Design of experiments for smoke depollution from the output of diesel engine

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The context of this work is the study of a catalytic depollution system, the post-treatment through NOx trap of smoke produced by diesel engines. Kinetic models developed to represent this physico-chemical phenomenon depend on parameters (pre exponentional factors, activation energies, adsorption constants) that cannot be obtained from theoretical consideration. Therefore, experiments are necessary to calibrate the model.

The aim of this work is to propose a criterion for experimental designs adapted to kinetic parameters identification, considering that:

- the kinetic model does not fit well experimental data,
- the model is highly non linear and can be express by $y = f(x, \beta)$, where y is the response vector (for example the content of unburned hydrocarbons), x the experimental conditions and β the kinetic parameters of the model denoted by the function f

In order to solve this problem, we propose to consider that the differences observed between the kinetic model and experimental data can be represented by a realization of a Gaussian process. Gaussian Process often accounts for correlated errors due to the lack of fit.. Thus, we suppose the following model

$$y = f(x, \beta) + z_{\sigma^2,\theta}(x),$$

where $z_{\sigma^2,\theta}(x)$ is a centred Gaussian process with the Gaussian covariance kernel specified by the variance σ^2 and the scale parameters θ. This approach is commonly used in the field of computer experiments and is known as kriging However, in traditional use the trend is linear and the trend parameters estimation and its uncertainty are well known and obtained thanks to an analytical formula.

The first difficulty in our framework is to estimate the parameters considering the non linear trend. Similarly to nonlinear regression the traditional analytical formula for β is replaced by a minimisation procedure. This procedure was tested on a simplified kinetic application and gave good results. Besides, we show how the knowledge of derivatives provides useful information for kriging evaluation in that particular kinetic application. Since differentiation is a linear operator, the derivative of a Gaussian process is another Gaussian process. Thus we can use GPs to make predictions about derivatives, and also to make inference based on derivative information.

The second issue is the approximation of the kriging prediction variance. Two different ways to compute prediction variance are proposed and compared. The first is based on a generalization of the classical formula for prediction variance. Alternatively, we propose a Bayesian approach to account uncertainty in parameters inference.

Finally we propose designs of experiments adapted to our model and based on the calculus of prediction variance. Our final goal is to combine this knowledge of uncertainty and input variables uncertainties in order to propose an optimal design of experiments, which can be compared to classical ones: D-optimal Designs adapted to non linear problems or traditional space filling designs adapted to Gaussian Process.

All these methods are developed and tested on the catalytic system, i.e. on the diesel engines smoke post-treatment.

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