINES KERNEL FUNCTION

KAZEEM ADEWALE OSUOLALE

Department of Statistics, University of Ibadan, Nigeria
E-mail: ka.osuolale@ui.edu.ng; whereisqosimadewale@gmail.com

Abstract - Computer experimentation technique has been commonly applied as an alternative approach to physical experiment in engineering, science and technology in the recent time. It is more accepted than the classical physical experiments due to its flexibility when developing computer experiments and building metamodels of computer models. Sometimes, it is used to complement or serve as a proxy to real life or physical experiments. Experimental design is rapidly growing since it is useful to both physical processes and computer or simulation models. In this study, an Orthogonal Array Latin Hypercube Design, OA (N, k) LHD was used to develop simple pendulum computer experiments. The OA (49, 3) LHD was adopted in the development of simple pendulum computer experiments using a simple pendulum model. This model was used to simulate a simple pendulum experiment that is conventionally performed in the laboratory. A Support Vector Regression (SVR) model was employed as a computer based metamodel to mimic the simple pendulum computer model in order to reduce the required computational efforts in running the computer codes and predict the stoppage time of pendulum at untried inputs. The SVR algorithm was used for modelling and analysing simple pendulum computer experiments. MATLAB 2016 software was used to implement the SVR algorithm with B-Splines kernel function so that the SVR model adequately captures non-linearities in the simple pendulum computer model. The e-insensitive loss function was set at e=0.05 and C=8 in order to control the support vector regression model. Results obtained using the SVR model with B-Splines function trained with only 85.7% of the experimental runs with zero bias. The fitted SVR model predicted values that were close to the test data as shown in Figure 1.

Index Terms - Computer Experiments, B-splines Kernel Function, SVR Model, Orthogonal Array Latin Hypercube Design, Simple Pendulum Computer Model.

I. INTRODUCTION

Conventional experimental design has its origin from the theory of Design of Experiments (DOE) when physical experiments are carried out (Montgomery, 2001) whereas space-filling designs are more connected with computer experiments. Computer experimentations differ greatly from physical experiments because they deal with functions that are considered to have more complex behaviour without random error since the typical computer experiments are expected to be deterministic in nature. For instance, the simple pendulum model which has been used as a computer model by Osuolale et al. (2014a) is deterministic. This same model has been considered in this study.

Computer experiments are more commonly employed in engineering, science and technology because the conventional physical experiments could require more cost in term of time, money and some other resources for its implementation. Some circumstances may require that computer experiments be conducted prior to laboratory or physical experiments so that computer experiments can serve as a prototype for the real life situations. A computer experiment is carried out by using data obtained from a mathematical model, known as a computer model in lieu of the physical process (Osuolale et al., 2014a). The Orthogonal Array Latin Hypercube Design (OALHD) originally constructed by Osuolale et al. (2014b) is adopted in the development of a computer experiment and the SVR model is used to emulate the simple pendulum computer model.

II. MATERIALS AND METHODS

Modelling and analysis in this study were performed using 9.0.0.341360 (R2016a) MATLAB software. Orthogonal array-based Latin hypercube design (OALHD) was used to develop a computer experiment using a simple pendulum model and the SVR model was subsequently used to serve as an emulator of a simple pendulum computer model. The constructed OA (49, 3) LHD and its plot for projection properties among the three input variables are given in Table 1 and Figure 1(Osuolale, et al., 2014b), respectively. A simple pendulum experiment has been proposed as a novel application in the field of computer experiments by Osuolale et al. (2014a). Osuolale et al. (2015) have also investigated a simple pendulum model using a Gaussian process model as an emulator.

The adopted OA (49, 3) LHD was scaled according to the assumed range of the input variables given in Table 1 using:

$$y_{OALHD} = \frac{y_{data} - y_{datamin}}{y_{datamax} - y_{datamin}} \qquad (1)$$

$$y_{data} = y_{OALHD}(y_{datamax} - y_{datamin}) + y_{datamin}$$

Table 1. Input and output variables for training datasets

Variable	Variable name	Minimum	Maximum
X_1 (L)	Length (m)	0.2	0.49
X_2 (θ)	Angle (degree)	5	42.59
X_3 (M)	Mass (kg)	0.01	0.0459
Y	Stoppage Time (s)	-	-

The scaled OA (49, 3) LHD was used to develop a simple pendulum computer experiment using the non-linear differential equation as its model (MATLAB Basics, 2003) to produce the output of a simple pendulum computer experiment.

$$ML^2\frac{d^2\theta}{dt^2} + b\frac{d\theta}{dt} + MgLsin(\theta) = 0$$

$$\frac{d^2\theta}{dt^2} = \frac{-b\frac{d\theta}{dt} - MgLsin(\theta)}{ML^2} \qquad (2)$$

where

$y = \frac{d^2\theta}{dt^2}$ = stoppage time of the pendulum bob

M = mass of the pendulum bob(kg)

L = length of the pendulum(m)

θ = the pendulum displacement angle (degree)

b = coefficient of friction (Ns/rad)

g = acceleration (ms^{-2}) due to gravity

The coefficient of friction is denoted by b in Equation 2 and is fixed at 0.02Ns/rad and the acceleration due to gravity, g is given as 9.81 ms^{-2}. The scaled input variables and the output simulated from a simple pendulum computer model now constitute the experimental outcomes for the training datasets.

Table 2. Simple Pendulum Computer Experimental Data Based on the Assumed Ranges for Training Datasets

Run	X_1	X_2	X_3	Y
1	0.2270	8.4470	0.0119	8.8500
2	0.2319	12.8375	0.0129	8.2200
3	0.2368	17.2279	0.0139	7.5800
4	0.2418	21.6184	0.0150	6.9700
5	0.2467	26.0088	0.0160	6.3900
6	0.2516	30.3993	0.0170	5.8500
7	0.2565	34.7898	0.0181	5.3300
.	.	.	.	.
.	.	.	.	.
.	.	.	.	.
31	0.3745	19.7368	0.0186	3.5100
32	0.3794	24.1272	0.0125	4.4200
33	0.3843	28.5177	0.0135	3.3100
34	0.3892	32.9081	0.0145	2.8400
35	0.3942	37.2986	0.0155	3.2500
36	0.3991	11.5830	0.0178	2.6300
37	0.4040	15.9735	0.0188	3.3100
38	0.4089	20.3640	0.0126	2.4800
39	0.4138	24.7544	0.0136	2.6200
40	0.4187	29.1449	0.0147	3.1600
41	0.4237	33.5353	0.0157	3.7300
42	0.4286	37.9258	0.0167	3.5000
43	0.4335	12.2102	0.0189	2.4000
44	0.4384	16.6007	0.0128	2.5400
45	0.4433	20.9912	0.0138	3.1300
46	0.4482	25.3816	0.0148	3.7300
47	0.4532	29.7721	0.0158	4.3400
48	0.4581	34.1626	0.0169	4.1900
49	0.4630	38.5530	0.0179	4.8600

III. MODELLING AND ANALYSIS OF SIMPLE PENDULUM COMPUTER EXPERIMENTS

A Support Vector Regression (SVR) model was investigated as an alternative technique for approximating a simple pendulum computer model. This model was employed as a metamodel to abate the computational efforts in using computer codes. A metamodel is referred to as a model utilized to mimic another model. A myriad of techniques have been discussed in the literature for creating metamodels (Strogatz, 2003). Some of these techniques include response surface modelling (Myers and Montgomery, 1995), Radial Basis Functions (Dyn, et al., 1986; Fang and Horstemeyer, 2006) and Multivariate Adaptive Regression Splines (Friedman, 1991). Osuolale et al. (2018) has also modeled and analysed simple pendulum computer experiments using a SVR with Gaussian Radial Basis Function(GRBF). The SVR algorithm (Gunn, 1998) was adopted for modelling and analysing simple pendulum computer experiments with B-Splines kernel function to ensure that the SVR efficiently captures non-linearities in the simple pendulum model. The SVR problem can be formulated as the minimization of the following function:

$$\frac{1}{2}\|w\|^2 + C\sum_{i=1}^{n}\left(\xi_i + \xi_i^*\right) \qquad (3)$$

$$such\ that \begin{cases} y_i - (w.x_i) - b \le \varepsilon + \xi_i^* \\ (w.x_i) + b - y_i \le \varepsilon + \xi_i \\ \xi_i^*, \xi_i \ge 0 \end{cases} \qquad (4)$$

where C is a positive constant or the penalty parameter and ε is the insensitive zone which can be chosen by the user. The parameter ε determines the width of the epsilon insensitive zone. The optimization problem in Equation (3) and the constraints in Equation (4) can be written as a Lagrangian function:

$$L = \frac{1}{2}\|w\|^2 + C\sum_{i=1}^{n}\left(\xi_i + \xi_i^*\right) - \sum_{i=1}^{n}\alpha_i(\varepsilon + \xi_i - y_i + (w.x_i) + b) - \sum_{i=1}^{n}\alpha_i^*(\varepsilon + \xi^*{}_i + y_i - (w.x_i) - b) - \sum_{i=1}^{n}\left(v_i\xi_i + v_i^*\xi_i^*\right) \qquad (5)$$

where v_i and v_i^* are additional slack variables. The dual form optimization problem is given as:

$$\max imize \begin{cases} -\frac{1}{2}\sum_{i,j=1}^{n}(\alpha_i - \alpha_i^*)(\alpha_j - \alpha_j^*)(x_i.x_j) \\ -\varepsilon\sum_{i=1}^{n}(\alpha_i + \alpha_i^*) + \sum_{i=1}^{n}y_i(\alpha_i - \alpha_i^*) \end{cases}$$

$$such\ that \begin{cases} \sum_{i=1}^{n}(\alpha_i - \alpha_i^*) = 0 \\ (\alpha_i - \alpha_i^*) \in [0, C] \end{cases} \qquad (6)$$

and **w** is given as:

$$w = \sum_{i=1}^{n}(\alpha_i^* - \alpha_i)x_i \qquad (7)$$

The linear regression expressed can be written as:

$$f(x) = \sum_{i=1}^{n}(\alpha_i - \alpha_i^*)(x_i.x_i) + b \qquad (8)$$

where (x_i, x_i) is the dot products of two points and the variables
$\propto_i, \propto_i^*$ and b are estimated by the SVR algorithm following Smola and Scholkopf (2004). Replacing the dot products $(X_i.X_i)$ with a kernel function, K, in the approximation function, equation (8) becomes the nonlinear SVR approximation as:

$$f(x) = \sum_{i=1}^{n} (\alpha_i - \alpha_i^*) K(x_i.x_j) + b \qquad (9)$$

where $K(x_i.x_j) = B_{2N+1}(x_i - x_j^T)$ is the B-Splines kernel function and the algorithm adopted actually implements the model as:

$$\{N_s, \beta, bias\} = f(Xdata(X), Ydata(Y), kernel(Ker), Cost(C), loss, insensitivity(\epsilon)) \quad (10)$$

The three variables involved as shown in Table 2 were normalized to reduce the dimension effect of each design variable and prevent an erratic prediction of the SVR model. The results are provided in Table 3.

Table 3: Results of SVR Using B-Splines Function

SVR Using B-Splines Function			
SV **Bias** **Sum Beta** **$\|w_0\|$^2**	42(85.7%) 0.000 0.030001 0.351313	C e	8 0.05

The results presented in Table 3 showed that SVR model using B-Splines function trained with 85.7% of the experimental data. The B-Splines SVR has zero bias and it also indicated that not all the data generated from the experimental runs are support vectors. The regression model was controlled by the loss function, the kernel and additional capacity control, C. The e-insensitive loss function was utilized with e=0.05 and C=8. The results presented in Table 3 showed that SVR model using B-Splines function trained with 85.7% of the experimental data . The B-Splines SVR has zero bias and it also indicated that not all the data generated from the experimental runs are support vectors. The regression model was controlled by the loss function, the kernel and additional capacity control, C. The e-insensitive loss function was utilized with e=0.05 and C=8. A simple pendulum computer experiment was performed with the test data to assess the prediction accuracy of the SVR model. This assessment makes it possible to find out how well the SVR model predicts the output of the experiment at untried inputs. The assumed range of design variables for the test data and the experimental data for the test data were given in Table 4 and Table 5, respectively.

Table 4. Input and output variables for test datasets

Variable	Variable name	Minimum	Maximum
X_1 (L)	Length (m)	0.2	0.49
X_2 (θ)	Angle (degree)	5	42.59
X_3 (M)	Mass (kg)	0.01	0.0459
Y	Stoppage Time (s)	-	-

Table 5. Simple Pendulum Computer Experimental Data Based on the Assumed Ranges for Test Datasets

Run	X_1	X_2	X_3	Y
1	0.5466	47.3786	0.0517	17.21
2	0.5551	52.9557	0.0531	21.1
3	0.5635	58.5328	0.0546	12.94
4	0.572	64.1098	0.056	23.71
5	0.5805	69.6869	0.0575	24.66
6	0.589	75.264	0.059	24.08
7	0.5974	80.841	0.0604	24.27
.	.	.	.	.
.	.	.	.	.
.	.	.	.	.
31	0.8009	61.7197	0.0613	48.69
32	0.8093	67.2967	0.0525	43.55
33	0.8178	72.8738	0.054	44.72
34	0.8263	78.4509	0.0554	48.64
35	0.8348	84.0279	0.0569	29.68
36	0.8432	51.3622	0.06	37.93
37	0.8517	56.9393	0.0615	51.12
38	0.8602	62.5164	0.0527	46.74
39	0.8687	68.0934	0.0542	52.62
40	0.8771	73.6705	0.0556	48.22
41	0.8856	79.2476	0.0571	40.95
42	0.8941	84.8247	0.0586	45
43	0.9026	52.159	0.0617	63.09
44	0.911	57.736	0.0529	49.04
45	0.9195	63.3131	0.0544	50.27
46	0.928	68.8902	0.0558	47.65
47	0.9365	74.4672	0.0573	65.4
48	0.9449	80.0443	0.0588	69.66
49	0.9534	85.6214	0.0602	72.98

The three variables were also standardized for the purpose of prediction since the training datasets used to build the model were normalized.

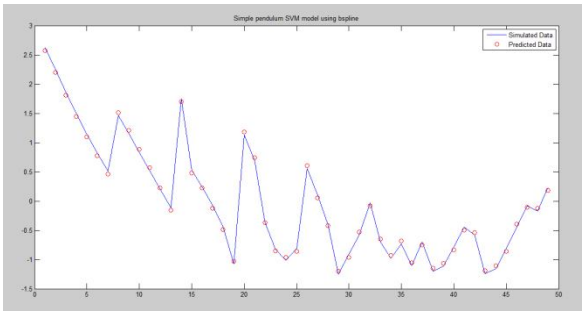


Figure 1: Graph of the Predicted y against Simulated Output

The graph in Figure 1 for SVR with B-Splines kernel function showed the plot of the predicted y against the simulated output. The SVR model with B-Splines function gave rough approximations of the test data. The predictions were not exact but close to the simulated output. SVR model did not interpolate the test data and therefore regarded as an approximating model.

DISCUSSION OF RESULTS

The OA (49, 3) LHD was used to develop a simple pendulum computer experiment by scaling OA(49, 3)LHD and then applied Equation 1 to obtain the experimental output. The scaled input variables and the output obtained constitute the experimental results for the training data sets. The B-Splines Support Vector Regression (BSVR) model was fitted using the training data sets. The BSVR model showed that trained with 85.7% of the experimental data with zero bias. The test data were also simulated using a 49-run experimental design in order to test the accuracy of the BSVR model. These test data were used on the fitted SVR model to predict the stoppage time of pendulum and the result of the predictions were close to the test data as shown in Figure 1. This indicates that the fitted BSVR model is fairly efficient at modelling and predicting the stoppage time of a pendulum.

CONCLUSION

This study has dealt with modelling and analysis of simple pendulum computer experiments using a support vector regression model with B-Splines function. The SVR model with B-Splines kernel function modelled the simple pendulum computer experimental data fairly well with zero bias and predicted the stoppage time of pendulum better, though the predicted output did not give exact estimates for the simulated output. The SVR model predicted the simulated output differently and is therefore termed an approximating model of a simple pendulum model. This study concluded that SVR model with B-Splines function is good at modelling and predicting the stoppage time of simple pendulum using a 49-run experimental design. Comparisons of the outcomes of the Support Vector Regression (SVR) model with both B-Splines and Gaussian Radial Basis Function (GRBF) kernel functions shall be made so as to identify the one with minimal error as well as prediction accuracy for future research.

REFERENCES

[1] J. Smola, and B. Scholkopf, "A tutorial on support vector regression," Statistics and Computing, vol. 14, pp. 199–222, 2004.

[2] N. Dyn, D. Levin, and S. Rippa, "Numerical procedures for surface fitting of scattered data by radial basis functions," SIAM Journal of Scientific and Statistical Computing, vol. 7, pp. 639-659, 1986.

[3] H. Fang, and M. F. Horstemeyer, "Global response approximation with radial basis functions," Journal of Engineering Optimization, vol. 38, pp. 407-424, 2006.

[4] J. H. Friedman, "Multivariate adaptive regressive splines," The Annals of Statistics, vol. 19, pp. 1-67, 1991.

[5] S. R. Gunn, "Support vector machines for classification and regression," Technical Report, University of Southampton, 1998.

[6] MATLAB Basics, "Matlab/simulink tutorial (2nd Ed.)," School of Electrical, Electronic and Computer Engineering, University of Newcastle Upon Tyne, 2003.

[7] D.C. Montgomery, " Design and analysis of experiments (5th Ed.)," John Willey and Sons, Inco., New York, 2001.

[8] R. H. Myers, and D. C. Montgomery, "Response surface methodology: Process and product optimization using designed experiments," Wiley Series in Probability and Statistics. New York, NY: John Wiley and Sons, 1995.

[9] K. A. Osuolale, W. B. Yahya, and B. L. Adeleke, " Performing a simple pendulum experiment as a demonstrative example for computer experiments,".Annals. Computer Science Series, vol. 12, pp. 33-38, 2014a.

[10] K. A. Osuolale, W. B. Yahya, and B. L. Adeleke, "Construction of space-filling designs for three input variables computer experiments,". WASET, International Journal of Computer, Control, Quantum and Information Engineering, vol. 8, pp. 1624-1628, 2014b.

[11] K. A. Osuolale, W. B. Yahya, and B. L. Adeleke, "Modelling and analysis of simple pendulum computer experiment," Proceedings of the International Conference on Computer Science Research and Innovations (CoSRI), University of Ibadan,2015.

[12] K. A. Osuolale, W. B. Yahya, and B. L. Adeleke, "Modelling and analysis of simple pendulum computer experiment using a support vector regression model," Thailand Statistician, 2018 (To appear).

[13] S. Strogatz, "The real scientific hero of 1953," New York Times, March 4, Editorial/Op-Ed., 2003.

★★★