Analysis of Parameter Variability in Integrated Devices by Partial Least Squares Regression

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***Abstract*—This paper focuses on the application of the partial least squares (PLS) regression to the uncertainty quantification of the responses of complex stochastic systems. It considers the development of a surrogate model using a limited set of training samples in order to estimate statistical quantities of the system output with relatively low computational cost compared to the standard brute force Monte Carlo (MC) simulation. The performance and the strength of the proposed modeling scheme is investigated for an integrated voltage regulator (IVR) with 8 random variables. The results highlight the ability of the PLS regression to deals with complex nonlinear problems with very few principal components, also providing important insights about the input variables.**

***Index Terms*—Machine learning, uncertainty quantification, surrogate model, PLS regression, sensitivity analysis, integrated voltage regulator (IVR).**

I. Introduction

Uncertainties associated with fabrication process, tolerances and unknown parameters in complex electronic systems may generated large and uncontrolled variations of the system outputs, which can lead to a potential failure of the system. In advanced electronic systems, the number of parameters impacting the variability of output signals is so large that the brute force Monte Carlo (MC) approach turns out to be inefficient.

For the above reason, in the last decades, various surrogate modeling techniques such as Polynomial Chaos (PC) expansion and its variant [1]–[3] and Machine Learning-based regressions [4]–[7] have been successfully proposed as viable and efficient alternatives to the plain MC simulation.

This paper investigate the accuracy and the strength of an alternative technique for the uncertainty quantification, namely the partial least squares (PLS) regression [8]. Such technique allows building a compact surrogate model of the output of a generic stochastic system as a function of its uncertain parameters. Similarly to the principal component analysis (PCA) [9], PLS allows to reduce the problem dimensionality using a limited number of components while mapping the relationship between input and output variables. This feature allows to capture the most prominent input variables of the systems. Moreover, the surrogate model can then be used to compute statistical moments and the probability density function (PDF) of the output of interest. In Sec. III, the proposed PLS regression is adopted to predict the efficiency of an integrated voltage regulator (IVR) as a function of 8 stochastic parameters.

II. Partial Least Squares (PLS)

Given a limited set of L training samples $\{(\mathbf{x}_i, y_i)\}_{i=1}^{L}$, with $\mathbf{x}_i \subseteq \mathbb{R}^D$ and $y_i \subseteq \mathbb{R}$ generated by the full-computational model $\mathcal{M}$ (i.e., $y_i = \mathcal{M}(\mathbf{x}_i)$), the PLS regression allows defining a reduced set of the input variables, called principal components, which better explain the behavior of the system response y as a function of the input $\mathbf{x}$ [8].

First, the input matrix $\mathbf{X} = [\mathbf{x}_1, \ldots, \mathbf{x}_L]^t$ of size $(L \times D)$ and the response vector $\mathbf{y} = [y_1, \ldots, y_L]^t$ are centered and reduced in order to avoid a bias of the input variables having large values and strong variations. Then, the first principal component $\mathbf{t}^{(1)}$ is computed by searching the best direction $\mathbf{u}^{(1)}$ maximizing the squared covariance between $\mathbf{t}^{(1)} = \mathbf{X}\mathbf{u}^{(1)}$ and $\mathbf{y}$ as:

$$\mathbf{u}^{(1)} = \arg \max_{\mathbf{u}^t\mathbf{u}=1} \mathbf{u}^t\mathbf{X}^t\mathbf{y}\mathbf{y}^t\mathbf{X}\mathbf{u}. \tag{1}$$

The above optimization problem (1) is maximized when $\mathbf{u}^{(1)}$ is the eigenvector of the matrix $\mathbf{X}^t\mathbf{y}\mathbf{y}^t\mathbf{X}$ associated with the eigenvalue with the largest absolute value. The vector $\mathbf{u}^{(1)}$, called *loading vector*, corresponds to the $\mathbf{X}$ weights of the first component. Then, the residual matrix of $\mathbf{X}^{(0)} = \mathbf{X}$ and $\mathbf{y}^{(0)} = \mathbf{y}$, which are denoted by $\mathbf{X}^{(1)}$ and $\mathbf{y}^{(1)}$, are computed as:

$$\begin{aligned} \mathbf{X}^{(1)} &= \mathbf{X}^{(0)} - \mathbf{t}^{(1)}\mathbf{b}^{(1)}, \\ \mathbf{y}^{(1)} &= \mathbf{y}^{(0)} - \mathrm{w}_1\mathbf{t}^{(1)}, \end{aligned} \tag{2}$$

where $\mathbf{b}^{(1)}$ represents a vector of size $(1 \times D)$ including the regression coefficients of the local regression of $\mathbf{X}$ onto the first principal component $\mathbf{t}^{(1)}$ of dimension $(L \times 1)$, and w_1 is the regression coefficient of the local regression of $\mathbf{y}$ related the first principal component $\mathbf{t}^{(1)}$. The equation (2) corresponds to the local regression of $\mathbf{X}$ and $\mathbf{y}$ onto the first principal component.

The second principal component, which is orthogonal to $\mathbf{t}^{(1)}$, is computed via the PLS again by solving the problem

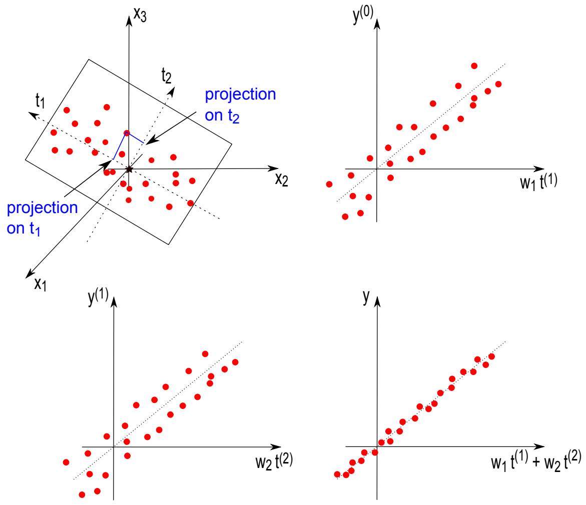

Fig. 1. Top left represents the construction of two principal components in the initial X space. Top right and Bottom left illustrate the prediction of $y^{(0)}$ and $y^{(1)}$, respectively. Bottom right shows the final prediction of the output y.

in (1) where $\mathbf{X}$ and $\mathbf{y}$ are replaced by $\mathbf{X}^{(1)}$ and $\mathbf{y}^{(1)}$, respectively. The same iterative scheme can be used to compute the rest of the components. A graphical interpretation in a three-dimensional example with two principal components is depicted in Fig. 1.

Usually, the number of principal components q are selected by retaining the one minimizing the root mean square error (RMSE) computed between the model predictions and the training samples used to build the model. The principal components, accounted for within the PLS regression, define a new coordinate system which corresponds to a rotation of the initial system in the parameter $\mathbf{x} = [x_1, \ldots, x_D]^t$. The r-th component of the new coordinate system, denoted $\mathbf{t}^{(r)}$ with $r = 1, \ldots, q$, is given by:

$$\mathbf{t}^{(r)} = \mathbf{X}^{(r-1)}\mathbf{u}^{(r)} = \mathbf{X}\mathbf{u}_*^{(r)}. \tag{3}$$

The relationship between the vectors $\mathbf{u}^{(r)}$ and $\mathbf{u}_*^{(r)}$ are defined through the matrices $\mathbf{U} = \left[\mathbf{u}^{(1)}, \ldots, \mathbf{u}^{(q)}\right]$ and $\mathbf{U}_* = \left[\mathbf{u}_*^{(1)}, \ldots, \mathbf{u}_*^{(q)}\right]$ as follows:

$$\mathbf{U}_* = \mathbf{U}\left(\mathbf{B}^t\mathbf{U}\right)^{-1}, \tag{4}$$

where $\mathbf{B} = \left[\mathbf{b}^{(1)^t}, \ldots, \mathbf{b}^{(q)^t}\right]$.

The PLS regression can be suitably adopted to identify the importance of each input parameter via a variable selection method such as the variables importance projections (VIP) [10]. The VIP score for the input variable j is defined as:

$$VIP_j = \sqrt{\frac{D \cdot \left(\sum_{r=1}^{q} R^2(\mathbf{y}, \mathbf{t}^{(r)}) \cdot (\mathbf{u}^{(rj)} / \left\|\mathbf{u}^{(rj)}\right\|)^2\right)}{\sum_{r=1}^{q} R^2(\mathbf{y}, \mathbf{t}^{(r)})}} \tag{5}$$

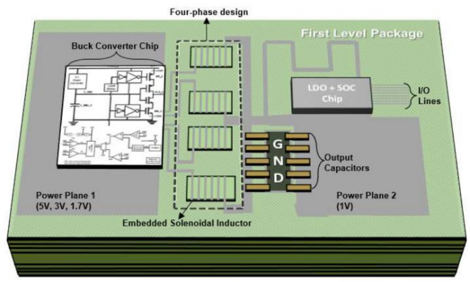

Fig. 2. Illustration of the two-chip SiP IVR architecture [11].

TABLE I
UNCERTAIN GEOMETRICAL PARAMETERS OF THE SOLENOIDAL INDUCTOR USED FOR THE IVR.

Uniform random variables		Unit	$\mathcal{U}\,[Min; Max]$
Gap between windings	g	mil	$\mathcal{U}\,[4; 6]$
Size of via	s_v	μm	$\mathcal{U}\,[80; 120]$
Copper Trace Width	w_v	mil	$\mathcal{U}\,[9; 11]$
Copper Thickness Bottom	$t_{c,b}$	μm	$\mathcal{U}\,[64; 96]$
Copper Thickness Top	$t_{c,t}$	μm	$\mathcal{U}\,[64; 96]$
Dielectric Thickness	t_d	μm	$\mathcal{U}\,[180; 220]$
Dielectric Width	w_d	mil	$\mathcal{U}\,[59.4; 60.6]$
Magnetic Core Width offset	Δw_m	mil	$\mathcal{U}\,[9; 11]$

where $\mathbf{u}^{(rj)}$ is the weight of the j^{th} variable in component r and $R^2(\mathbf{y}, \mathbf{t}^{(r)})$ is the percentage of $\mathbf{y}$ explained by the component r.

The VIP value is a weighted sum of squares of the PLS weights ($\mathbf{u}^{(rj)}$), which takes into account the explained variance of each PLS dimension. The input variable with a VIP score greater than one is generally considered to have a significant impact on the response $\mathbf{y}$ [10].

III. Application Examples

The integrated voltage regulator shown in Fig. 2 is considered with the objective of estimating its power conversion efficiency. The architecture consists of a system-in-package solution with an integrated inductor on an organic package with a solenoid structure with a Nickel-Zinc ferrite magnetic core [11].

The goal of this study is to evaluate the impact of 8 stochastic geometrical parameters of the integrated inductor (see Table I) on the IVR efficiency for 5V:1V conversion ratio at the frequency of 100 MHz [4], [6]. The efficiency is calculated via an extensive model that accounts for switching and conduction losses of power switches, DC, power delivery network (PDN) and AC losses of inductor and output capacitance by relaying on the results of the full-wave solver of Ansys HFSS [11], [12].

We now analyze the effect of uncertain input parameters on the IVR efficiency E_{ff}. In order to do that, we construct

TABLE II

EVALUATION OF THE ACCURACY OF THE PLS REGRESSION MODEL W.R.T THE NUMBER OF PRINCIPAL COMPONENTS.

Method	Number of Components	RMSE	$\hat{\mu}$	$\hat{\sigma}$	t_{model}*	t_{cost}
MC	–	–	67.01	0.31	–	7 days
PLS	1	0.162	67.01	0.28	<1s	<1s
	2	**0.158**	67.01	0.28	<1s	<1s
	3	0.158	67.01	0.28	<1s	<1s
	4	0.158	67.01	0.28	<1s	<1s
	5	0.158	67.01	0.28	<1s	<1s

* In addition to 200 LHS simulations which took 3 h 27 min.

a PLS regression model with [13] using 200 realizations from Latin Hypercube sampling (LHS) and a number of principal components varying from 1 to 5. An evaluation of the performance of each PLS model is performed by comparison with the brute force MC simulation. Table II shows, from 10000 realizations, a comparison of various PLS models with an increasing number of components and MC simulation, by computing the RMSE, the mean value $\hat{\mu}$ and the standard deviation $\hat{\sigma}$. We see that the PLS model with one principal component provides a RMSE equal to 0.162, while the PLS models with 2 to 5 principal components provide a RMSE of 0.158. As the PLS surrogate model with 2 components achieves the lowest RMSE, i.e. 0.158, the minimum number of components is retained. It is worth noting that the accuracy of this PLS model is very close to LS-SVM surrogate model with a RBF kernel, i.e. with a RMSE of 0.155, and better than the sparse PC which has a RMSE of 0.170 as presented in [4]. This result points out to the ability of the PLS surrogate model to estimate the main variability of a complex output while reducing the dimensionality of the problem, i.e. from 8 original variables to 2 principal components. This feature of the method is very interesting and will be exploited in the following to hierarchize the effect of the uncertain parameters on the IVR efficiency.

For the purpose of illustration, we compare in Fig. 3 the predictions of the PLS regression model with 2 principal components with 10000 MC realizations. As the scatter plot is very well aligned along the dashed line, we then deduce that there is a good agreement between the PLS model and MC simulation. As far as the variability of the IVR efficiency is concerned, a representation of the PDFs estimated by the PLS surrogate model and by MC simulation with 10000 realizations is given in Fig. 4. It can be observed that the PLS surrogate model reproduces well the central tendency of the output estimated by MC simulation, although some discrepancy exists for the left tails of the PDFs. In terms of computational cost, 10000 MC simulations took about 7 days while the PLS surrogate model required less than 1 s to carry out the predictions. It is important to mention that this comparison does not include the computational cost related to the generation of the training data set (200 simulations), which needed about 3 h 27 min as shown in Table II.

In addition to the variability of the output, the PLS model provides a sensitivity analysis of the model response. The

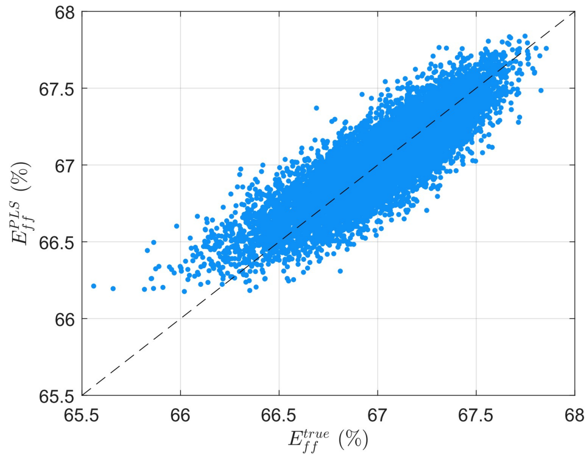

Fig. 3. Scatter plot of the IVR efficiency computed by the PLS surrogate model and by the real numerical model with 10000 MC realizations. The dashed-line illustrates a good correlation between the models.

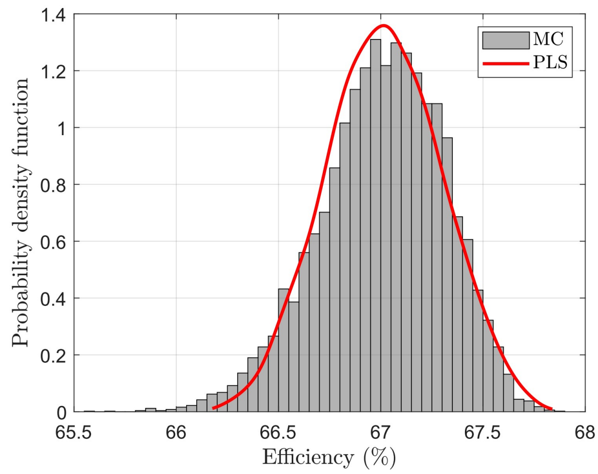

Fig. 4. PDFs of the IVR efficiency estimated by the PLS surrogate model (solid curve) and by MC simulation (histogram) from 10000 MC realizations.

histogram in Fig. 5 illustrates the VIP scores calculated via the proposed PLS-based surrogate. The VIP scores indicate the impact of the input random variables on the efficiency E_{ff}. We see that the main variability of E_{ff} is related to 3 variables, i.e., the copper thickness bottom $t_{\text{c,b}}$, the copper thickness top $t_{\text{c,t}}$ and the copper trace width w_v of the inductors, as their VIP scores are greater than or equal to the threshold of 1, as suggested by [10]. Other variables, such as the size of via s_v and the dielectric thickness t_d, have less impact while the dielectric width w_d, the gap between windings g and the magnetic core width offset Δw_m of the inductors have an insignificant effect on the variability of the response E_{ff}.

Furthermore, at 100 MHz, total losses of the IVR system are dominated by switching and conduction losses of power switches and the resistive loss due to the PDN [11]. Since the DC resistance of the inductor impacts the finite resistance of the PDN, its AC losses become less important. Hence,

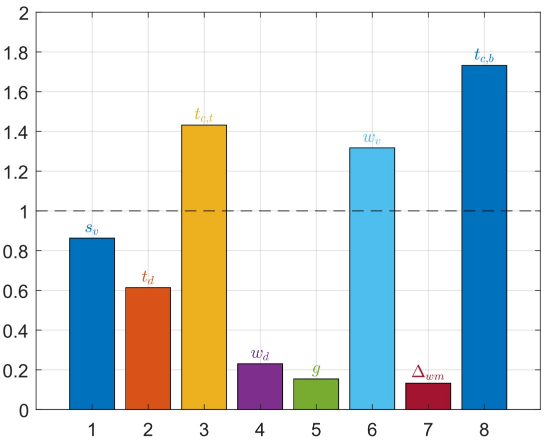

Fig. 5. Variable Importance in Projection (VIP) scores of the IVR efficiency E_{ff}. Input variables having a VIP score greater than or equal to 1 have an important impact on the variability of the IVR efficiency E_{ff}.

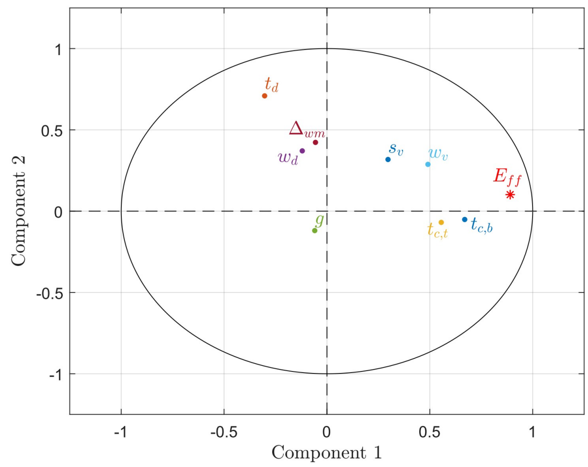

Fig. 6. Correlation circle representing the projection of the input variables and the output variable (IVR efficiency E_{ff}). The variables are represented through their projections onto the plane defined by the first two PLS components. A positive correlation is highlighted between the input variables s_v, w_v, $t_{c,t}$, $t_{c,b}$ and the output variable E_{ff} as they are projected in the same direction and at a large distance from the origin.

the parameters of the inductor directly influencing its DC resistance become more important and have more effect on the IVR efficiency. This confirms that the sensitivity analysis illustrated in Fig. 5 is coherent since it presents a more significant impact of the parameters that directly affect the DC resistance than the other parameters related to the magnetic material.

Based on the projection provided by the PLS surrogate model, we can also display the variables on the 2 components. Figure 6 shows the correlation circle to highlight the correlation between the input variables and the output. This graph is obtained by computing the correlation between the principal components (i.e., the 2 axes of the graph) and the original variables (input variables and output). We can see that the distance between the output E_{ff} and the input variables such as the copper thickness bottom $t_{\mathrm{c,b}}$, the copper thickness top $t_{\mathrm{c,t}}$ and the copper trace width w_v of the inductors is very short. This means that they are highly positively correlated. In other words, large values of those input variables will lead to an increase of the IVR efficiency E_{ff}. Concerning the other variables, the size of vias s_v is positively correlated with the output E_{ff} but with less impact, while other variables seem to have a negligible effect.

IV. Conclusions

This paper presents a PLS surrogate model, with a very low computational cost compared to MC simulation, for the uncertainty quantification in high-dimensional space. This PLS surrogate model allowed to efficiently estimate the efficiency of an IVR characterized by 8 uncertain input variables.

Additionally to a good estimation of the first two statistical moments, the PLS surrogate model also provides a sensitivity analysis of the model response at a negligible computational cost. Using this sensitivity analysis, the designer may identify the uncertain input variables affecting the most the variability of the output of the system. Also, the designer may determine the configurations of input variables allowing to improve the performance of the system during the design stage.

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