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# A Kriging modeling approach applied to the railways case

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**Abstract**

This paper deals with Kriging modeling applied for optimizing the braking performances for freight trains. In particular, it focuses on mass distribution optimization to reduce the effects of in-train forces among vehicles, e.g. compression and tensile forces, in-train emergency braking. Kriging models are applied with covariance structure based on the Matérn function, and by introducing specific input parameters to better outline the payload distribution on the train, by also evaluating the shape of the payload distribution. Satisfactory results have been obtained considering compression forces, tensile forces and their sum, and by also evaluating residuals and diagnostic measures.


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## 1. Introduction

Among the different statistical models applied to engineering and technological issues, Kriging modeling is one of the most important since it allows for using simulations through computer experiments and, further, to deal with a specific and suitable covariance structure for data. Moreover, through the Kriging modeling, the experimental region is investigated by considering the reliability of prediction, e.g. the Kriging variance, which is smaller when the predicted point is located nearby the training set of starter data ($X$) and larger as moving away from $X$. In literature, starting from the seminal contribution of Sacks et al. (1989), the studies on Kriging have been particularly developed since 2000. Regarding to the definition of the covariance structure for the stochastic part of the model, novel issues are suggested by Del Castillo et al. (2015), while Pistone and Vicario (2013) focus a peculiar attention on the strong correlation for spatial data. Zhou et al. (2011) deal with Kriging modeling by also considering qualitative variables. Arcidiacono et al. (2012) have also developed research activities with the support of Lean Six Sigma. However, Kriging modeling approach was more appropriate for this particular application: when considering computer experiments and Kriging

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modeling, a crucial feature is the design of such an experiment. In this regard, Space-Filling design are widely accepted as one of the most appropriate one. This is mainly due to the fact that they allocates the design points as uniformly as possible in order to observe the response in the entire design space. The most widely used class of Space Filling design for computer experiment is that of Latin Hypercube Design (LHD) introduced by McKay et al. (1979). This work is based on the research of Arcidiacono et al. (2017) where the innovative contribution consists in applying Kriging models to the railway field, in order to optimize the payload distribution of freight trains. In particular, the procedure is applied to evaluate the braking performance (considered in terms of in-train forces exchanged by consecutive vehicles of train) of a freight train transporting scrap material. Kriging modeling is applied by investigating the whole experimental region of a simulated experimental design generated by LHD based on Sobol sequencies, which ensures a valid choice of simulated trains. In order to increase the accuracy of the obtained results, the computer experiments are performed through the software TrainDy by Cantone (2011), whose pneumatic model is described by Cantone et al. (2009) and is certificated internationally for this type of calculation. The manuscript is organized as follows. In Section 2 the basic theoretical and modeling issues on Kriging methodology are briefly described. In Section 3 the Kriging model results related to the optimization of the payload distribution of freight trains are reported. Future research that are currently carried out are briefly described in Section 4.

## 2. Kriging methodology: theoretical issues

The seminal contribution of Sacks et al. (1989) introduced a concept of simulated designs substantially different by the physical and classical experimental designs of Cox and Reid (2000): the observation is predicted according to a simulated model of the process under study in order to deeply analyze the causal relationships between input and output variables. The seminal paper of Sacks et al. (1989) was the fundamental source for many and interesting papers published during 1980's and 1990's, where the basic theory of Kriging method for statisticians was developed; these new inputs introduced and faced a new concept of design and simulations, where the concept of deterministic model and the concept of experimental design were really changed.

Lets start by considering a set $S$ of $n$ experimental points $x_i \in X$ (input) and the corresponding response values (output) $y_i$, $i = 1, \ldots, n$, e.g. $S = \{(x_1, y_1), \ldots, (x_i, y_i), \ldots, (x_n, y_n)\}$. Therefore, the set of trials $X$ is selected within the experimental region, and each $y_i$ is the realization of a random variable $Y(X)$. The Kriging method is carried out in order to predict new simulated observations on the basis of the information gained through $S$. The final aim is an optimal prediction of $Y$ through a statistical model involving a deterministic part, $\mu(x)$ also named trend function, and a stochastic part, $Z(x)$ the latter replacing the error component for a standard statistical model, as in the following formula:

$$Y(x) = \mu(x) + Z(x) \tag{1}$$

The main type of Kriging mainly applied could be summarized as follows:

1. Ordinary Kriging that assumes a non random constant deterministic part ($\mu(x) = \mu$) so as in this case the trend function does not vary in time and space, while Z(x) identifies a spacial stochastic process that here reduces to the covariance between any two points.
2. Universal Kriging that assumes a no more constant trend that is modeled through some regression function $f(x)$.

Prediction is based on the allocation of a simulated experimental point by taking into account the covariance structure of the data and the set $S$ of starting real experimental data. To this end, in order to achieve a satisfactory prediction, it is relevant to define a fitting measure which assures: i) the best identification for the covariance structure; ii) the assumption of unbiasedness. In the literature, some measures are defined, also depending on the estimation method applied (Maximum Likelihood (ML), Ordinary Least Squares (OLS), moments method) and also depending on what we know of the real process, in particular when the covariance structure is unknown.

When considering the Kriging modeling applied at improving the assembling of freight trains, estimates are performed trough the ML method following the Empirical Best Linear Unbiased Predictor (EBLUP) property. In general, the covariance function mostly applied are related to the exponential, Gaussian and spherical models: in our case we apply the Matérn covariance function introduced by Rasmussen and Williams (2006). Moreover, computational problems and jumps may be encountered during simulations and, to this end, a nugget parameter has been introduced. The inclusion of this coefficient allows to avoid instability, e.g. it may be viewed as a noise added to the process variance. In particular, we consider a nugget equal to zero, but we also investigated for the presence of the nugget. A last remark is relating to the reliability of predictions; in general, the predicted value $\hat{Y}(x)$ is estimated by involving the correlation matrix and therefore by considering the correlation among the simulated point and the training set of starting data ($X$). Therefore, the error in prediction is useful for two aims: i) to evaluate the applied covariance structure for the Kriging model and ii) to evaluate the reliability of prediction, e.g. the Kriging variance, which is smaller when the predicted point is located nearby $X$ and larger as moving away from $X$.

### 2.1. Kriging modeling: input and output variables

In order to build the model, we have defined a strategy for representing a train in the design space, for further details see Arcidiacono et al. (2017). The main chosen characteristic is the payload distribution of the entire train. In particular, we consider three payload distributions: uniform, triangular and trapezoidal. We denote by B the length of the train and by Q the area of each distribution, corresponding to the total payload on the train. We consider that: i) wagons and the total payload are chosen *a-priori* and ii) wagons and the total payload are the same for every train evaluated in the Kriging model. Therefore, every distribution share the same base (B) and it has the same area (Q). To describe it mathematically, we define two discrete variables, e.g. $h$ and $x$, that could univocally represent the payload distribution on the entire train. Through the input variable $h$, it is possible to define the shape of the payload distribution, which can gradually change from the uniform shape to the triangular one. Through the input variable $x$, it is possible to identify the position of the maximum load along the length of the train.

The optimal solution searched through the Kriging model is the best payload distribution along the train. It guarantees an emergency braking with the minimum in-train forces between wagons, both in compression and in tensile. Therefore, the estimated response variables are the in-train forces computed at 2 m and at 10 m; at each position, the minimum value (in absolute sense) is considered of the in-train forces occurring in the previous 2 m or 10 m. The true values of compression and tensile forces are calculated to evaluate the proposed model through the TrainDy software by Cantone (2011). This software developed by Cantone et al. (2009) is internationally certified for the computation of in-train forces of freight trains.

## 3. Simulations and results

The Kriging method is applied building a model by considering the sum of compression and tensile forces as output. A cross-validation has also been carried out in order to verify the applied Kriging model for each monitored force. The prediction model has been trained through 360 simulations while the remaining 40 have been applied to validate the results. The diagnostic results, calculated for each force ($R^2$ index), show that the models are highly predictive, as reported in Table 1. The Kriging model related to the sum of forces (compression and tensile at 2 m) yields the best performance. Model results are evaluated also considering the residuals. In Table 2 diagnostic results are summarized according to the Max Absolute Error (MaxAE), the Max Relative Error (MRE), the Mean Absolute Error (MAE) and the Error Mean (EM).The largest MRE value occurs for simulations that are in the boundary region of the design space. The largest MAE value, for all the observed forces, is one order of magnitude less than the simulated. These results can be consider satisfactory for this case study. Regarding the nugget parameter, it can be viewed as a constant that can be determined by statistical and numerical criteria since grants numerical stability and predictive accuracy. When considering the semivariogram function we pay our attention to the maximum value for the semivariogram when the stationarity is achieved, e.g the sill and the range, where the latter is the distance fixed by the point where sill is achieved. In the case study we have calculated different semivariograms also by adding a small noise to the process variance by choosing a nugget equal to 0.01. As shown in Table 3, we achieved a better result only for the model related to sum of forces at 2m. For all the models we reached satisfactory results in terms of small errors (Table 2) especially when considering the magnitude of forces.

Table 1. $R^2$ related to cross-validation.

| In-train forces | $R^2$ |
|---|---|
| Compression forces at 2m | 0.997 |
| Compression forces at 10m | 0.992 |
| Tensile forces at 2m | 0.972 |
| Sum of forces: compression at 2m+tensile at 2m | 0.994 |

Table 2. Diagnostic measures by monitored forces 80% loading.

| In-train forces | MaxAE [N] | MRE [%] | MAE [N] | EM [N] |
|---|---|---|---|---|
| a-Compression forces at 2m | 1468 | 3 | 363 | 44 |
| b-Compression forces at 10m | 2918 | 6 | 598 | 271 |
| c-Tensile forces at 2m | 1403 | 6 | 413 | 197 |
| d-Sum of forces: a+c | 2556 | 3 | 541 | 249 |

Table 3. Variogram measures and Likelihood functions by monitored forces 80% loading.

| Monitored forces | Sill | Range | Nugget | Likelihood |
|---|---|---|---|---|
| a-Compression forces at 2m | 0.4456 | 1.0778 | 0.0 | 577.1359 |
| | | | 0.01 | 437.3442 |
| b-Compression forces at 10m | 0.2323 | 0.4608 | 0.0 | 218.8910 |
| | | | 0.01 | 189.2757 |
| c-Tensile forces at 2m | 0.2804 | 0.4129 | 0.0 | 181.7518 |
| | | | 0.01 | 90.7234 |
| d-Sum of forces: a+c | 0.3458 | 0.5341 | 0.0 | 680.2857 |
| | | | 0.01 | 720.5227 |

## 4. Future research

Further developments are currently underway. The train, divided in several subsections, is investigated in order to better understand the effective optimization of in-train forces through the payload distribution. Moreover, a new LHD has been generated based on a new type of orthogonal arrays, called strong orthogonal arrays, and recently developed by He and Tang (2013). This new type of LHD, called Strong Orthogonal Array based LHD (SOA-LHD) is a further development of the Orthogonal Array based LHD (OA-LHD), illustrated by Tang (1993). Tang (1993) has demonstrated the excellent space-filling properties of the SOA-LHD. With respect to the design generated by Arcidiacono et al. (2017), the SOA-LHD allows us to obtain very good properties of space-filling with a lower number of experimental runs. In particular, we have generated two SOA-LHDs with 40 and 64 experimental runs, a significantly lower number of runs with respect to the LHD based on Sobol sequencies with 400 runs applied by Arcidiacono et al. (2017), and the obtained results are very satisfactory. To the better of our knowledge, this is the first time that the SOA-LHD is going to be applied to a real case study, e.g. in the railway field. This research is currently underway also for dealing with the subsequent application of Kriging modeling.

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