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# Smart Input Space Sampling Combined with Kriging-Partial Least Square Regression for EMC Risk Analysis at PCB Level with Many Variables

A. Plot

Univ Rennes, INSA Rennes, CNRS, IETR UMR 6164, F-35000 Rennes, France *Thales SIX GTS France* F-49300 Cholet, France alexandre.plot@thalesgroup.com P. Besnier Univ Rennes, INSA Rennes, CNRS, IETR UMR 6164, F-35000 Rennes, France philippe.besnier@insa-rennes.fr B. Goral Thales SIX GTS France F-49300 Cholet, France benoit.goral@thalesgroup.com

*Abstract*—This article describes an advanced methodology for training surrogate models (SMs) in order to study the sensitivity of many geometrical parameters of printed circuit boards (PCBs) for a quicker investigation of routing rules regarding potential electromagnetic compatibility (EMC) or signal integrity (SI) issues. This methodology consists in two steps. First, it retains only the sensitive parameters of the input space that mostly explain the several output observations. Second, it consists in training iteratively several competing SMs, selecting the most efficient one, regarding training time and/or accuracy. Here, the kriging-partial least square Regression (K-PLS) is identified as a relevant method for the considered case study, which consists of a 17-parameter multiple outputs crosstalk scenario. An extreme value analysis is provided as an outcome for a possible adjustment of design rules.

Index Terms—Surrogate model, EMC risk analysis, Morris analysis, kriging, Partial least square, K-PLS, Design rules.

#### I. INTRODUCTION

This paper presents a methodology for training a surrogate model to approximate the behavior of a complex model, in the context of EMC studies at PCBs level. Multilayer PCB design, in an industry that aims to densify, miniaturize, and integrate increasingly innovative functionalities, requires the creation of routing guidelines to reduce the risk of non-compliant electromagnetic compatibility (EMC) tests. These guidelines can be provided using reliable numerical simulations. These simulations, which involve solving Maxwell's equations using 3D numerical solvers, are time-consuming and resourceintensive, especially when performing parametric analysis with a large number of parameters. Building a surrogate model trained from a limited amount of runs of the initial solver is a solution to overcome this hurdle. Surrogate models have become very popular in different engineering field [1] because of their ability to carry out costly operations such as problem optimisation [2] [3], parametric analyses [4] [5] or extreme values analyses [6]. Several types of SMs are available in the literature such as kriging, support vector machine, decision trees or neural networks to name a part of them.

In the EMC domain, kriging method have been successfully applied to a variety of scenarios [7] [8] [9] [10] [11] [12]. This does not mean by any way that this is the best ML method for EMC scenario; but it remains a good candidate for surrogate modelling. However, like other machine learning (ML) methods, kriging suffers from what is known as the curse of dimensionality. Specifically, an increase in the number of variables leads to an exponential increase in the number of data required for surrogate model training [13]. In more details, kriging involves calculating a covariance matrix that becomes larger as the number of input variables increases. This results in a longer computation time when inverting the covariance matrix. Moreover, the resulting kriging model becomes increasingly voluminous at the same time.

Several proposals have been made to deal with this problem. Some of these methods, called "dimensionality reduction" methods [14] [15], allow to decrease the complexity of the problem by studying the relationships between the variables and the output of interest. The principal components analysis (PCA) allows to identify the main components of the problem by calculating the eigenvalues and eigenvectors of the covariance matrix, thus allowing to project the data into a lower-dimensional space. Alternatively, the partial least square method allows to identify the linear combination of the predictor variables that best explains the output. It reduces the dimensionality of the data by projecting it onto a new set of orthogonal variables, called latent variables, which are linear combinations of the original variables.

Recently, [16] has implemented a surrogate model that combines Kriging and PLS. The idea is to reduce the number of hyperparameters to be optimized in kriging and to define a new covariance matrix (kernel) using the weights of PLS. Based on analytical functions and a specific industrial scenario, the results presented in this paper show that K-PLS can substitute simple Kriging while significantly reducing the learning time and error.

Another limitation in building a SM is determining the appropriate size of the learning sample. The amount of data

needed for a precise SM is unknown beforehand. A potential solution is to use a gradually increasing sample size design of experiment (DOE) until a specific error criterion is reached. An Iterative-LHS-Morris method was presented in [12] to further reduce the required sample size.

This paper extends the concept presented in [12] in several ways. Whereas the pre-selection of relevant variables is still performed through a Morris analysis a more suitable error criterion is used for the convergence of the iterative model. Then, the K-PLS SM is used in competition with the kriging SM. Finally, a 17-parameter multiple outputs crosstalk scenario is investigated, highlighting the relevance of the K-PLS regression. Section II provides a rapid overview of kriging and K-PLS SMs whereas section III recalls the principle of Morris analysis and its operation. Section IV provides both the algorithm and the presentation of the updated error criterion, as applied to the use case in Section V.

#### **II. SURROGATE MODELS**

A surrogate model is a black-box representation of a complex model. It is used to predict the output of the model based on a set of input parameters. The two methods used in this paper are briefly discussed in this section.

#### A. Kriging

The kriging method consists in approaching the response of a model with M inputs variables described by an input vector  $\mathbf{X}$  of the corresponding size. The response  $f(\mathbf{X})$  is then evaluated from:

$$\forall x \in D^M, f(\mathbf{X}) = \mu(\mathbf{X}) + \varepsilon(\mathbf{X}) \tag{1}$$

In this equation,  $\mu$  is a deterministic function of X and represents the mean or the trend of the process. For an ordinary kriging, it is considered as a known constant. The term  $\varepsilon$  is a Gaussian process of random variables which is found by optimizing hyperparameters from known values. The Gaussian process  $\varepsilon$  is supposed to be stationary (regarding the first and the second moment), which means that the dependence function between random variables  $\varepsilon(X_1)$  and  $\varepsilon(X_2)$  does not depend on their local coordinates in the input space. It is generally defined as a function of the Euclidean distance between  $X_1$  and  $X_2$  only. Thus, the correlation function Ccan be written as:

$$\forall \mathbf{X_1}, \mathbf{X_2} \in D^M \times D^M, C(\|\mathbf{X_1} - \mathbf{X_2}\|_{\theta})$$
(2)

where  $\theta$  is the vector of the *M* hyperparameters. A typical parameterized correlation function must be selected. These hyperparameters are then determined by optimization. A commonly used function is the exponential one:

$$C(h,\theta) = exp(-\theta|X_1 - X_2|) \tag{3}$$

The training phase consists in optimizing the hyperparameters by maximizing a likelihood function which is computationally expensive for high dimensions (high M) of the input space. Futhermore, the resulting model requires a large memory space. Its combination with PLS, i.e. the K-PLS method, provides an interesting solution.

#### B. Kriging - Partial Least Square

Maximizing the likelihood function of Kriging can be time consuming when the dimension of the covariance matrix is large. This issue can be resolved by combining the PLS method and the kriging model.

PLS is a widely-used solution for high-dimensional problems. It is a statistical method that identifies the linear combinations input variables  $\mathbf{X}$  and output variables  $\mathbf{y}$  that maximize their corrrelation. This is achieved by projecting initial inputs into a new parameter space defined by h principal components also called latent variables,  $h \ll M$ . In other words, PLS aims at finding the best directions of  $\mathbf{X}$  space that explains the output  $\mathbf{y}$ . More details on how the exponential kernel is built from PLS coefficient can be found in [16].

## III. SMART SAMPLING USING MORRIS ANALYSIS AS A PREPROCESSOR

#### A. Concept

The Morris method is a global sensitivity analysis method based on measuring the variations of the output corresponding to the variation of one parameter at a time. This method is particularly effective when the number of parameters is large because it only requires a small number of model realizations.

The Morris method consists in calculating an elementary effect caused by the variation of a  $\Delta$  step of a given input. The elementary effect for the input  $x_i$  of **X** is calculated as follows:

$$E_i(\mathbf{X}) = \frac{f(x_1, ..., x_i + \Delta, ..., x_M) - f(x_1, ..., x_i, ..., x_M)}{\Delta}$$
(4)

where  $\mathbf{X} = (x_1, ..., x_i, ..., x_M)$  is a given random realization of X and  $\Delta$  is the experiment step which is equal to a multiple of  $\frac{1}{p-1}$  where p is the number of grid levels (grid is built from input space).

The calculation of elementary effects for all M inputs is repeated r times to achieve r independent trajectories. Then, the mean over all trajectories of the absolute value of the elementary effect of the *i*-th input parameter and the standard deviation are calculated such as:

$$\mu_{i} = \frac{1}{r} \sum_{t=1}^{r} |E_{i}^{t}|$$
(5)

$$\sigma_i = \sqrt{\frac{1}{r} \sum_{t=1}^r \left( E_i^t - \frac{1}{r} \sum_{t=1}^r (E_i^t) \right)^2}$$
(6)

Thus,  $\mu$  is the average of elementary effects over all trajectories, providing the overall influence of the input  $X_i$  on the output variations. As far as the average standard deviation  $\sigma_i$  = is concerned, it measures the non-linear influence of the other inputs and their interactions.

Based on the values of  $\mu_i$  and  $\sigma_i$ , it is possible to classify input variables into 3 categories: i)negligible effects ii) large linear effects without interactions iii) large non linear effects.

The total cost of Morris experiment is r(M + 1) (i.e. the number of calls to the model). This is the result of changing one variable at a time for each trajectory once a first random input vector is initialized. In the Morris analysis, the main factors influencing the precision of the result are r and p. For all analysis in this paper p = 4 and r = 10 are used, based on the analysis in [19], where the authors demonstrated that this choice produced satisfying results.

#### B. selection of influential parameters

As detailed in [12],  $\mu_i$  is first normalized to their total sum over the *M* variables. Then, the cumulative contribution for a subset of input variables is computed by summing their normalized contributions after sorting them in decreasing order. The retained subset of influential parameters is defined such as its cumulative contribution is greater of equal to 80%, assuming that this group of variables is sufficient to predict the output response with an acceptable approximation. Thus, the other ones (with the lowest  $\mu$  values) are discarded from the SM construction and are fixed to their nominal values.

#### IV. MULTI-MODELS ITERATIVE LEARNING

#### A. Concept

An iterative learning algorithm of the SM was proposed in [12]. The enrichment method is preserved and improved by adding multi-metamodels learning. The method is summarized in the algorithm below. It involves first building an initial LHS-type experimental design of size  $N_{ini}$  whose outputs are calculated using the simulator. Several metamodel methods (here kriging and K-PLS) are trained and their prediction accuracy are compared. The initial sample is then enriched with several points, also evaluated by the simulator, forming a new experimental design of larger size. The different metamodels are retrained. This loop is repeated until the satisfaction criterion is met for one SM at least.

 $N_{ini}$  sets the initial number of experiments contained in the DOE. A rule of thumb consists of choosing  $N_{ini} = 10 \times M$ .  $N_{step}$  defines the number of points added at each iteration. It can be constant or evolving during the iterative process to avoid a too marginal evolution of the sample size. The algorithm is based on LHS enrichment, which consists in adding new points to an existing DOE, preserving the LHS nature of the complete sample.

#### B. Prediction error and criterion for accuracy

The presented iterative learning scheme is based on calculating a prediction error that measures the degree of confidence of predictions. Several methods and metrics for calculating error exist. One of them consists of isolating an independent sample from the training on which each meta-model is evaluated and an error is calculated. However, this method is not appropriate since it creates a dependence between the error on the test sample.

#### Algorithm 1 Iterative sampling approach

- 1: **Input** : A costly function f with M parameters
- 2: **Output** : A Kriging surrogate model  $\hat{f}$
- 3: Generate an initial DOE  $X = [x_1, ..., x_{N_{ini}}]^T$  of size  $N_{init}$  using LHS
- 4: Call f to compute the output of each experiment of DOE  $y = [f(x_1), ..., f(x_{N_{ini}})]^T$
- 5: Train the different metamodels using X and y
- 6: While stopping criterion is not met do
- 7: Add new points:
- 8: Generate  $N_{step}$  points based on the initial DOE and using iLHS technique  $X' = [x'_1, ..., x'_{N_{step}}]^T$
- 9: Call f to compute the output of the added points  $y' = [f(x'_1), ..., f(x'_{N_{step}}]^T$
- 10: Update information:
- 11:  $X = X \cup X' \text{ and } y = y \cup y'$
- 12: Train the different metamodels using the new DOE with added points
- 13: **return** The final metamodel  $\hat{f}(x)$  with the lowest prediction error among all the trained metamodels

A best suited method is introduced here. It uses a validation method called the k-fold cross validation. It consists in splitting the dataset into k groups of samples of equal sizes. Training is done using k - 1 folds, and the fold left is used for test. The prediction error is calculated as follows:

$$\epsilon_{i}^{k} = \frac{|max(\hat{Y}_{i}, Y_{i}) - min(\hat{Y}_{i}, Y_{i})|}{min(\hat{Y}_{i}, Y_{i})}$$
(7)

where  $Y_i$  is the output of the test fold to be predicted and  $\hat{Y}_i$  is the output predicted by the surrogate model built up from the other k - 1 folds.  $\epsilon_i^k$  is a relative error which corresponds to the i-th error of the k-th fold. The operation is repeated by selecting another test fold among the predefined ones. The k-fold cross validation is more expensive in terms of computation time as it requires to train k different metamodels. The advantage of this method is that it offers a statistical overview of the prediction error over the entire dataset.

A decision criterion must be fixed so that a reliable metamodel is obtained. We choose to use the median which is a good indicator of the global predictions of the surrogate model. This criterion is based on the median relative error of  $\epsilon_i^k$  that is computed for all the samples of each fold and for all the folds. A median relative error of less or equal 20% is selected.

Since a SM is built up for each frequency of analysis this condition has to be fulfilled for all SMs.

#### V. APPLICATION TO A USE CASE

#### A. Presentation of the test case

The proposed methodology and the criterion defined for each step are going to be tested on a 17-parameter test case represented in Fig. 1.

The case study represents a situation of inter-track crosstalk frequently encountered in PCBs. It consists of 3 microstrip lines with 3 openings in the ground plane under each of them. The scenario is configured with 17 variables, the ranges of which are summarized in the table below.



Fig. 1. Schematic of the case study and its 17 parameters.

TABLE I PARAMETERS DEFINITION

Parameter	Description	Range (mm)
$L_1, L_2, L_3$	Length of traces	20 - 200
$W_1, W_1, W_1$	Width of traces	0.1 - 0.6
$L_{f1}, L_{f1}, L_{f1}$	Length of openings	0.1 - 20
$W_{f1}, W_{f2}, W_{f3}$	Width of openings	0.1 - 20
h	Height of dielectric	0.08 - 0.8
$h_2$	Height of solder mask	0.04 - 0.4
$d_{w1}, d_{w2}$	Traces separation	0.5 - 15
$W_p$	Width of ground plane	20 - 40

This scenario presents an interest in terms of EMC study as it allows for the simultaneous study of three potential impacts on EMC performance:

- The effect of openings on the return current associated with each microstrip line
- The proximity effect of traces on the crosstalk level
- The impact of the ground plane width on the return current

This analysis focuses on the different S parameters of the lines and, in particular, on the insertion loss of microstrip line 1 ( $S_{21}$ ), the crosstalk level between microstrip lines 1 and 2 ( $S_{41}$ ), and the crosstalk level between microstrip lines 1 and 3 ( $S_{61}$ ). These three S parameters are computed using CST MW studio (using the finite integration technique in the time domain) in 350 MHz to 2 GHz frequency range.

#### B. Application of Morris analysis

The Morris analysis is computed independently for the three outputs  $S_{21}$ ,  $S_{41}$  and  $S_{61}$ . Since M = 17 and using r = 10,  $N = (M + 1) \times r = 180$  input data are required. Moreover, frequencies are treated independently, meaning a

Morris analysis is performed for each frequency. There are 1001 uniformly spaced frequencies from 350 MHz to 2 GHz. The results, introduced in Fig. 2, are presented through boxplots showing the spread of sensitivity indices over frequency.



Fig. 2. Results of Morris analysis:  $\mu$  box-plots of each of the 17 parameters for  $S_{61}$  (top left),  $S_{41}$  (top right),  $S_{21}$  bottom). The spread of  $\mu$  over frequencies (whiskers), the median (orange bars) and the mean(green triangles) are indicated.

From these boxplots, relevant parameters of the scenario can be clearly identified. As an example, only 4 parameters seem to be influential  $(L_1, L_{f1}, W_{f1} \text{ and } h)$  to explain the  $S_{21}$  output. This result was expected since these parameters are related to intrinsic parameters of the first microstrip line and its associated opening that influence its insertion loss performance. Regarding  $S_{41}$ , the most important parameter appears to be  $d_{w1}$  which is the distance between the first and second line. $W_{f1}$  and  $W_{f2}$  are also important parameters, since they indirectly set the distance between the lines. Finally, only a few parameters seem to have marginal influence on the  $S_{61}$ output.

Different parameter selections are possible based on the observed output. The adopted methodology consists of only eliminating non-influential parameters for all outputs. It means that the selection made have to satisfy the defined criteria for all the three outputs.

As a result, the selection made is composed of 12 parameters:  $L_1$ ,  $L_2$ ,  $L_3$ ,  $L_{f1}$ ,  $L_{f2}$ ,  $L_{f3}$ ,  $W_{f1}$ ,  $W_{f2}$ ,  $W_{f3}$ ,  $d_{w1}$ ,  $d_{w2}$  and h. For this group of parameters, the cumulative contribution is computed:

$$\mu_{cumulated} = \mu_{L_1} + \mu_{L_2} + \dots + \mu_h \tag{8}$$

The results, illustrated in Fig. 3, confirm that for the three considered outputs, 12 parameters are sufficient to explain more than 90% of the variations of outputs, i.e. well above the required criterion of 80 %.

Some strong variations of the cumulative contribution of  $\mu$  can be observed on the  $S_{41}$  curve around 1.6 GHz and 1.2 GHz. These are due to outliers of some of the eliminated parameters.

To sum up this part, we managed to identify 12 parameters out of the initial 17 that explain over 80 % of the observed outputs. The remaining 5 parameters are therefore considered



Fig. 3. Cumulative contribution over frequency for 12 selected parameters:  $(S_{61} \text{ top left}, S_{41} \text{ top right}, S_{21} \text{ bottom}).$ 

to be non-influential and can be set to their nominal values. Therefore, the following iterative learning process is applied for this set of 12 parameters and the obtained SM will be compared to the the one obtained with the whole set of 17 parameters as a reference.

#### C. Application of iterative learning

The metamodels corresponding to the three outputs  $S_{21}$ ,  $S_{61}$ and  $S_{41}$  are now being iteratively trained. In order to validate the parameter selection previously carried out, a comparative approach is being conducted. Thus, for each output, two metamodels are iteratively trained: one with the 17 initial variables and one with the 12 selected variables. Surrogate models are then denominated as follows:  $SM_X^Y$  where SM is either KRG or K-PLS, X is either  $S_{21}$ ,  $S_{61}$ ,  $S_{41}$  and Y is 17p or 12p.

First, kriging metamodels are compared in Fig. 4 where the median relative error evolution is plotted according to the number of iterations for the three considered outputs and for both 12-parameter (following Morris analysis) and 17parameter cases (reference).



Fig. 4. Median relative error evolution for the 12-parameter and 17-parameter cases (reference). SM ( $S_{61}$  top left,  $S_{41}$  top right,  $S_{21}$  bottom).

The median relative error of the  $S_{21}$  metamodel is always below 20%, whether for 12 or 17 parameters. This can be explained by a dependency on a small number of input parameters. Regarding  $S_{41}$ , the target error of the metamodel with 12 parameters is reached with 3206 training points, which is 1332 less realizations than the SM with 17 parameters.

Finally,  $KRG_{S_{61}}^{17p}$  does not converge, and the iterative learning process was stopped due to excessive computation time. On the contrary, the  $KRG_{S_{61}}^{12p}$  reaches the threshold error with 4616 training points.

Reducing the number of parameters allows the target error to be reached quicker, which reduces the number of simulations required for learning. For comparison, the total simulation time for the 4616 realizations and learning of  $KRG_{S61}^{12p}$  is 16 hours, compared to 19 hours for  $KRG_{S61}^{17p}$  which didn't reach the error goal. This means that we obtain a metamodel with lower error and at the same time a lower simulation and training time.

#### D. Application of K-PLS

This part describes the application of K-PLS with h = 3 latent components to further accelerate the computations. We are only interested in  $S_{61}$  here as it is the most difficult output to predict. The performance of K-PLS will be compared to kriging, more specifically the training will be carried out on the basis of the 4616 realizations obtained at the last iteration of the iterative algorithm. The resulting errors for K-PLS and kriging are represented in box-and-whisker plots in Fig. 5 to visualize the dispersion (in frequency and across the different folds).



Fig. 5. Boxplot representation of error for both KRG and K-PLS

The training times and median errors are given in table. II. The error is slightly higher but the gain in training time is significant (about 5 times faster).

TABLE II Performances of Kriging against K-PLS

Metamodel	Median relative error (%)	Training time (min)
Kriging	19.87	83
K-PLS (h=3)	21.09	18

#### E. Validation

In the previous sections, we saw that reducing the number of parameters and using K-PLS significantly accelerated the learning process. This final section aims to compare the  $KPLS_{S_{61}}^{12p}$  metamodel to the  $KRG_{S_{61}}^{17p}$  metamodel in terms of accuracy on an extreme value analysis. This analysis is particularly useful for defining routing rules. Indeed, it makes it possible to identify parameter values leading to extreme situations (high values of  $S_{61}$  in our case).

To illustrate this analysis, we focus on 2 particular parameters (h and  $d_{w1}$ ) which are the most influential according to Morris sensitivity analysis. A Monte Carlo-type sample is constructed and evaluated from both  $KRG_{S_{61}}^{17p}$  and  $KPLS_{S_{61}}^{12p}$ . Realizations beyond the empirical 95% quantile of the output distribution are isolated. They represent a group of configurations with the highest crosstalk level between microstrip lines 1 and 3. Distributions of h and  $d_{w1}$  belonging to this group of extreme values is displayed in Fig. 6 and compared to their initial uniform distribution of the total sample.



Fig. 6. Compared extreme values analyses of h and  $d_{w1}$  obtain with  $KRG_{S_{61}}^{17p}$  on the left and  $KPLS_{S_{61}}^{12p}$  on the right

The distributions obtained with KRG or K-PLS are similar, which confirms that the combination of Morris analysis and K-PLS method are useful to reduce both the simulation time and training calculation time. K-PLS can be definitely considered as a competitive candidate among different SMs. According to this extreme value distribution, decisions can be taken regarding further limitation of h or the prescription of a new minimum distance for  $d_{w1}$  if necessary.

#### VI. CONCLUSION

In this article, we presented a new method to accelerate the learning of metamodels, which are then used to extract PCB design rules. This method is based on the use of MORRIS analysis to eliminate unimportant parameters and iterative learning for which the K-PLS was introduced to accelerate the learning process. The application of this method to a case study with 17 parameters demonstrated its effectiveness. Other learning methods such as support vector machine, decision tree or gradient boosting may be easily added to the iterative learning to compete with kriging and K-PLS.

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