UMEMA
10-11 December 2018, Split, Croatia
4th Workshop Uncertainty Modeling for Engineering Applications

SVM and LS-SVM for the Uncertainty Quantification of Complex Systems

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Abstract. This paper investigates the application of the support vector machine and the least-squares support vector machine regressions to the uncertainty quantification of complex systems. The feasibility and the accuracy of the above techniques are demonstrated by predicting the efficiency of an integrated voltage regulator with 8 stochastic parameters.

I. INTRODUCTION

In the last decades, several mathematical tools have been proposed for the statistical analysis of complex systems affected by uncertainty parameters. Among the state-of-the-art techniques, polynomial chaos (PC) [1] expansion represents a well-established approach which have been successfully applied as an alternative to the standard Monte Carlo (MC) technique for the design exploration in different fields.

Recently, *machine learning* techniques have enjoyed widespread applications in different research areas. Support vector machine (SVM) [2] and least-squares support vector machine (LS-SVM) [3] regressions can be considered as promising candidates for the uncertainty quantification of system, for which compact surrogates with multiple parameters can be built.

This work investigates the application of the above machine learning techniques to the statistical analysis of a realistic structure with 8 uniformly distributed stochastic parameters. The results of the SVM and LS-SVM have been compared with the ones obtained via a sparse PC regression.

II. PROBLEM STATMENT & PROPOSED MODELING TECHNIQUES

Let us consider a set of L training data $\{(\mathbf{x}_i, y_i)\}_{i=1}^{L}$ provided by a generic nonlinear system $y = \mathcal{M}(\mathbf{x})$ as a function of the input parameters $\mathbf{x} = [x_1, \ldots, x_d] \in \mathbb{R}^d$. Our goal is to find an accurate surrogate $\tilde{\mathcal{M}}$ such that:

$$y_i \approx \tilde{\mathcal{M}}(\mathbf{x}_i), \;\; \text{for } i = 1 \ldots L. \tag{1}$$

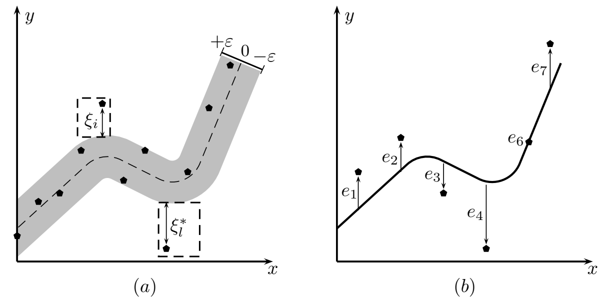

Fig. 1. Graphical interpretation of the SVM (panel (a)) and the LS-SVM (panel(b)) regressions.

II.1. SVM & LS-SVM REGRESSION

Let us consider the following non-linear regression:

$$M_{SVM,LS\text{-}SVM}(\mathbf{x}) = \sum_{i=1}^{L} \beta_i K(\mathbf{x}_i, \mathbf{x}) + b \tag{2}$$

where $\beta_i \in \mathbb{R}$ are scalar coefficients, $K(\cdot,\cdot) : \mathbb{R}^d \to \mathbb{R}$ is the *kernel function* and $b \in \mathbb{R}$ is the bias term. The goal of the SVM and the LS-SVM regressions is to estimate the optimum set of β_i and b by solving two different optimization problems.

Figure 1(a) provides a graphical interpretation of the optimization problem behind the SVM regression [2]. The underlying idea is to minimize the positive ξ_i and negative ξ_i^* deviations larger than ε between the model predictions and the training samples. The above constraints, along with the one on the model flatness, lead to a complex optimization problem which allows estimating the parameters β_i and b in (2).

The LS-SVM regression provides an alternative interpretation of the above optimization problem without losing the advantages of the standard SVM regression [3]. It minimizes the error e_i shown in Fig. 1(b) computed between the model prediction and the training samples in the L^2 norm. The above constraint, along with the one on the model flatness, allows estimating the parameters β_i and b via the solution of a least-square problem.

II.2. Sparse PC Expansion

As a reference for the performance of the above advocated techniques, we consider the classical Sparse PC

Table 1. Performance comparison of the considered regression techniques.

Method	Kernel Regression	RMSE	Mean $\hat{\mu}$ $\hat{\mu}_{MC}$=67.008	Std. Dev. $\hat{\sigma}$ $\hat{\sigma}_{MC}$=0.305
SVM	Linear	0.1585	67.018	0.275
	Poly Order 2	0.1785	67.037	0.299
	Poly Order 3	0.4281	67.000	0.522
	RBF	0.1658	67.035	0.277
LS-SVM	Linear	0.1580	67.019	0.281
	Poly Order 2	0.1663	67.037	0.291
	Poly Order 3	0.4434	67.000	0.539
	RBF	**0.1552**	67.022	0.280
Sparse PC	Order $\leq$ 10	0.1696	67.023	0.278

method, based on the following expansion:

$$\mathcal{M}_{PC}(\mathbf{x}) = \sum_{\boldsymbol{\lambda}\in\mathbb{N}^d} \boldsymbol{a}_{\boldsymbol{\lambda}} \Psi_{\boldsymbol{\lambda}}(\mathbf{x}), \tag{3}$$

where $\boldsymbol{a}_{\boldsymbol{\lambda}}$ are the unknown coefficients and $\Psi_{\boldsymbol{\lambda}}$ are the multivariate orthonormal polynomials.

For a given order h, usually the PC coefficients $\boldsymbol{a}_{\boldsymbol{\lambda}}$ can be estimated via non-intrusive techniques by truncating the polynomial expansion in order to preserve a total degree $\leq h$. The total number of required coefficients defined as $\frac{(d+h)!}{d!h!}$ blows up for large values of d and h.

The *sparse* PC approach with an adaptive degree h [1] can be used to overcome the above issue. In fact, it allows selecting the variables having the most impact on the model response, thus minimizing the number of polynomial basis required in the regression. This approach represents a powerful tool for the uncertainty quantification in high-dimensional space and for strongly nonlinear problems.

III. APPLICATION EXAMPLE

The SVM and LS-SVM regressions with polynomial and RBF kernel have been used to predict the impact of 8 uncertain parameters with uniform distribution on the efficiency of an integrated voltage regulator (see [4] for additional details).

The above regressions and the sparse PC regression have been trained with the 200 samples of a latin hypercube calculated via the full-wave solver of ANSYS. The predictions of each surrogate are then compared with the results of a MC simulation with 10000 samples.

Table 1. provides a detailed comparison among the accuracy of the three approaches in terms of the root mean square error (RMSE), mean value $\hat{\mu}$ and standard deviation $\hat{\sigma}$. From the results, the LS-SVM regression with RBF kernel provides the most accurate prediction. However, a remarkable accuracy is also achieved by the linear LS-SVM and SVM regressions and by the sparse PC expansion. Also, Fig. 2 provides an illustrative comparison among the PDFs and the scatter plots generated from the predictions of the LS-SVM regression with RBF kernel, the sparse PC expansion and the MC simulations. All the results confirm once again the good accuracy achieved by the SVM-based surrogates.

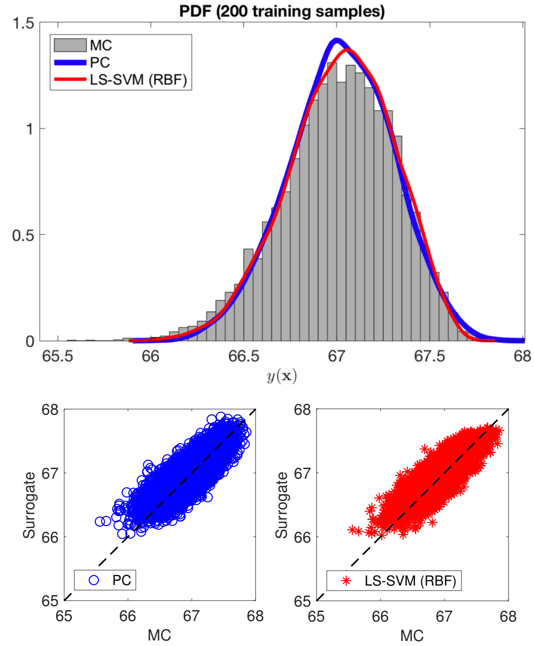

Fig. 2. Top Panel: comparison of the PDFs obtained from a 10000 samples MC simulation (gray bins) and the ones predicted by the LS-SVM with RBF kernel (red curve) and the PC expansion (blue curve). Bottom Panel: scatter plots obtained by comparing the MC results with the ones predicted by the LS-SVM and PC surrogates.

IV. CONCLUSIONS

Two promising alternatives based on the SVM and the LS-SVM regression have been proposed for the generation of compact surrogate models of complex systems with several parameters. From the illustrated results, the LS-SVM regression can be considered as a viable solution for the uncertainty quantification, since, for the specific example considered in this work, it produces more accurate predictions than the PC expansion.

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