

Simulation and optimization of engine performance using Kriging model and Genetic Algorithm

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Abstract

In order to optimize the performance of a diesel engine subject to legislative constraints on the pollutants emissions, it is necessary to improve the design of combustion engines, and identify how design parameters affect engine behavior. One of the specificity of this work is, that we don't have a physical model of engine behavior under all possible operational conditions. A powerful strategy for engine modeling is to build a fast emulator of the engine based on carefully chosen observations, made according to an experimental design. In this paper, we propose an emulator based on Kriging model adapted to take into account a number of input parameters greater than 3, while existing software don't deal with this case. This model has allowed us to predict the behavior of the engine, and was adopted to optimize the fuel consumption within constraints on the emission of NO_x (nitrogen oxide) using Genetic Algorithm.

1 Introduction

The use of statistics in engineering increases rapidly. As engineering systems become more complex, the problems faced by engineers also increase in complexity. For some design problems, no physical model exist and empirical studies must be developed and executed in order to optimize engineering systems for performance and compliance to regulations. This holds particularly in the field of combustion engine design, where typically, the engine is controlled by a great number of parameters, in order to meet multiple performance objectives.

The compression ignition heterogeneous combustion process of the diesel engine is highly dependent on fuel injection parameters. Therefore, precise control over fuel injection, is essential to control combustion processes. In previous studies, results have indicated multiple injections with exhaust gas recirculation EGR can provide substantial reduction in emission of NO_x from diesel engines (2). Thus, the current objective is to develop an efficient strategy to optimize operating parameters of diesel engines with injection and EGR capabilities. However, optimization is not limited to injection and exhaust gas recirculation (EGR) parameters. Variables such as engine speed, pressure in the rail injection, pressure and temperature in admission manifold... must be included which can provide important information on the formation of the pollutants.

Strategies based on Lolimot (Local Linear Model Tree), Zeldovich mechanisms (7) have been developed in order to predict emissions of NO_x (4). In the first case, the corresponding model can lead to singular points which reduces the precision of the results. In the second case, the results are not satisfactory enough.

Several models have been developed to predict the various responses (fuel consumption, NO_x) from variable entries above. We choose the Kriging model, which gives the best results. Software such as R and Matlab contain a toolbox for the use of this method. But unfortunately, they are restricted to less than 3 dimensions. Adapting the method to higher dimensions has been considered, and more generally in (1), we have proposed an innovative approach for functional data. The performance of this model is due to its ability to take into account the spatial dependence of data, and has a minimal variance estimators without bias. Once the adjusted model is tested and validated, the stage of the research of optimal designs is achieved by using genetic algorithms.

This paper is organized as follows: In the first section, the ordinary Kriging techniques are given. In the second section details of Genetic Algorithm method are recalled. In the last section numerical results and implementation of process are given.

2 Ordinary Kriging Techniques

Kriging methods are used frequently for spatial interpolation of soil properties ((14), (15)). Kriging is a linear least squares estimation algorithm. It is a tool for interpolation, the aim is to estimate the value of an unknown real function Z at a point x_0^* , given the values of a function Z at some other points x_1, \dots, x_n , where $x_i \in \mathfrak{R}^d$ for each $i = 1, \dots, n$.

2.1 Ordinary Kriging

The ordinary Kriging estimator $\hat{Z}(x_0^*)$ is defined by:

$$\hat{Z}(x_0^*) = \sum_{i=1}^n \lambda_i Z(x_i). \quad (1)$$

where m is the number of surrounding observations $Z(x_i)$ and λ_i is the weight of $Z(x_i)$. The weights should sum to unity in order to make the estimator unbiased:

$$\sum_{i=1}^n \lambda_i = 1. \quad (2)$$

The weights are also determined such that the Kriging variance is minimal.

This leads to a classical optimization problem with equality constraint. The Lagrange multiplier theory is used in order to work out this problem. This gives a linear system to be solved (9)

2.2 Semi-variogram

The semi-variogram is a function representing the spatial dependency, and has been obtained from the stationarity definition. In fact, this stationarity hypothesis is an indispensable condition for the use of the Kriging method. It is based on the assumption of intrinsic stationarity for spatial data. The variation of a data set, is only dependent on distance r between two locations where the variables values are $Z(x_i + h)$ and $Z(x_i)$ with $r = |h|$, can be given by the following semi-variogram:

$$\hat{\gamma}(r) = \frac{1}{N(r)} \sum_{N(r)} [Z(x_i) - Z(x_j)]^2 \quad (3)$$

where

$$N(r) = \{(i, j) \text{ such that } |x_i - x_j| = r\} \quad (4)$$

where $N(r)$ is the pair number of $Z(x_i + h)$ and $Z(x_i)$ and $\hat{\gamma}(r)$ is the experimental semivariogram.

The experimental semi-variogram presented in equation 3 estimates the theoretical semi-variogram only for a finite number of distances. Moreover, it does not necessarily forms a valid semi-variogram. this means, that maybe it does not concern a negative conditionally function. The experimental semi-variogram is then modeled by a function of negative conditional type and is defined for all distances. This modeling makes the Kriging possible.

A variogram model must be fitted to such semi-variogram. Various form of variogram model are available. In addition to select the model, this one must be adjusted of variogram experimental. This means that the parameters of model must be estimated. This adjustment can be done with the eyes, but it is usually done with an estimation method such as the weighted least squares or maximum likelihood method.

Finally the weights λ_i in (1) are computed by solving the following system:

$$A\Lambda = B \text{ with}$$

$$A = \begin{bmatrix} \gamma(r_{11}) & \gamma(r_{12}) & \dots & \gamma(r_{1n}) & 1 \\ \gamma(r_{21}) & \gamma(r_{22}) & \dots & \gamma(r_{2n}) & 1 \\ \dots & \dots & \dots & \dots & \dots \\ \gamma(r_{n1}) & \gamma(r_{n2}) & \dots & \gamma(r_{nn}) & 1 \\ 1 & 1 & \dots & 1 & 0 \end{bmatrix} \quad (5)$$

$$\Lambda = [\lambda_1 \quad \lambda_2 \quad \dots \quad \lambda_n \quad \lambda]^T \quad (6)$$

and

$$B = [\gamma(r_{01}) \quad \gamma(r_{02}) \quad \dots \quad \gamma(r_{0n}) \quad 1]^T \quad (7)$$

Where λ is the Lagrange multiplier.

The variance of the estimate s_i^2 , ie the square of the standard error at each point is obtained by the relationship:

$$s_i^2 = \Lambda^T . B \quad (8)$$

If we assume that the estimation errors are normally distributed around the true value, then the probability that the true value will be in $Z(x_i) \pm s_i$ is 68 %, while the probability that the true value will be in $Z(x_i) \pm 2s_i$ is 95 %, (9).

2.3 Krigin Emulator Validation

The true test of the quality of the fitted emulator model is its ability to predict the response at untried factor values. In order to maximally exploit the data to aid model fitting, the emulators are validated using leave-one-out cross validation. This process involves taking the fitted model and re-fitting it to a subset of non using experimental data. More precisely, for an experiment with d design factors $y = y_1, \dots, y_d$, the set of n experimental design points $X = x_1, \dots, x_n$ and responses $Z = z_1, \dots, z_n$, contain the information used to build the Kriging model. Cross validation involves predicting at each design point in turn when that point is left out of the predictor equations.

Let $\hat{Z}(x_i)$ be the estimate of the $Z(x_i)$ based on all the design points except x_i . The prediction error (the estimated root mean square error, RMSE) is then calculated as:

$$RMSE = \sqrt{\frac{1}{n} \sum_{i=1}^n [Z(x_i) - \hat{Z}(x_i)]^2}$$

An other index of the accuracy of the emulator is expressed as a percentage of the range of the response Z ,

$$\%RMSE = 100 \times \frac{RMSE}{\max(Z) - \min(Z)}$$

3 Optimization of the Calibration

Optimization of the response model has undergone much research to identify a suitable search strategy. Early success were reported with gradient techniques, but problems with local minima, increasing problem dimensionality and requirement to cope with discrete input variables caused its abandonment in favor of genetic algorithm approach. Details of this method are given in section 3.2.

3.1 Formulation of problem

We recall that our goal is to minimize the consumption of diesel engine with respect to European laws on emissions of NO_x . In this case solving an optimization problem with constraints is required. The optimization problem is given by:

For the objective $f(Y)$,
 Find $Y = \{y_1, y_2, \dots, y_d\}$
 which minimizes $f(Y)$
 subject to constraints $g(Y) - threshold < 0$
 and $y_i^l \leq y_i \leq y_i^u \quad i = 1, 2, \dots, d$

This problem is converted to an optimization problem without constraints, using the external penalty method. In the present study, it is proposed that the objective function should be a Kriging model of Consumption.

$Y = \{y_1, y_2, \dots, y_d\}$ array of control factors such as engine speed, pressure rail injection...

$g(Y)$ Kriging model for NO_x It is important to realize that objective functions can be a function of output variables. For instance, it could be the weighted sum of responses, to reflect the relative importance of each output variable.

3.2 Genetic Algorithm

Genetic Algorithms are a family of computational models inspired by evolution. These algorithms encode a potential solution to a specific problem on a simple chromosome-like data structure and apply recombination operators to these structures, so as to preserve critical information. Genetic algorithms are often viewed as function optimizers although the range of problems to which they have been applied is quite broad. An implementation of a genetic algorithm begins with a population of typically random chromosomes. Then, it evaluates these structures and allocates reproductive opportunities, in such a way that those chromosomes which represent a better solution to the target problem have more chances to reproduce, than those chromosomes which are poorer solutions.

3.2.1 Selection

Tournament selection is a useful and robust selection mechanism commonly used by genetic algorithms which runs a "tournament" among a few individuals chosen at random from the population and selects the winner (the one with the best fitness) for crossover. Selection pressure can be easily adjusted by changing the tournament size. If the tournament size is large, weak individuals have a small chance to be selected. Tournament selection pseudo code is:

- choose k (the tournament size) individuals from the population at random.
- choose the best individual from pool/tournament with probability p .
- choose the second best individual with probability $p(1-p)$.
- choose the third best individual with probability $p((1-p)^2)$.
- and so on...

Tournament selection has several benefits: it is efficient to code, works on parallel architectures and allows the selection pressure to be easily adjusted.

3.2.2 Crossover

Crossover is a genetic operator that combines (mates) two chromosomes (parents) to produce a new chromosome (offspring). The idea behind crossover is that the new chromosome may be better than both of the parents if it takes the best characteristics from each of the them. Crossover occurs during evolution according to a user-definable crossover probability.

3.2.3 Mutation

Mutation is a genetic operator that alters one or more gene values in a chromosome from its initial state. This can result in entirely new gene values being added to the gene pool. With these new gene values, the genetic algorithm may be able to arrive at better solution, than it was previously possible. Mutation is an important part of the genetic search which helps to prevent the population from stagnating at any local optima. Mutation occurs during evolution according to a user-definable mutation probability. This probability should usually be set fairly low (0.01 is a good first choice). If it is set to high, the search will turn into a primitive random search.

4 Numerical results

This subsection will be devoted to the presentation of the numerical results obtained for a both output variables NO_x and consumption. In the beginning, we give the mathematical model used to adjust the experimental variogram and the corresponding graph for each output variables. Variography modeling is a critical step and most difficult in the construction of a Kriging model. For this reason, several models were adjusted and then compared. It was difficult to select the better model by eye. The cross validation has facilitated the work. It allows us to select the one, that minimizes the root mean square error. For the

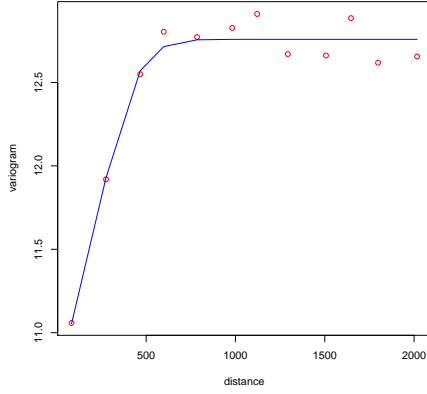


Figure 1: Experimental and Gaussian model variogram in the case of NO_x

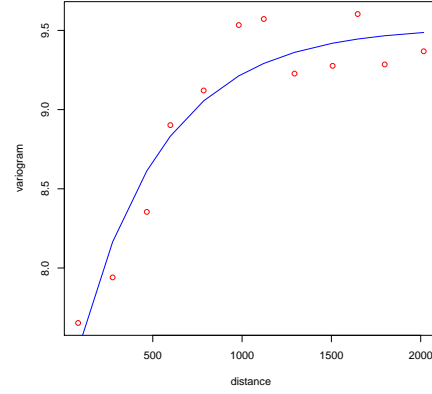


Figure 2: Experimental and exponential model variogram in the case of consumption

NO_x variable, the model used is a Gaussian model given by equation:

$$\gamma(r) = c_0 + c.(1 - \exp(-\frac{r^2}{a^2})) \quad \text{as } r \geq 0, \quad (9)$$

The value of parameters model was founded using the least square method:

where $c_0=10.929$, $c=1.829$, $a=309.559$. For the Consumption variable, the model used is an exponential model given by equation:

$$\gamma(r) = c_0 + c.(1 - \exp(-\frac{r}{a})) \quad \text{as } r \geq 0, \quad (10)$$

where $c_0=7.106$, $c=2.415$, $a=477.444$.

where:

- r is the distance

- c_0 is the Nugget effect

- $c_0 + c$ is the sill correspond to the variance of $Z(x)$

- $\sqrt{3}a$ and $3a$ is a range (the distance at which the variogram reaches the sill) for the Gaussian and exponential model respectively (13).

Figures 1 shows the experimental variogram (red points), and Gaussian model(blue curve) corresponding to NO_x response.

Figures 2 shows the experimental variogram (red points), and exponential model(blue curve) corresponding to consumption response.

This tool measures the variability of NO_x and consumption as a function of distance, we notice that when the distance reached the range $535 = \sqrt{3}a$ (Figure 1) and $1300 = 3a$ (Figure 2), the variation becomes stationary. This is explained by the fact that, we can have a similar behavior of consumption and NO_x on two different operating points, thus with a pattern of different control parameters

Figures 3 and 4 show the Cross-validation plots for the Kriging model corresponding to the Gaussian and exponential variogram respectively. The plots contain the measured, the Kriging estimated value and a 10% errors bands.

The accuracy of predictions was similar for both training and performance validation data. Accuracy was good for both of responses and still within 10% for the majority of operating conditions. By against, graph 4 presents some observations which are poorly estimated. This is because they are far from the cloud of points used to be adjusted. On the other hand, this bad estimate is due to the experimental design used. The classical and optimal designs, in particular the D-optimal, are not suitable for Kriging which is based on measuring similarity between sites. Indeed, the optimal design allows to test just a small number of levels for each variable and tend to generate points on the edges of the experimental field (10). This distribution of points, which is optimal to fit a polynomial model, can not pick up any irregularities inside the experimental field, which is the

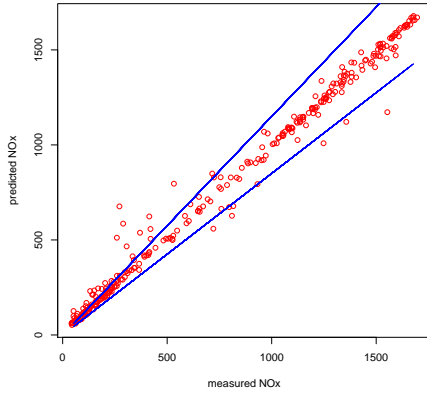


Figure 3: Measured and Kriging predicted NOx[ppm] with $\pm 10\%$ error bands

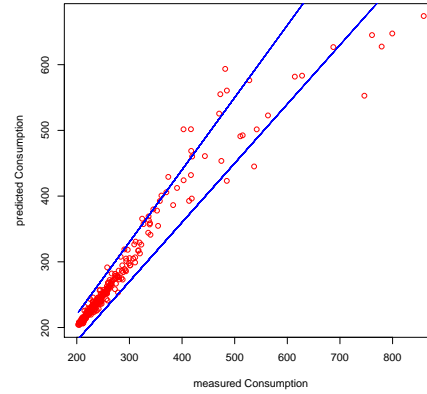


Figure 4: Measured and Kriging predicted specific consumption [g/kWh] with $\pm 10\%$ error bands

case of some poorly estimated points. To address this problem, we recommend to use an appropriate designs for Kriging, belonging to the class 'space filling designs', such as Latin hypercubes that provide a good spatial distribution of points of the plan and have an optimal plan for the model (12), (11)

The emulator model is fitted to each response in turn and the RMSE, percentage RMSE are recorded. These results are presented in Table1

	NO_x	Consumption
RMSE	61.4	27.16
%RMSE	3.64	4.1

Table 1: Kriging RMSE end %RMSE for each response

The percentage RMSE results show that model have a RMSE less than 5% of the range of the response data. This indicates roughly that if the emulator is used to predict the response at a new input setting, the error of prediction can be expected to be less than 5% when compared with the true value.

4.1 Implementation

After we have used and validated the Kriging model to predict both responses NO_x and consumption, in the below step, we present a methodology which we advocate for optimization phase. The results obtained using genetic algorithms are also presented.

The implementation of the optimization process of the diesel engine operating parameters is given in Figure5:

The configuration adopted of genetic algorithm parameters is given in Table2. The continuous Genetic

Population size	100
probability of Crossover	0.7
probability of mutation	0.1
type of coding	real coding

Table 2: Genetic Algorithm configuration

Algorithm (which means that we have used a real coding) is chosen for the following reasons:
 -The traditional binary representation used for genetic algorithms creates difficulties for optimization problems with high numerical precision.

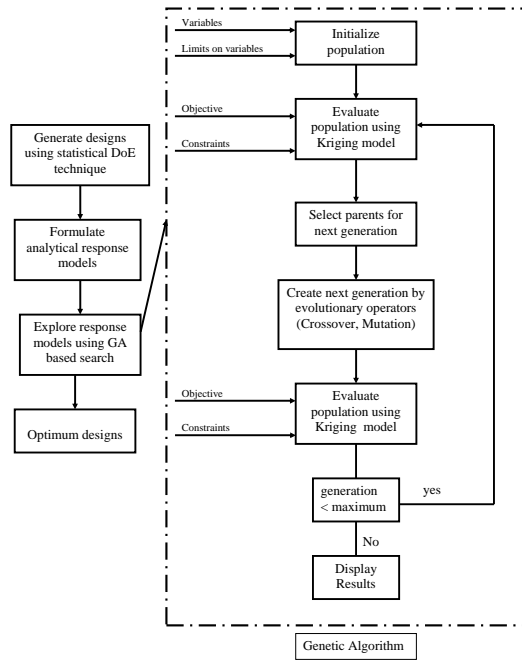


Figure 5: Optimization process using Genetic Algorithm

-Solving algorithm is costly in time.

-The crossover and mutation operators may be unsuitable (creation of chromosome outside the area research). A major improvement, is then to use real numbers directly.

Using the above approach has allowed us to find the best values of input parameters that minimize the consumption of diesel within constraints on the NO_x emission. In Figure 6 we show the optimal design consumption corresponding to the optimal input parameters. Indeed, the values of consumption and NO_x which appear in Figure 6 correspond to the 100 best values optimal factors obtained by the process of optimization (Figure 5) evaluated by the Kriging model.

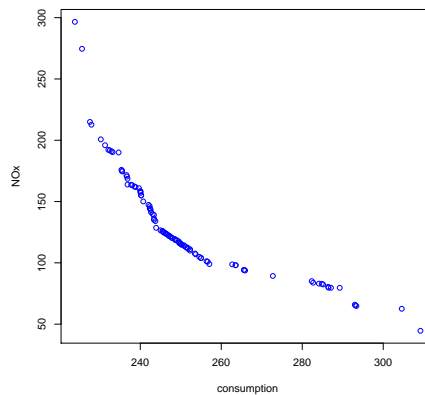


Figure 6: optimal design of Specific consumption [g/kWh]

5 Conclusion

This paper describes an emulator for pollutant emissions and of performance of compression ignition engine. The effort has been put into building a model based on the Kriging method. The resulting model

can be used to predict the different responses of engine, it is easy to generalize for various diesel engine configurations. These models are also suitable for real time simulations. The predictions obtained by this emulator are satisfactory and improve the results obtained by using a physical model or statistic methods (Lolimot) given by S.Castric et al (3).

Genetic algorithm optimization is a robust tools able to deal with practical engine responses. It can be incorporated into an approach which takes advantage of available computing power to perform optimization in a reasonable times.

A strategy for optimization of engine operating parameters was demonstrated. It was also show that the use of this new strategy provides an efficient means by which operating parameters can be optimized, especially when we don't have a physical model.

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