MODELING AND ESTIMATION OF POLLUTANT EMISSIONS

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Abstract: The European laws lead to the increase of emission constraints. In order to take into account these constraints, automotive constructors are obliged to create more and more complex systems. This paper presents two stage approaches for the prediction of NOx (nitrogen oxide) emissions, which are based on an ordinary Kriging method. In the first stage, a reduction of data will take place by selecting signals with correlations studies and by using a fast Fourier transformation. In the second stage, the Kriging method is used to solve the problem of the estimation of NOx emissions under given conditions. Numerical results are presented and compared to highlight the effectiveness of the proposed methods.

1 INTRODUCTION

The diesel engine is an internal combustion engine. At each cycle during the intake stroke, the combustion chamber receives a mixture of air and vaporized fuel via the injector (their flows are measured and controlled). Afterwards fuel vapor and air are compressed and ignited.
The mixture air-fuel is not stoechiometric during the combustion process. The unfortunate consequence is the creation of pollutants. In order to limit this problem, the European laws increase the constraints on pollutant gas emissions.
The main aim is the minimization of the NOx emissions under some constraints based on the Kriging model, by making a compromise with engine performance. In this case multi-objectives optimization will be considered. Then, it is necessary to simulate the pollutant behavior which is the subject of this paper.

A physical phenomenon model has been developed by S.Castric et al (S. Castric, 2007) in order to simulate the engine behavior. It takes into account the input parameters (fuel mass flow, air mass flow, exhaust gas recirculation ratio,...) and gives the corresponding state variables, particularly pressure, temperatures, fresh gas mass, mixed gas mass, and burned gas mass. It leads to a good representation of the experiment results. Strategies based on Lolimot (Local Linear Model Tree) and Zeldovich mechanisms (Heywood, 1988) have been developed in order to predict emissions of NOx (Castric, 2007). 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. On the other hand, the trend surfaces can be used, but it is difficult to go deeper with this approach because it consists of a classical regression based on the assumption of independence of observations, which is rarely checked with spatial data (S. Baillargeon, 2004).

Our choice is the Kriging method which takes into account the dependence of spatial data and has a variance that is minimal among estimators without bias. Moreover it leads to efficient results.

This paper is organized as follows: In the first section, the ordinary Kriging techniques are recalled. In the second section, two different approaches for modeling our problem are proposed. An efficient reduction model strategy is considered in order to apply the kriging method. Finally the Kriging method is applied to the reduced model. In the last section, numerical results are given followed by a short discussion.

2 ORDINARY KRIGING TECHNIQUES

Kriging methods is used frequently for spatial interpolation of soil properties. Kriging is a linear least squares estimation algorithm. It is a tool for interpolation, which is to estimate the value of an unknown real function F at a point x_0^*, given the values of a function Z at some other points $x_1,....x_n$.

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. 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. It gives a linear system to be solved (Davis.J.C, 1986)

2.2 Semivariogram

The semi-variogram is a function representing the spatial dependency, and has been obtained from the stationarity definition. It is based on the assumption of intrinsic stationarity for spatial data, the variation of a data set that 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:

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

where

$$N(r) = \left\{(i,j) \quad tel\ que \quad \left|x_i - x_j\right| = r\right\} \quad (3)$$

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

A variogram model should be fitted to such semivariogram. Different form of variogram model are available. In this study a power model was used:

$$\gamma(r) = C_0 + m.r^d \quad as \ \ h \geq 0, \ \ 0 < d < 2 \quad (4)$$

where C_o is called the nugget effect, The least square method was used to estimate the parameters of experimental variogram and variogram models.

2.3 Cross-Validation

To evaluate the reliability of kriging estimation, cross-validation was used,and the mean square error (MSE) of the kriging-estimated values had been calculated.

The mean error ME is a measure of the estimation bias, and it should be close to zero for unbiased methods.

3 DESCRIPTION OF TWO MODELS

S. Castric et all (Castric, 2007), have developed a physical model for modeling the engine behavior, in order to minimizing the NOx emessions. To do this, he has divided into two sub-model: The first is a physical model, making the link between the input parameters and state variables. The second study the impact of the latter on NOx, the second part was not completely done. In this work, we are inspired of this original idea to give the two modelings below.

3.1 First Modeling

The first one consist of studying the impact of input parameters on the NOx without taking into account the state variables. In this case, a model will be built by taking into consideration 8 input parameters like:
pressure in the rail injection,the exhaust gas recirculation ratio..., with the corresponding value of the NOx flow.
The choice of these parameters was recommended by experts, and multiple regression to study the impact of these parameters on the NOx, was confirmed it.

3.2 Second Modeling

The second one consist of studying the impact of state variables on the NOx, which is tantamount to build a model that uses ten state variables like: cylinder low pressure, temperature in the cylinder...
which are each one represented by a vector of 1334 components and the corresponding value of NOx flow.

3.3 Model Reduction

The data of the first model can be directly used for applying the Kriging method. It is not the case for the second one. In the latter case, the data have to be reduced.

The reduction process begins by studying the different correlations between the state variables and their corresponding p-value. The criterion which has been chosen consists in testing the p-value: if it is inferior to 0.05 the correlation is considered significant.

This analysis allows us to retain two state variables only: the cylinder low pressure P and the mixed gas temperature in the cylinder T_e.

In the second step, the number of components of the two remaining signals is reduced. It has been accomplished by using the discrete Fourier transform. The function fft of Matlab returns the discrete Fourier transform (DFT) of a vector, computed with a fast Fourier transform (FFT) algorithm. After calculating the coefficients, a minimum number of these are retained. This number allows to reproduce the initial signal with a relative error of order 10^{-2}, which is reached with only 40 Fourier coefficients. The reduction of the number of points of each signal is tantamount to minimizing the number of Fourier coefficients representing that signal.

The two retained signals, representing respectively the cylinder low pressure and the temperature of the mixed gas in the cylinder, have been reduced to a number of 40 Fourier coefficients. Each signal has been reconstructed from these 40 coefficients with an acceptable error.

The following table presents the relative error committed, for the reconstruction of the two signals from the 40 selected coefficients.

Type of signal	relative error
Cylinder low pressure	0.01
Temperature of the mixed gas	0.02

4 NOX ESTIMATION

4.1 Numerical Results using the First Model

This subsection will be devoted to the presentation of the numerical results obtained in the case of the first modelisation, more precisely we give the mathematical model used to adjust the experimental variogram and the corresponding graph.

The model used in this part is given by equation 5. where:
$C_0 = 9.909432.10^{-1}$, $m = 5.281263.10^{-8}$, and $d = 1.798734$

Figure 1 shows the experimental semi-variogram and the mathematical model which adjusts it. This model has the power form, without bearing and with a nugget effect C_0 . Several models were adjusted and then compared, it was difficult to select the better model by eye.The cross validation has facilitated the work. She allows us to select the one, that minimizes the mean square error, which is presented in this Figure.

Type of Indice	Value
Mean Error	0.1082633
Mean square error	11.23740

Finally the kriging model is obtained and Figure 3 illustrate the comparison between measured and simulated emissions of NOx by using this first model.

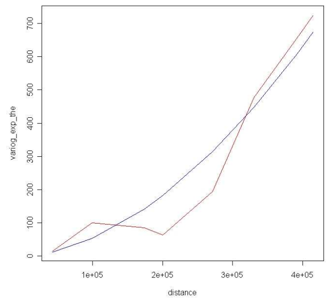

Figure 1: Experimental semivariogram and semivariogram model obtained using the input parameters.

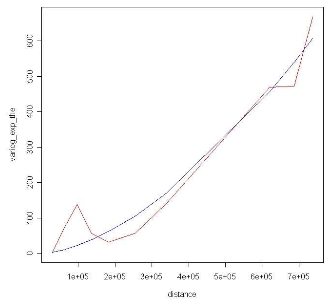

Figure 2: Experimental semivariogram and semivariogram model obtained using low pressure and temperature.

4.2 Numerical Results using the Second Model

This subsection is devoted to the presentation of the numerical results obtained in the case of the secon modelisation more precisely we give the mathematical model used to adjust the experimental variogram and the corresponding graph

The model used in this part is given by equation 5. where:
$C_0 = 9.917759.10^{-1}$, $m = 1.277732.10^{-}7$, and $d = 1.648926$.

Figure 2 shows the experimental semi-variogram and the mathematical model which adjusts it. This model has the power form, without bearing and with a nugget effect C_0 . Several models were adjusted and then compared, it was difficult to select the better model by eye. The cross validation has facilitated the choice.

Type of Indice	Value
Mean Error	0.205614
Mean square error	10.45415

The green straight lines in the Figure 3 and 4 is the regression straight lines of NOx values estimated

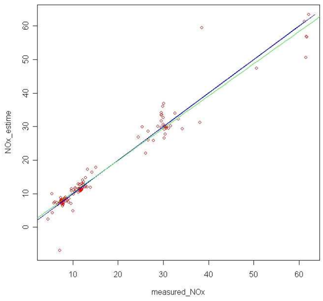

Figure 3: The scatter plot of the observed and predicted values of NOx, using the Kriging method (first model).

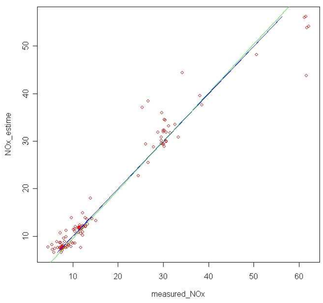

Figure 4: The scatter plot of the observed and predicted values of NOx, using the Kriging method (second model).

by the model, on the values of NOx observed. We notice that this straight lines coincide with the Black straight lines given by equation $y = x$, which is why the estimate obtained is effective

Both experimental variogram calculated in the framework of these two approaches are almost similar. We notice that the two sructures spatial show a strong dependence.

In both cases the estimations and the results given by cross-validation are good. On the other hand, it is clear that, for some experiments, the first one is the best, and, for other experiments, it is the second one which gives the best results.

These results impel us to adopt, in future work, a combination of these models in order to optimize the estimation of NOx emissions.

5 CONCLUSIONS

This paper describes a pollutant emissions simulator of compression ignition engine. The effort has been put into building a model based on the kriging method. The resulting model can predict engine pollutant emissions and can be used to predict the engine performance and noise, it is easy to generalize for various diesel engine configurations. This model is also suitable for real time simulations. The predictions obtained by this simulator are satisfactory compared to the results obtained by using of a physical model given by S.castric et al (Castric, 2007). Our future aim is to estimate the engine performance by using the proposed model. This latter will be adopted in order to make the multi-objective optimization, using the stochastic methods.

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